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Science and Mathematics Education Centre

Learners' Mental Models of Chemical Bonding

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**"This thesis is presented as part of the requirements for the award of the Degree of
Doctor of Science Education
of the
Curtin University of Technology"**

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I, Richard Coll, a candidate for the degree of Doctor of Science Education (ScEdD) at Curtin University of Technology, certify that the work presented in this thesis is my own. I have not been enrolled for another tertiary award during the term of my ScEdD without the knowledge and approval of the University.

Candidate's Signature

19-10-99

Date

Dedication

This thesis is dedicated with much love to my mother, Nancy Teresa Coll, and the memory of my father the late Kevin Patrick Coll.

Abstract

The research reported in this thesis comprised a cross-age inquiry of learners' mental models for chemical bonding. Learners were chosen purposefully from three academic levels—senior secondary school (Year-13, age range 17-18 years old), undergraduate (age range 19-21 years), and postgraduate (comprising MSc and PhD; age range 22-27 years). The principal research goal was to establish learners' preferred mental models for the concept of chemical bonding. Other research goals were to establish if and how learners made use of analogy to understand chemical bonding and to establish the prevalence of learners' alternative conceptions for chemical bonding. The research inquiry was conducted from within a constructivist paradigm; specifically the researcher ascribed to a social and contextual constructivist belief system.

Based on a review of the science education literature a decision was made to classify mental models into four classes according to the typology of Norman (1983), namely, the target system, a conceptual model, the users' or learners' mental model and the scientists' conceptualisation. A conceptual theme for the inquiry was developed based on this typology resulting in the identification of target systems—metallic, ionic and covalent bonding. Subsequently, target models for each of the three target systems were identified, namely, the *sea of electrons model* and the *band theory* for metallic bonding; the *electrostatic model*, and the *theoretical electrostatic model* for ionic bonding; and the *octet rule*, the *valence bond approach*, the *molecular orbital theory* and the *ligand field theory* for covalent bonding. A conceptual model, consisting of a summary of the salient points of the target models, was developed by the researcher. Once validated by four of the instructors involved in the inquiry, this formed the scientists' conceptualisation for the target models.

Learners' mental models were elicited by the use of a three phase semi-structured interview protocol for each of the three target systems based on the translation interface developed by Johnson and Gott (1996). The protocol consisted of showing participants samples of common substances and asking

them to describe the bonding in these materials. In addition, participants were shown Interviews About Events (IAE) focus cards which depicted events involving chemical bonding or contained depicted models of bonding for the three target systems. Transcriptions of audio-tapes combined with diagrams produced by the participants formed the data corpus for the inquiry. Learners' mental models were compiled into inventories for each of the target systems. Examination of inventories enabled identification of commonality of views which were validated by four instructors—two instructors from the teaching institutions involved in the inquiry, and two instructors independent of the inquiry.

The research reported in this thesis revealed that learners across all three academic levels preferred simple or realist mental models for chemical bonding, such as the sea of electrons model and the octet rule. Learners frequently used concepts from other more sophisticated models to aid their explanations when their preferred mental models were found to be inadequate. Senior level learners were more critical of mental models, particularly depicted models provided on IAE focus cards. Furthermore, senior level learners were able to describe their mental models in greater detail than their younger counterparts. However, the inquiry found considerable commonality across all three levels of learner, suggesting mental models are relatively stable.

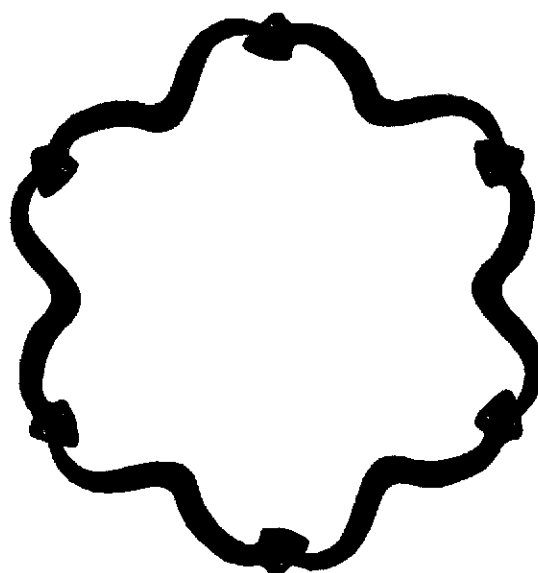
Learners' use of analogy was classified according to Dagher's (1995a) typology, namely, simple, narrative, peripheral and compound. Learners' use of analogy for the understanding of chemical bonding was found to be idiosyncratic. When they struggled to explain aspects of their mental models for chemical bonding, learners made extensive use of simple analogy, that typically involved the mapping of a single attribute between the target and source domains. There did not appear to be any correlation between academic ability or academic level and use of analogy. However, learners made greater use of compound analogy for the target systems of metallic and ionic bonding, mostly as a result of the use of analogical models during instruction.

This inquiry revealed prevalent alternative conceptions for chemical bonding across all three academic levels of learner. This is a somewhat surprising result considering that the mental models preferred by learners were typically simple, realist models they had encountered during instruction. Learners' alternative conceptions often concerned simple conceptions such as ionic size, the presence of charged species in non-polar molecular compounds, and misunderstandings about the strength of bonding in metals and ionic substances. The inquiry also revealed widespread confusion about intermolecular and intramolecular bonding, and the nature of lattices structures for ionic and metallic substances.

The inquiry resulted in a number of recommendations. It is proposed that it may be more beneficial to teach less content at the introductory level, that is, delivering a curriculum that is more appropriate for non-specialist chemistry majors. Hence, one recommendation is for instructors to examine the intended curriculum carefully and be more critical regarding the value of inclusion of some course content. A second recommendation is that sophisticated models of chemical bonding are better taught only at advanced stages of the degree program, and that teaching from a constructivist view of learning may be beneficial. The third recommendation relates to the fact that learners spontaneously generated analogies to aid their explanations and conceptual understanding, consequently, learners may benefit from greater use of analogy during instruction.

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I turned my chair to the fire and dozed. Again the atoms were gambolling before my eyes. This time the smaller groups kept modestly in the background. My mental eye, rendered more acute by repeated visions of this kind, could now distinguish larger structures, of manifold conformation; long rows, sometimes more closely fitted together; all twining and twisting in snakelike motion. But look. What was that? One of the snakes had seized hold of its own tail, and the form whirled mockingly before my eyes. As if by a flash of lightening I awoke. (Kekulé, cited in Hill & Holman, 1983, p. 495)

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CHAPTER ONE
INTRODUCTION

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CHAPTER ONE

INTRODUCTION

Overview of the Chapter

This chapter comprises an introduction to the thesis. It begins with the background and justification for the inquiry followed by the nature, scope and purpose of the inquiry. The assumptions and terms used in the thesis are detailed next along with a discussion of the significance of the inquiry. The chapter concludes with a description of the context and an outline of the organisation of the thesis.

1.1 Background and Justification for the Inquiry

This inquiry consists of an investigation into learners' mental models of chemical bonding. In selecting this area of research, I have been influenced by my university learning and teaching experiences in New Zealand and in a number of developing countries in the Pacific and the Caribbean. As a result of these experiences, I came to the conclusion that the teaching of abstract concepts such as atomic structure and chemical bonding is very challenging for many learners. I also observed that in spite of instruction, many learners retained and used simple, rather limited models for atomic structure and chemical bonding. Evidence that this situation also prevails at the University of Waikato was obtained from a rudimentary study carried out during 1996 as part of the coursework carried out during my ScEdD. In the study, a cross-section of third-year chemistry majors were asked to draw a representation for the electronic structure of hydrogen and carbon—only two out of 25 produced a diagram that was in reasonable agreement with the currently accepted scientific model. Further support for the above view comes from reports in the science education literature which have found that learning abstract science concepts is a complex and

difficult task for many learners (e.g., Banerjee, 1995; Banerjee & Power, 1991; Bodner, 1991; Boo, 1998; Kogut, 1996; Nakhleh, 1992; Shiland, 1997).

A number of authors have highlighted the importance of models in science, and some of the most important models used in chemistry are those for atomic structure and chemical bonding (Gilbert, S.W., 1991; Greca & Moreira, 1997; Grosslight, Unger, Jay, & Smith, 1991; Harrison & Treagust, 1996; Vosniadou, 1994; Zumdahl, 1989). The possibility that chemistry majors may progress onto postgraduate work whilst retaining limited or erroneous models is of concern (Camacho & Cazares, 1998; Justi & Gilbert, 1999). The fact that these graduates gained high grades for their chemistry courses throughout their degrees suggests that they were able to reproduce the currently accepted scientific models when required, for example, in tests and examinations (see also, Rop, 1999). Hence, it seems likely that these individuals retain several models in their minds at the same time.

1.2 Nature and Scope of the Inquiry

This inquiry comprises an in-depth investigation into learners' mental models for chemical bonding. The inquiry is a cross-age inquiry and the sample consisted of 24 learners from learning institutions within the Waikato region—eight from each of three levels of learning, senior secondary school (ca. 18 years old), undergraduate (ca. 20-21 years old), and postgraduate (ca. 25 years old). This is a naturalistic qualitative inquiry conducted within a constructivist paradigm in which data were elicited and refined through interview-participant interaction. The principal data collection technique consisted of semi-structured interviews and included the use of Interviews-About-Events focus cards (Carr, 1996).

1.3 Purpose of the Inquiry

The purpose of this inquiry was to gain an understanding of learners' mental models for chemical bonding.

The research goals for this inquiry are to:

1. Establish if there are preferred mental models for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.
2. Establish the prevalence of the use of analogies for the understanding of the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.
3. Establish the prevalence of alternative conceptions for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

1.4 Assumptions and Definition of Terms

The following assumptions are central to this inquiry:

1. Individuals are purposeful beings who construct knowledge in ways that are meaningful to them for the purpose of understanding the material world, and to cope with learning experiences.
2. The construction of knowledge is influenced by the learners' context, including social interactions, peers and cultural background.
3. Personal constructs held by learners may at times be in conflict with scientific views; learners do not necessarily attribute such constructs a lower status than the scientific view.
4. Learners benefit by developing conceptual understandings that are in broad agreement with the scientific view or are consistent with experimental observation.

A number of terms are used frequently throughout this thesis—consequently, it is beneficial to make clear the meaning ascribed them in this research report.

Chemical bond—a force that holds groups of atoms together and makes them function as a unit (Pauling, 1960; Zumdahl, 1989).

Concept—a general view of things and events, which is used as a basis for thought, commonly expressed using symbolic language. Concepts range from those easily imagined, like plant and animal, to the highly abstract, like atom or force (Page & Thomas, 1979).

Conceptual understanding—the ability of a learner to relate newly acquired concepts to prior existing knowledge in a substantive, non-arbitrary way (Ausubel, 1968).

Rote learning—the arbitrary, verbatim and non-substantive incorporation of new concepts by the learner, with no attempt made to link such concepts to existing knowledge (Ausubel, 1968).

Scientific view—the consensual peer-negotiated view held by the scientific community at large (Summers, 1992).

Alternative conceptions—beliefs that differ from the scientific view and from the intended outcomes of instruction, but which are meaningful to the learner. Such views also are referred to in the literature as misconceptions, alternative frameworks, children's science, and world-views depending on the epistemological perspective of the author (Driver, 1981).

Mental model—the researcher's interpretations of a learners' mental representations for a concept (Harrison & Treagust, 1996; Norman, 1983; Vosniadou, 1994).

Analogy—a correspondence in some respects between concepts that are otherwise dissimilar, consisting of mapping between similar features of those concepts (Thiele & Treagust, 1995).

1.5 Significance of the Inquiry

The findings from this inquiry will provide chemistry educators with an understanding of the preferred mental models for the concept of chemical

bonding for secondary, undergraduate and postgraduate chemistry learners. The inquiry will provide recommendations for the appropriate use of mental models and analogies for the teaching of the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

1.6 Context of the Inquiry

The New Zealand school education system has undergone dramatic and complex changes in the last two decades (Bell, B. 1991; Bell, B., Jones & Carr, 1995, 1996; Department of Education, 1987; Matthews, 1995; Ross, 1984). New Zealand changed from a fragmented national curriculum to a more coherent structure to deal with Year-1 to Year-13 learners. Curriculum and administrative reviews carried out from 1984-87 resulted in the formulation of the *National Education Guidelines* containing the *National Education Goals* which specified the Ministry's overall objectives, the *National Administration Guidelines* which specified the administrative framework necessary to achieve these objectives, and the *New Zealand Curriculum Framework* (Ministry of Education, 1993a, 1993c). The *National Education Guidelines* and *New Zealand Curriculum Framework* detail the elements deemed fundamental to teaching and learning in New Zealand schools, comprising seven essential learning areas and eight essential skills. Curriculum documents incorporating essential skills were subsequently developed for each of the learning areas for Year-1 to Year-13. Similarly, national curriculum statements were developed for science, physics, chemistry, biology, and technology for Year-11 to Year-13. The science curriculum comprised achievement aims and objectives with specific content to be selected by schools (Ministry of Education, 1993b), whereas for the subject curricula content was prescribed by the New Zealand Qualifications Authority (NZQA) (Ministry of Education, 1996a, 1996b, 1996c, 1996d). In addition to providing content prescriptions, the subject curricula were linked to the aims and objectives and essential skills expressed in the *National Education Guidelines*, the *New Zealand Curriculum Framework*. For example, school curriculum was

expected to incorporate generic skills such as communication and literacy skills provided in the *New Zealand Curriculum Framework* as well as appropriate content detailed in the subject guidelines. A key philosophy of the curriculum documents was a shift from an exclusive science-for-some content-driven teaching approach, towards a more inclusive science-for-all learner-centred approach (Clark, 1996). Program development is now substantially school-based and each school is required to develop its own teaching approach with performance evaluated by an independent Government appointed body, known as the Education Review Office (ERO). In spite of the curriculum reviews there has been little change to the fundamental chemistry taught and topics like balancing equations, stoichiometry, atomic theory and chemical bonding still form the basis of chemistry learning in New Zealand secondary schools.

Science and technology has undergone spectacular growth in recent times with significant impact on society (Halloun, 1998; Harding & Vining, 1997). There is now increasing Government emphasis placed on the production of a more skilled workforce and consequent demand for access to higher education (Fensham, 1980; Kings, 1990; Laws, 1996). A number of in-depth studies spread over nearly a decade, resulted in the New Zealand Government imposing a partial user-pays system as a means of funding increased demand for tertiary education (Hawke, 1988; Todd, 1994). Tertiary education fees are presently funded by loans at well above market rates. At the time of writing, collective student debt totalled in excess of 3 billion New Zealand dollars, and universities were experiencing a contraction in rolls (Cassie, 1999).

The learning institutions involved in this inquiry comprised two secondary schools and a tertiary institution in the Hamilton Metropolitan area, the major city of the Waikato province—a wealthy dairy farming area. The secondary schools were single-sex integrated schools in a high-decile suburb (decile rating 7). Decile rating is a measure of the schools' community wealth and communities are rated on a scale of 1A to 10, with 1A being poorest and 10 wealthiest (Education Review Office, 1999, August 7). Integrated schools were

private schools that have been subsumed into the state schooling system, whilst retaining some aspects of their origins such as religious affiliation. The University involved in this inquiry was the University of Waikato, possessing a roll of approximately 10,000 equivalent full-time students (EFTS) with the roll for the School of Science & Technology approximately 1000 EFTS. The School has undergone significant contraction in recent years with the Department of Chemistry experiencing a decrease in enrolment of around 30% over the last five years. The Chemistry Department comprises 15 academic staff with a wide range of research interests. In recognition of recent advances in science, a number of applied chemistry and multidisciplinary courses have been introduced latterly. In spite of this, the Department is still rather traditional in outlook; for example, until 1998 chemistry majors were required to complete all core chemistry courses (i.e., organic, inorganic, and physical) to the third-year level. Now learners may choose three third-year courses from the core courses and third-year analytical chemistry. The traditional views of Departmental staff also are evident in course prescriptions, with strong emphasis placed on theoretical chemistry, particularly atomic structure and chemical bonding. Likewise teaching methodology is typically transmissive in nature (Coll, 1997a) as is reportedly common in science faculties in other tertiary institutions (Laws, 1996).

1.7 The Organisation of the Thesis

This thesis is organised into eight chapters. Chapter 2 comprises the first part of the literature review. It consists of a review of relevant literature of science education inquiries, namely learners' mental models, the use of analogies for conceptual understanding, and learners' alternative conceptions for chemistry and chemical bonding. Chapter 3, which provides the theoretical framework for the inquiry, begins with a discussion of the salient features of paradigms, ontology, epistemology and methodology. This is followed by a description of the development of the constructivist paradigm and the chapter concludes by considering the relevance of the constructivist paradigm for this inquiry. Chapter

4 consists of a description of the methods and methodology used in the inquiry, beginning with a description of methodologies used in science education inquiries, with particular emphasis paid to naturalistic and qualitative means of inquiry. The chapter describes the development of the interview protocol, followed by a description of the data collection strategies employed. The data analysis procedures are described next, along with a description of the measures taken to maintain the trustworthiness of the inquiry. The chapter concludes with a consideration of the ethical issues pertinent to the inquiry. Chapter 5 consists of a description of the pilot study undertaken in Australia, including a discussion of the implications of the pilot study for the main inquiry. The results of the data collection based on clinical interviews, together with data analysis, and discussion of results are reported in Chapters 6 and 7. The format for the presentation of the results and discussion follow that of the research goals outlined in Section 1.3 (p. 3), with learners' mental models for chemical bonding reported in Chapter 6, and learners' use of analogies and alternative conceptions for chemical bonding in Chapter 7. The thesis concludes with Chapter 8 which consists of a discussion of the implications of the research findings for teaching and learning, along with suggestions for future research.

1.8 Summary

This chapter has provided an introduction to the inquiry. The background and justification were described first and used to provide the scope of the inquiry followed by a description of the research goals. A description of the assumptions and definition of relevant terms followed, and the chapter concluded with comments on the significance of the inquiry, the context of the inquiry, and the organisation of the thesis. Chapter 2 represents the first part of the literature review and comprises a review of relevant studies in science education—the use of models and modelling in the sciences, the use of analogy and learners' alternative conceptions for chemistry and chemical bonding.

CHAPTER TWO

LITERATURE REVIEW:

RELEVANT STUDIES IN SCIENCE EDUCATION

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CHAPTER TWO
LITERATURE REVIEW:
RELEVANT STUDIES IN SCIENCE EDUCATION

Overview of the Chapter

This chapter comprises a review of relevant studies in the science education literature, focusing on the research goals described in Chapter 1 (p. 3). As this inquiry is concerned with learners' preferred mental models in science and science education, the first section considers the use of models and modelling in chemistry and the sciences, beginning with a discussion of the purpose, importance, and characteristics of models. Typologies of models are described next, followed by a description of mental models, and the section concludes with a description of learners' use of mental models.

The second section is based on the second research goal, and comprises a review of reports of learners' use of analogies in science and chemistry. The section begins with a definition of analogy followed by a description of the use of analogy for concept generation, and concludes with a description of the use of analogies in chemistry teaching.

The third research goal relates to learners' alternative conceptions for chemical bonding. Hence, the third section in this chapter consists of a review of studies of learners' alternative conceptions for the sciences and the concept of chemical bonding. The section begins with a description of the foundations of the alternative conception movement and concludes with a description of specific alternative conceptions encountered in chemistry and chemical bonding.

2.1 Models and Modelling in the Sciences and Science Education

2.1.1 *The Purpose, Importance and Characteristics of Models*

Researchers have identified three principal purposes for modelling in the sciences: to produce simpler forms of objects or concepts, to provide stimulation and support for the visualisation of some phenomenon and to provide explanations for scientific phenomena (Gilbert, J.K., 1980; Gilbert, J.K., & Rutherford, 1998a, 1998b; Suckling, Suckling, & Suckling, 1978). Modelling involves the transfer of some aspects or features of the source of the model to the target of the model (Brodie et al., 1994) (Figure 2.1).

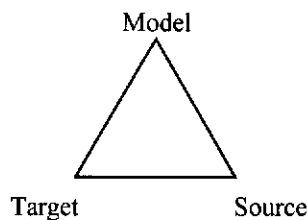


Figure 2.1 The relationship between a model, its source and target
(After Brodie et al., 1994)

Since modelling inherently involves simplification, the extent to which the target and source share attributes varies, that is, the model comprises an approximation or less accurate representation of the target. However, Maksic (1990) points out that any loss of accuracy is compensated for by gains in clarity.

A salient feature of all models [is] that they represent an approximate description of the corresponding complex systems—the so called objects, originals or prototypes. In modelling we sacrifice perfect truthfulness because the object is distorted by simplification. This is, however, more a strength than a weakness because a model gains greatly in transparency and conceptual clarity. It deliberately neglects the less relevant details and emphasizes the most important facets...It should always be kept in mind that a

model is different, and sometimes quite different, from its object in very many ways. It is also useful to remember that a reliable model exhibits the essence of the property or a phenomenon under study, since attention is focused only on selected and dominant features. (Maksic, 1990, p. xiv)

Consequently, the use of a model enables the scientist or novice to recognise the key aspects of the target without becoming distracted by extraneous detail (Gilbert, J.K., & Boulter, 1998). Further detail may be subsequently introduced, but the initial grasping of an abstract concept is most easily achieved when the concept has been stripped to the bare necessities required for understanding.

It is the function of the model to provide the student with a basic outline of the 'forest' before he [sic] is able to differentiate the 'trees.' When confronted with the 'trees' he [sic] has a much greater opportunity to place them in their proper perspective. (Weller, 1970, p. 118)

Because the purpose of models and modelling varies, models themselves vary considerably from the simple to the extraordinarily complex (Gilbert, J.K., & Osborne, 1980). As Zumdahl (1989, pp. 197-198) puts it, models vary "from simple models to predict approximate behaviour and more complicated models to account very precisely for observed quantitative behaviour".

Models and modelling are of such importance in science that the appropriate use of models is seen by many as central to an understanding of science (Gilbert, J.K., & Boulter, 1998; Harrison & Treagust, 1996, Ingham & Gilbert, 1991). As Harrison and Treagust (1998) put it "modelling is the essence of scientific thinking". Whilst models and modelling in some form are used in all sciences and also the humanities, they have particular importance in chemistry and physics since these disciplines involve many complex and abstract concepts. Zumdahl (1989) asserts that models and modelling are of such importance in chemistry, that it is difficult to conceive of understanding chemistry without an

understanding of models and their use. Even stronger views are held regarding the importance of models and modelling in the sciences (e.g., Hammond, Osteryoung, Crawford & Gray, 1971). S.W. Gilbert (1991) suggests that it is more appropriate to define science as a process of model building rather than as adherence to the scientific method. Such a view recognises the common ground among scientific fields using diverse methodologies.

There are a number of characteristics that models must possess, namely, self-consistency, simplicity, stability, flexibility, utility, and the ability to fail. It is likely that scientists, teachers, and science education researchers would agree with all but the last characteristic, which at first sight seems rather surprising. Maksic (1990), however, asserts that the necessity for a model to fail arises naturally from the nature of models and modelling. A model is a representation of an object or concept and not the reality, consequently "a model that is never wrong would represent the truth. Flaws are inevitable and important" (Maksic, 1990, p. xxv). Maksic further cautions that whilst a close match between the predictions of a given model and experimental data indicates that a model is reliable, this should not be taken to infer that it is somehow a copy of reality. Furthermore, complex and sophisticated quantitative models are not necessarily superior to their simpler qualitative counterparts. Nevertheless, simple qualitative models, despite their apparent lack of accuracy, possess value since they are easier to understand and remember.

2.1.2 Typology of Models: Towards a Definition of Models

Consensus about the fundamental importance of models masks considerable semantic variation in the use of the terms model and modelling. For example, knowledge models, scale models, target systems, mental models, expressed models, consensus models, enactive models, historical and teaching models have been identified (Brodie, et al., 1994; Gilbert, J.K., & Boulter, 1998; Harrison & Treagust, 1998; Justi & Gilbert, 1999; Smit & Finegold, 1995; Suckling et al., 1978). Examination of the meaning ascribed to such models reveals the broadness of such model typologies. Knowledge models are scientists'

tools used to understand reality and scale models are engineers' models constructed to represent external characteristics (Heaton, 1991; McCabe, Smith, & Harriott, 1993). Target systems are models represented in common experience, whereas mental models are deemed private, personal representations of the target. Expressed models are those made evident by an individual through action, speech or writing. Consensus and historical models are those which have been subject to testing by some social group (e.g., the scientific community) or over time, and which have agreed merit. Enactive models are models of behaviour, and teaching models are models using during instruction.

The science and science education literature contains a variety of typologies or classification schemes based on the nature of the model. Such schemes are typically dependent both on the nature of the model and the domain of scientific inquiry, hence they are appropriate for the sciences and chemistry. From these typologies a number of model types have been identified (Figure 2.2), and these are described briefly here.

Models have been classified broadly as physical and conceptual/symbolic (Brunner, 1967; Suckling et al., 1978). Physical models include scale/iconic models used to represent form or external characteristics (Black, 1962; Harré, 1970; Smit & Finegold, 1995; Tomasi, 1988), maps and diagrams such as reaction schemes and metabolic pathways (Harrison & Treagust, 1996), and formulae (Harrison & Treagust, 1996; Trindle, 1984). Analogue models may be physical or conceptual/symbolic, and are models which possess one or more of the target models' attributes (Black, 1962; Duit, 1991; Peierls, 1980; Tomasi, 1988). Conceptual/symbolic models represent mental constructs, in other words, mental models (Brunner, 1967; Suckling et al., 1978). Conceptual/symbolic models include empirical models, models which relate variables to theory (Suckling et al., 1978), and a standard, something to be imitated such as a model of a process (Harrison & Treagust, 1996; Peierls, 1980).

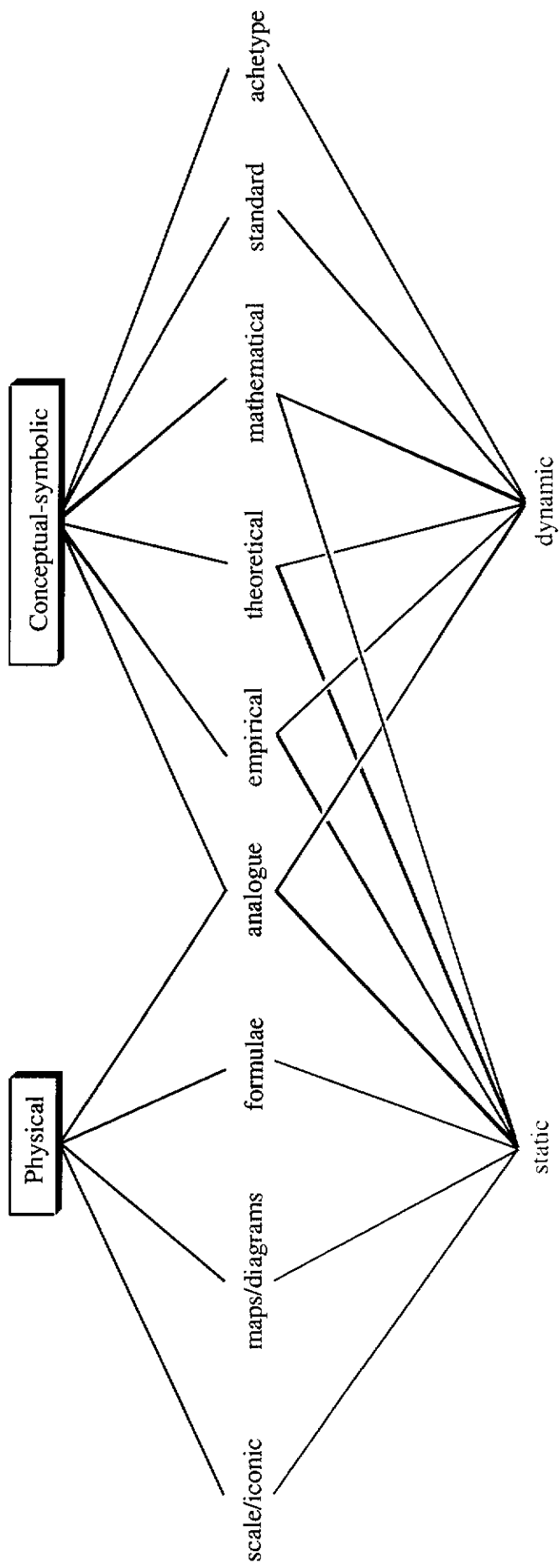


Figure 2.2 Models identified in the science education literature

An archetype consists of a constructed model which is used to describe some phenomena, the model drawing on concepts and terms from a variety of other domains (Gilbert, J.K., & Osborne, 1980). Theoretical models are models used to represent abstract phenomenon such as lines of force or bonding (Gilbert, J.K., & Osborne, 1980; Harrison & Treagust, 1996; Trindle, 1984), and mathematical models comprise physical properties like density or physical processes and mathematical equations (e.g., $F = ma$, $pV = nRT$) (Barrow, G.H., 1996; Moore, W.J., 1972, 1982).

Physical and conceptual/symbolic models may be static or dynamic; with a number of models being both static and dynamic (Comba, & Hambley, 1995; Maksic, 1990). For example, scale models and maps and diagrams are typically static in nature (Walton, 1978), a standard and archetype models are more commonly dynamic, whereas mathematical models and theoretical models may be either static or dynamic (Maksic, 1990). However, these model types are not exclusive either and, for example, a physical model may also be an analogue model, and a mathematical model also be a theoretical model. Tomasi (1988) points out that any overlap of model types may result in confusion. Such confusion is exacerbated by the complex relationship between theory and experiment (De Posada, 1999; Franco et al., 1999; Maksic, 1990). According to Maksic, theory and experiment are inextricably entwined. A natural transmission or conduit exists between experiments and theory, and between quantitative and qualitative models. So, for example, while a mathematical model comprising sophisticated calculations of wavefunctions results in considerable detail about atomic structure, simple pictorial representations arising from these calculations serve to focus on chemically interesting aspects of the structure (Trindle, 1984; Tsaparlis, 1997).

2.1.3 Fundamental Properties of Models: The Nature and Limitations of Models

Models possess a number of fundamental properties. First, models are human inventions and are thereby based on an incomplete understanding of how

nature works (Carr & Oxenham, 1985; Ganguly, 1995; Greca & Moreira, 1997). Consequently, most models are wrong in some key aspect (Tomasi, 1988; Trindle, 1984). The fact that a model possesses limitations does not necessarily mean it should be automatically discarded—particularly if it is not easily replaced. Consider the simple Aufbau principle, a model used to explain the electron configurations for the elements.

Chromium and copper do not agree with the predictions [of the Aufbau principle]. Detailed studies show that the [observed] configurations of chromium and copper result from complex electron interactions that are not taken into account in the model. But this does not mean that we should discard the simple model that is so useful for most atoms. Instead, we should apply it with caution and not expect it to be correct in every case. (Zumdahl, 1989, p. 344)

The pragmatic use of models that are known to possess limitations is one of the characteristics that differentiates the expert from the novice (Gilbert, J.K., & Osborne, 1980; Grosslight et al., 1991). Williamson and Abraham (1995) believe that this is related to experts' greater ability to visualise abstract concepts.

Novices usually have incomplete or inaccurate models, whereas while those built by experts includes both sensory (or macroscopic) data from the physical world *and* [original italics] formal abstract constructs of the phenomena. (p. 522)

Research has indicated that experts see models in a functional, utilitarian manner compared with novices—that is, they recognise that models are intended to serve the user and, for example, frequently require modification as new experimental data are revealed (Borges & Gilbert, 1999). Grosslight et al. (1991) point out that novices think of models in concrete terms, effectively as scale models of reality (see also, Abell & Roth, 1992; Bent, 1984b; Carr, 1984; Clement, 1998). Some

models have proven spectacularly successful, for example, the Watson-Crick model for the structure of DNA (Rodley & Reanny, 1977; Watson & Crick, 1953), Einstein's relativity (Clark, R., 1973; Kline, 1985), and Schödinger's wave-mechanical model of the atom (Kline, 1985; Moore, W.J., 1989). Remarkably, if a given model proves highly successful, even the scientific community may fail to remember that it possesses limitations (Ben-Zvi & Genut, 1998; Carr & Oxenham, 1985; Ingham & Gilbert, 1991). Schrader (1984) sums up the situation concisely, stating that "some models are so powerful at explaining well understood observations that *they are regarded as facts* [italics added]" (p. 1001). Zumdahl (1989) supports Schrader's view:

A model is considered successful if it explains the known behaviour in question and predicts correctly the results of future experiments. It is important to understand that a model can never be proved absolutely true. In fact, *any model is an approximation* [original italics] by its very nature and is doomed to fail at some point. (p. 187)

Interestingly, Zumdahl (1989) points out that failure of a model is not necessarily a bad thing since it can help by alerting scientists to fundamental misconceptions and ultimately result in an improved understanding of the concept.

When a model is wrong, we often learn much more than when it is right. If a model makes a wrong prediction, it usually means we do not understand some fundamental characteristics of nature. We often learn by making mistakes. (p. 344)

This view is supported by others (e.g., Bent, 1984b; Brodie et al., 1994; Gilbert, J.K., & Osborne, 1980), and Schamp (1990, p. 16) argues that recognition of a models' limitations may serve to advance "understanding by emphasizing the *limitations* [original italics] of any one model rather than focusing on its

generality". There is an interesting illustration of this issue in the scientific literature. In the late 1970s, two scientists proposed an alternative model for the structure of DNA (Rodley & Reaney, 1977). This challenge to the successful and well established Watson-Crick model was highly controversial and acrimonious. Interestingly, it was well known that the Watson-Crick model possessed limitations—for example, the rapid unzipping of the DNA chain seemed inconsistent with the double-helix model (Crick & Klug, 1975; Rodley & Reaney, 1977). However, the remarkable success of the Watson-Crick model meant that many scientists were highly uncomfortable about any challenge to its correctness. Hence it seems that the social context may exert an influence on perceptions of the correctness or otherwise of a model, and there is a long history of such influence in the development of scientific theories such as evolution and creationism (Lühl, 1992; Laws, 1996; Matthews, 1995). Lühl argues that such an approach, what she refers to as the *historic-genetic method*, "is a way of showing high school students some of the complex interactions which lie behind the facts presented in science courses" (p. 193). The significance of this approach for the use of models and modelling in science education is that properly briefed learners "develop their understanding of physical modelling by learning to think in terms of models, and interpreting the ideas of important scientists in terms of models" (Lühl, 1992, p. 193). It would seem that such an approach may be of value in that an appreciation of the historical context of the development of scientific theories, including models, may help learners and scientists alike to remain conscious of the nature and limitations of models.

A number of authors have pointed out that it is common to use multiple models in science (e.g., Barnea, Dori, & Finegold, 1995; Birk & Abbassain, 1996); however, there is also considerable discrepancy between novices and experts in their recognition of the sense and purpose of multiple models (see, e.g., Clement, 1998; Grosslight et al., 1991). Despite this, the use of multiple models is particularly prevalent in chemistry, especially for the understanding of the abstract microscopic concepts of atomic structure and chemical bonding (e.g.,

Brodie et al., 1994; Comba & Hambley, 1995; Glynn & Duit, 1995; Kenan, Kleinfelter, & Wood, 1980; Zumdahl, 1989).

2.1.4 *Mental Representations, Mental Images, and Mental Models*

Scientists and learners construct mental representations in order to interpret their experiences and to make sense of the physical world. Like the term model, the terms mental representation, mental image, and mental model have been attributed a variety of meanings (e.g., Glynn & Duit, 1995; Hafner & Stewart, 1995; Harrison & Treagust, 1996; Vosniadou, 1994).

In 1983 Johnson-Laird proposed "the existence of at least three types of mental representations" (p. 165). First, propositional representations are interpreted to mean a mental representation consisting of a string of symbols composed from a finite vocabulary; that is the representation of verbal propositions. According to Johnson-Laird, a propositional representation is "a mental representation of a verbally expressible proposition" (p. 155). The most general way to represent this process is via mental language and the "mental language must have a vocabulary, a grammar, and a semantics" (p. 155). Second, mental images are seen by Johnson-Laird to possess a number of properties. The mental processes that result in mental images are similar to those underlying the perception of an object or picture. Third an image, which represents a coherent representation of a scene or object, is amenable to mental transformations in a continuous fashion. Images represent objects and are analogical in the sense that structural relationships exist between the image and object. Types of images correspond to sensory input and comprise, vision, audition, smell, taste, and kinesthesia (i.e., associated with muscle and nerve response). Ostensibly, these sensory responses trigger mental images that are dependent upon the frame of the subject (Horowitz, 1972; Kleinman, Griffin, & Kerner, 1987).

Mental models comprise specific knowledge about a particular situation or object(s), and may exert a great influence on an individuals' understanding and behaviour (Craik, 1967; Gentner & Stevens, 1983; Johnson-Laird, 1983; Medin

& Ross, 1992; Vosniadou, 1994). Mental models are distinguished from schemata in that they are not simply "filling in of expected values based on prior knowledge" (Medin & Ross, 1992, p. 353), rather they represent active constructs that are often spontaneous, and are frequently constrained by theories rather than empirically derived from experience (Norman, 1983; Hafner & Stewart, 1995). Mental models according to Johnson-Laird (1983) are analogical in nature, serving to relate the mental representation to the "state of affairs in the world" (p. 156). However, the extent of the analogical structure can vary considerably, "models of quantified assertions may introduce only a minimal degree of analogical structure" (Johnson-Laird, 1983, p. 156). A similar view of mental models to Johnson-Laird (1983) is held Vosniadou (1994) who sees mental models as analogues of mental representations—" [mental model] refer[s] to a special kind of mental representation, an analog representation, which individuals generate during cognitive functioning" (p. 48).

Mental models are of interest in this thesis for two reasons. First, they influence cognitive functioning (Vosniadou, 1994) and second, mental models can provide science education researchers with valuable information about the learners' conceptual framework, that is, the underlying knowledge structures (Vosniadou, 1994). Like models, mental models may serve a number of purposes. Mental models function to provide explanations and justifications and to serve as mnemonic devices for memory enhancement (Williams, Hollan, & Stevens, 1983). However, an important, often overlooked, function that mental models serve is to predict behaviour, particularly of physical systems.

It is important to clearly distinguish between the real world and the mental world, that is, the cognitive representation of the real world, and the mental model which is the representation of the mental world (Palmer, 1978). According to Palmer, a mental model, since it is a model of the mental world, is also a model of the real world. Palmer suggests that there are three levels of representational concepts; mental world, mental model and theorists' description of mental world and model. Holding a similar view of mental model to Palmer,

Paivio (1986) uses the term representation more explicitly to refer to *observable* psychological phenomena like language that have a representational function. According to Paivio, mental representations of an individual can be viewed as that individual's theory of the world and his or her interaction with it.

Mental models are considered by many authors to be functional evolving systems; that is, many mental models are incomplete and do not have clearly defined boundaries (e.g., Hafner & Stewart, 1995; Norman, 1983). Hence, mental models are often unscientific and quite unstable.

People's mental models are apt to be deficient in a number of ways, perhaps including contradictory, erroneous, and unnecessary concepts...as [social] scientists who are interested in studying people's mental models, we must develop appropriate experimental methods and discard our hopes of finding neat, elegant mental models, but instead learn to understand the messy, sloppy, incomplete, and indistinct structures that people actually have. (Norman, 1983, p. 14)

Mental models are causal and are functionally defined in the sense that they allow an individual to engage in description, explanation and prediction (Gilbert, J.K., & Rutherford, 1998a, 1998b; Hafner & Stewart, 1995). Mental models also may be defined in a structural sense and consist of objects, states that objects exist in, and process that are responsible for the objects changing states. Barsalou (1992) proffers another view of mental models in which he makes two assumptions about mental models. First, a mental model is a frame whose attributes and relations are analogous to the physical parts and relations of its category members. Second, a mental model must produce quasi-continuous simulations of events. However, like Norman (1983) and Hafner and Stewart (1995), Barsalou sees mental models as not necessarily complete or correct or even consistent, rather, "the representation must simply be an attempt to construct an analogous representation of physical structure" (p. 164).

There has been recent interest in the influence of social cognition on mental models (e.g., Anderson, T., Howe, & Tolmie, 1996; Glynn & Duit, 1995; Rogers & Rutherford, 1992). For example, T. Anderson et al. (1996) suggest that because older learners possess increased capacity of working memory, along with an ability to reflect on their own learning, there is a strong link between learners' working memory and metacognitive skills (Anderson, T., et al., 1996). Similarly, older learners and experts show greater capacity for solving problems that required the formation of multiple transitory mental models (Anderson, T., et al., 1996; Glynn & Duit, 1995; Larkin, 1983).

Mental models are unique to the observer: Norman (1983) and others (e.g., Glynn & Duit, 1995; Harrison & Treagust, 1996; Hesse, 1966; Johnson & Gott, 1996) warn that "discovering what a person's mental model is like is not easily accomplished" (Norman, 1983, p. 11). Norman suggests that it is no simple task to understand learners' mental models because they may behave quite inconsistently, and "believe one thing and act in a quite different manner" (p. 11). Hesse (1966) agrees that models represent personal constructs, but adds that this should not be taken to mean that they are used solely for purely subjective purposes. Hence, there is consensus that mental models are personal constructs and like other constructs are subject to social influence.

2.1.5 Typology of Mental Representations, Mental Images, and Mental Models

The research purpose for this inquiry is to investigate learners' mental models for chemical bonding. In this section, a typology of mental representations and mental models is developed from this review of the science education literature (Figure 2.3). Mental representations were classified into mental images, mental models and propositional representations by Johnson-Laird (1983). Similarly, Kleinman et al. (1987) classified mental images as, associate—that is, involving simple word association, real—that is, mental images that describe concrete or real-world experience, and model—a mental image that involves the description of an abstraction.

MENTAL REPRESENTATIONS

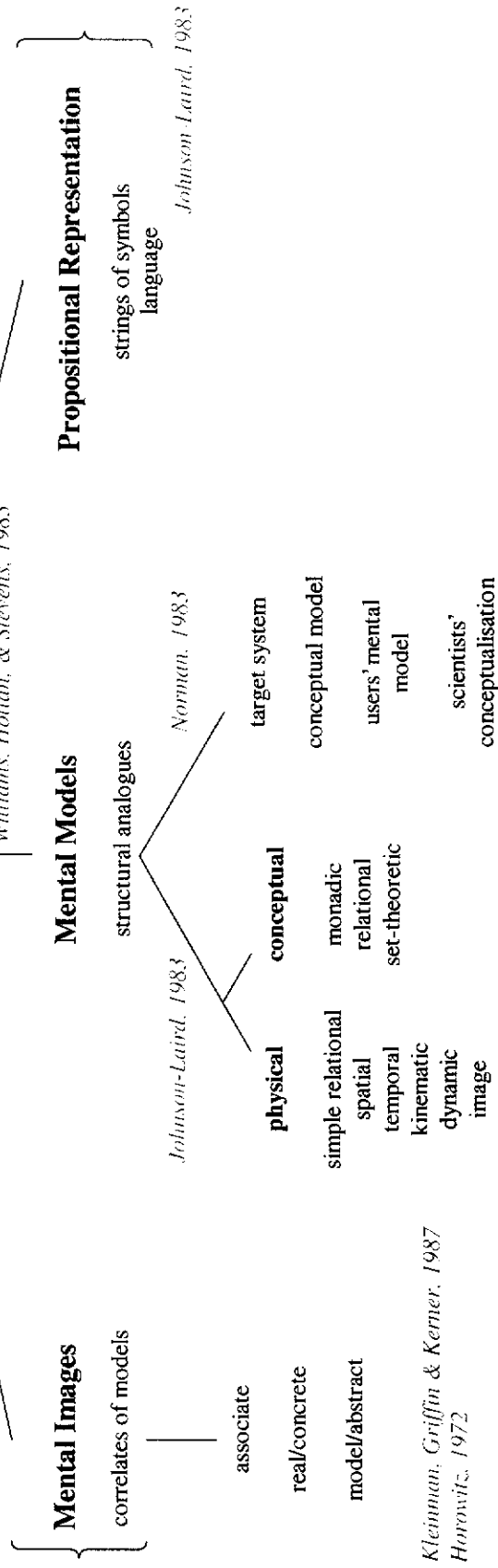


Figure 2.3 Typologies of mental representations and mental models identified in the science education literature

Mental models have been further classified using a number of typologies. Norman (1983) classified mental models as the target system—the system that the learner is attempting to study, the conceptual model of that system—an appropriate representation of the target system, the user's mental model of that system, and scientists' conceptualisation of the target situation.

Mental models can also be divided into physical and conceptual mental models, where "physical models represent the physical world; conceptual models represent more abstract matters" (Johnson-Laird, 1983, p. 422). Hence, physical mental models are mental constructs of physical entities—real or imagined, whereas conceptual mental models are mental constructs of concepts, models or abstractions.

Physical mental models are divided into simple relational, spatial, temporal, kinematic, dynamic and image. The simple relational model identified by Johnson-Laird shares similarities with scale models "a simple relational model is a static frame consisting of a finite set of tokens representing a finite set of physical entities" (p. 422). Mental tokens consist of a possible claim, decision, or action, relevant data and a warrant (Green, 1996). Spatial models are similar, consisting of relational models in which it is only spatial relations that are of interest. Temporal models consist of a sequence of spatial frames that occur in a temporal order. Kinematic models consist of temporal models that are psychologically continuous; that is, the model represents changes of the entities with no temporal discontinuities. A dynamic model is a kinematic model accompanied by causal relationships between frames. Finally, an image consists of a viewer-centred representation of visible characteristics.

Conceptual mental models were further classified by Johnson-Laird into monadic, relational and set-theoretic. A monadic model represents a set of assertions about individuals, whereas a relational model introduces a set of relations, frequently abstract, between the components of a monadic model. Set-theoretic models contain a finite number of tokens directly representing sets; the membership of the sets designated by members properties, abstract or real.

The treatment of mental models by Johnson-Laird (1983) is more general than that of Norman (1983)—the latter tending to focus on examples specific to the physical sciences (see also, Rogers & Rutherford, 1992). However, T. Anderson et al. (1996) argue that essentially Johnson-Laird proposes that humans model reality by manipulating internal symbols. That is, mental models function because the components of the mental model have the same relation-structure as that of the object or process being modelled. Interestingly, despite the difference in approach between Johnson-Laird and Norman, they share a number of similarities. For example, both view mental models as incomplete and believe that individuals' ability to operate their models is limited (see also, Anderson, T., et al., 1996; Barsalou, 1992; Glynn & Duit, 1995). The major point of difference between the two views lies in the stability of mental models. Johnson-Laird suggests that mental models are transitory, whereas Norman contends that models are held over long periods of time and are relatively stable. The typology proposed by Norman seems more appropriate for use in the sciences—Johnson-Laird's being too general. Hence, Norman's typology is that adopted for use in this inquiry.

2.1.6 Learners' use of Models and Mental Models in Chemistry and the Sciences

Many researchers argue that confusion in the use of models may have origins in the mode of instruction (e.g., Fensham & Kass, 1988; Harrison & Treagust 1996; Raghavan & Glaser, 1995). For example, Smit and Finegold (1995) found Southern African physical science teacher-trainees viewed models as in effect scale models of reality as a result of their exposure to medical models such as models of the human body, insects, skeletons and so forth. Similarly, Barnea et al. (1995) report that Israeli pre- and in-service chemistry teachers failed to distinguish between a mental image and concrete model, believing instead that a model is simply a way to describe a process or phenomenon; that is, they failed to realise that models also could be used for other purposes such as prediction.

A complication for instructors in using models in chemistry teaching is that sometimes the models used are attempting to model other models. As Walton (1978) puts it, "a major difficulty is that the atomic theory from which ideas of molecules and crystals derive is itself a model of the nature of matter" (p. 11). Weller (1970) suggests that this situation likely arises from the verbal shorthand that is so common among experts; the scientist is clear on what he or she means and when communicating with another like-minded expert no confusion arises. However, when the scientist is attempting to communicate with a novice or the general public, confusion between the model and the modelled arises because "in their own circle, as a matter of efficiency, the scientists, fully realizing the difference [between model and theory], may talk about the theory in terms of the model as if they were one and the same" (p. 116). This view is supported by Kleinman et al. (1987) who found that individuals retained an increased level of abstraction and number of images with increased educational level—culminating in an enormous number of mental images for faculty and post-doctoral research fellows. Typically, experienced chemists tended to suppress the associative image in favour of mental models, whereas undergraduate learners tended to conceptualise more by word association. An important difference between the two is that the images possessed by experts were not of real-world objects; rather they were of abstract images, that is, constructs based on abstract models. The view that learners prefer simple realist mental models is consistent across cultures. A study of high-achieving Portuguese learners' mental models for water and Australian senior secondary school learners' mental models for atomic structure revealed that learners preferred simple realist models such as space-filling models (Harrison & Treagust, 1996; Pereira & Pestana, 1991). Similarly Taber (1998) found that A-Level learners' preferred mental model for covalent compounds was the simple octet rule.

It seems that learners, unlike experts, fail to appreciate that the principal function of mental models in science is to aid in the understanding of some phenomenon; studies by Grosslight et al. (1991), Abell and Roth (1992) in the

biological sciences, Bent (1984b) in chemistry, and Raghavan and Glaser (1995) in physics support this conclusion. Mismatch between scientists' and learners' perceptions may be due to the inability of novices to operate at the formal level. For example, Gabel, Briner and Haines (1992) assert that chemistry can be described on three distinct levels, sensory, atomic/molecular, and symbolic. Commonly, a chemical substance is represented on the atomic/molecular level using models such as three-dimensional representations. However, many learners address chemical problems on one level alone, for example, using a purely symbolic approach. Consequently, some authors argue that it is essential for instructors to design problem-solving exercises that utilise all three levels in an integrated manner to foster genuine understanding, as opposed to merely achieving competence in the use of algorithms (Gabel et al., 1992; Nakhleh, Lowery, & Mitchell, 1996; Pestel, 1993).

Bent (1984b) suggests that learning the appropriate use of models is a complex task—making parallels between learning chemistry via models and learning a language, and argues that the difficulty arises during instruction, and models are often presented as abstractions outside the learners' framework. Bent recommends that chemistry instructors introduce a model when it is a necessary consequence or an immediate expression of an experiment or an observation and argues that "no model ought to be introduced unless its use can be made utterly clear to the student and unless it will be used again" (p. 777). Gabel et al. (1992) similarly argue that teachers should model the physical phenomena they are representing as often as possible. This may seem to be a simple solution, but it is difficult to see how the introduction of models can be avoided or reduced in disciplines like chemistry and physics, for which the use of models is highly prevalent.

One of the principal difficulties faced by learners in using two-dimensional structural models such as those presented in textbooks is responding appropriately to visual diagrammatic clues (Baker & Talley, 1972; Mathewson, 1999; Pribyl, & Bodner, 1987; Small, & Morton, 1983; Wartofsky, 1979; Weller,

1970). Learners' alternative conceptions can be triggered by inappropriate or misleading diagrams because diagrams highlight particular features, and resultant exaggeration may confuse the learners if taken literally. However, improvements in learners' ability to visualise models can occur after even a remarkably modest training program (Coleman & Gotch, 1998; Tuckey, Selvaratnam, & Bradley, 1991). Furthermore, the likelihood of inaccurate interpretation can be reduced by allowing learners to draw their own diagrams, and guiding them to be more critical of diagrams in textbooks and other curriculum material (Wheeler & Hill, 1990).

The use of combined manipulatives—two-dimensional representations, three-dimensional computer simulations, and three-dimensional ball-and-stick molecular models—has been reported to enhance learners' long term retention of depictions of molecular structure (Copolo & Hounshell, 1995; Rozzelle, & Rosenfeld, 1985). Learners using combined manipulatives "did not have to transfer a two-dimensional molecular representation into a three-dimensional mental model" (Copolo & Hounshell, 1995, p. 302); consequently, they were able to relate the two-dimensional representation to the concrete three-dimensional molecular model more effectively than using two-dimensional or three-dimension representations alone (Copolo & Hounshell, 1995; Glynn & Duit, 1995; Solomon, 1995). Solomon (1995) suggests that such analogue transfer is more straightforward when using mechanical models and the manifest differences between the mechanical model and theoretical model reduce the likelihood of model confusion.

Although some research studies have lauded the value of combined manipulatives, a number of authors argue that experience with physical or two-dimensional models alone serves to improve chemistry understanding of abstract concepts (e.g., Birk & Abbassian, 1996; Birk & Foster, 1989; Comba & Hambley, 1995; Gillespie, Spencer, & Moog, 1996a, 1996b; He, Liu, & Li, 1990; Streitberger, 1994; Taylor, A.P., & Williams, 1990). An example of the latter studies by Gabel and Sheerwood (1980) revealed that the manipulation of molecular models by high school chemistry learners over a long period of time led

to improved chemistry achievement for high school level learners as measured using a Piagetian style test. Interestingly, learners at both formal and concrete levels of development benefited from the use of models.

2.2 The Use of Analogy in Science Teaching and Learning

2.2.1 Definition of Analogy

Analogical models are similar in some respects to the target model and the use of analogy involves mapping or transferring shared attributes between the target and model domains (Duit, 1991; Holyoak & Thagard, 1996; Leatherdale, 1974; Sutton, 1993; Thiele & Treagust, 1995). Whilst some authors argue that any working model represents an analogy (see, e.g., Craik, 1967), Glynn, Britton, Semrud-Clikeman, and Muth (1989, p. 383) provide a more practical definition for analogy as "a correspondence in some respects between concepts, principles, or formulas otherwise dissimilar. More precisely it is a mapping between similar features of these concepts, principles and formulas". Authors use many different terms when discussing analogy; in general, target refers to the domain to be explained, whereas the terms source, base, anchor, and vehicle refer to the analog domain.

Analogical transfer can occur by a number of means. In (1989) Vosniadou proffering a simple mechanism, suggested that solving a problem about a target system (X) involves retrieving a source system (Y) which is similar to X in some way, mapping a relational structure from Y to X, and evaluating the applicability of this relational structure for X. Vosniadou states that for the analogical transfer process to work well "access to a productive analog must be based on similarity in some salient, easily accessible properties of the two systems" (p. 422).

A useful visualisation of mapping has been provided by Duit (1991) (Figure 2.4). In Duit's model there may be identical features in parts of the structures of the analog (R_1) and target (R_2); the model (R_m) represents the structural similarity—with analogy (A) representing the relation between the

analog and target. Duit notes that analogical transfer is symmetrical; that is, the terms target and analog do not "indicate some form of logical hierarchy" (p. 650). In other words, designation of target and analog are in a sense arbitrary and serve to describe the purpose of the analogy (see also, Duit & Glynn, 1996; Treagust, 1993).

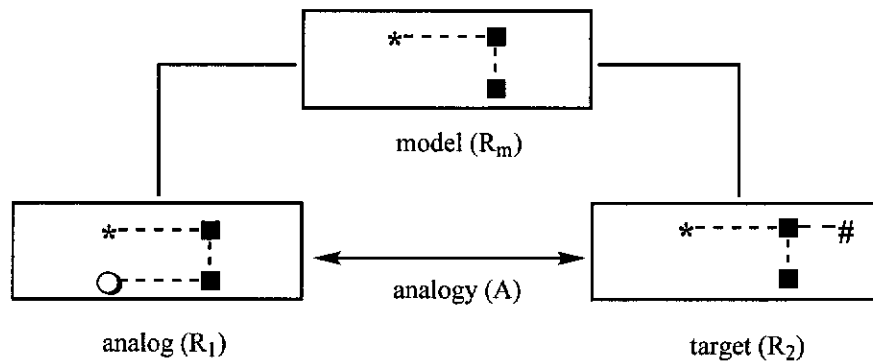


Figure 2.4 Analogical transfer by structural mapping between two domains (from Duit, 1991)

The traditional protocol employed for mapping analogical transfer is the overlap model attributed to Tversky (1977) in which "a set of qualitative concepts is shown to imply the model, which expresses similarity between objects as a linear combination of the measure of their common and distinctive features" (p. 327) (see also, Gilbert, J.K. & Osborne, 1980; Hesse, 1966). The basis of the overlap model is that a high degree of similarity indicates a good or successful analogy. In other words, the greater the match of knowledge between target and analog the better the analogy. According to this proposition, "an adequate analogue model will manifest a point-by-point correspondence between the relations it embodies and those embodied in the original" (Gilbert, J.K. & Osborne, 1980, p. 4). There are two forms of similarity, surface similarity which is perceptual in nature and cognitively primitive, and deep similarity which is based on perceptual similarity, and incorporates commonality in underlying properties (Rips, 1989; Vosniadou & Ortony, 1989).

Such a mapping process is reasonable for literal similarity comparisons such as scale models but does not provide a good overall account of analogy (Gentner, 1983, 1989). For example, a high degree of literal similarity may be of little value if it does not aid conceptual understanding. In contrast, even a small degree of overlap may be adequate if the features mapped serve to clarify counter-intuitive ideas or aid concept generation. According to Gentner (1983), "a theory based on the mere relative numbers of shared and non-shared predicates cannot provide an adequate account of analogy" (p. 156). Gentner offers an alternative, the structure-mapping theory which utilises different interpretation rules for mapping between analog and target domains. She identifies four forms of mapping—literal similarity, analogy, abstraction, and anomaly (Table 2.1).

Table 2.1 Mapping rules according to the structure-mapping theory (from Gentner, 1983)

Mapping	Number of attributes mapped	Number of relations mapped
literal similarity	many	many
analogy	few	many
abstraction	few	many
anomaly	few	few

The mapping rules depend only on syntactic properties of the knowledge representations, and these vary for each of the four cases. Literal similarity assesses both object characteristics and relations where the number of mapped predicates are compared with the number of non-mapped; for example, the solar system is compared with that in another galaxy. For analogy, relational predicates are of foremost importance and object attributes are largely ignored; for example, comparison of the hydrogen atom with our solar system. Abstraction is similar to analogy, excepting that there are fewer object-attributes

in the base domain, as well as few object-attributes in the target domain. The mapping for abstraction appears similar to analogy in that many relations but few attributes are mapped (Table 2.1). Anomaly, as the term implies, refers to situations in which there is little overlap of attributes or relations—Gentner offers the example, coffee is like the solar system.

An alternative to Tversky's (1977) overlap model and Gentner's structure-mapping model is the multiple-constraint theory (Holyoak & Thagard, 1996; Thagard, 1992). Multiple-constraint theory rests on two propositions. First, a source analog should have great semantic similarity, structural correspondence, and pragmatic relevance to the target; retrieving a potential source from memory is constrained by semantic similarity. The second restraint occurs when learners do not have to recall the analog, but are presented with both source and target. In this situation, individuals are simply involved in mapping between source and target and structural correspondence becomes the overriding concern. Analogical transfer is successful when the source analog is more familiar than the target, and there are strong semantic and structural correspondences between source and target. The main difference between Thagard's (1992) multiple-restraint theory and Gentner's (1983) structure-mapping theory is that for the former maintaining semantic and pragmatic constraints play a role in analogical mapping in addition to structural constraints. As Thagard puts it "when the stage of transfer is reached, what matters is whether the source analog can actually be used to understand or solve the target, so pragmatic matters dominate" (p. 539).

2.2.2 *The Role of Analogy in the Sciences*

Analogies can play a number of roles in science and four distinct functions have been identified, namely, discovery, development, evaluation and exposition (Cosgrove 1995; Holyoak & Thagard, 1996, 1997). Discovery occurs when analogy contributes to the formation or generation of a new hypothesis (Ganguly, 1995; Johnson-Laird, 1989; Stavy & Tirosh, 1993). When a hypothesis has been formulated, analogy may subsequently serve to further its

development from a theoretical or experimental perspective. Analogy also can play a role in the evaluation of a hypothesis, in marshalling of arguments for or against the hypothesis. Finally, analogies are commonly used to explain hypotheses to other people, particularly during instruction.

A series of great scientific analogies illustrate the role that analogy can play in concept generation during the development of scientific theories (Holyoak & Thagard, 1996; Sutton, 1993). The use of analogies in discovery is difficult to document, although there are numerous scientific theories for which analogy clearly contributed to some vital stage of a scientists' thinking, whether it was in discovery or the development of an idea. Literally hundreds of analogies have been used by scientists to aid conceptual understanding; Holyoak and Thagard (1996) identified 16 analogies that they perceive have played a pivotal role in theory development. Remarkably, they include only one analogy from chemistry—the famous example of Kekulé's snakes biting their tails used as a model for the structure of benzene (see this work, p. vi). Analogy likely plays a generative role when it occurs in situations for which prior knowledge is incomplete or poorly organized (Wong, 1993a, 1993b). Wong (1993a) argues that although analogical reasoning is typically seen as a process of schema transfer from a familiar domain into a problem situation, analogies can provide insight and inferences for individuals when spontaneously created. In such circumstances, individuals seek to find ways of making it easier to explain observed phenomena, and so develop their own analogies to advance their understanding (see also, Johnson-Laird, 1989). As Wong sees it, these generative analogies are dynamic tools rather than static representations used for understanding.

It has been suggested that analogies function best when they operate across domains because many of the formal scientific concepts in science teaching are outside the world experience of learners (Thagard, 1992; Vosniadou, 1989). However, Thagard (1992) cautions that "even if the teacher tries to use analogies to matters familiar to the students, failures can arise because the students' knowledge is not in fact organized the way the teacher thinks it is" (p.

541). Similarly, Duit (1991) argues that "familiarity is an ambivalent term" (p. 655), cautioning that "students quite often hold major misconceptions in areas where teachers and textbooks assume familiarity" (p. 655).

2.2.3 *The Use of Analogies in Chemistry Teaching*

Analogies are used extensively during chemistry instruction for a wide variety of purposes—to illustrate basic chemical concepts like solubility and kinetic theory (Coffman & Tanis, 1990; Taylor, N., & Coll, 1997), to model physical properties and the use of sophisticated instrumental techniques such as mass spectrometry and nuclear magnetic resonance (NMR) spectroscopy (Garde, 1986; Grim & Sarquis, 1995; Lee, A.W.M., 1985; Mabbott, 1988), to model molecular structure (Crane & Liu 1986; Schultz, 1986), to model chemical reactivity and equilibria (Marshall, J.K., 1984; Reingold, 1995), and to describe and understand stereochemistry (Barta & Stille, 1994; Mezl, 1996).

The chemical education literature abounds with descriptions of analogies and exhortations for their use. Pogliani and Berberan-Santos (1996) state there is considerable "educational value of the many analogies between human behaviour and chemical behaviour" (p. 950) and describe an analogy using the world-view notions of inflation and devaluation of motor vehicles to aid the understanding of chemical kinetics. However, in spite of the extensive use of analogy in chemistry teaching, there have been comparatively few studies about the use of analogy during instruction. Duit (1991) suggests this observation is true for the sciences in general, as he puts it "little is known about how analogies are used in the classroom" (p. 659) (see also, Ganguly, 1995).

Research has centred on two conceptual themes, the prevalence of analogy in curriculum materials such as textbooks and in classroom practice and learners' use of analogy or analog models. Dagher's (1995b) review of studies on the effectiveness of analogies in science education classified studies into one of two main categories according to whether the analogies were included in text or presented/facilitated by a teacher or researcher. She stated that the literature indicates that the level of guidance provided to readers, the degree of interaction

permitted, and the way the analogy is presented in textbook are the main factors that determine the effectiveness of learning via textbooks. For example, Vosniadou and Schommer (1988) found that five and seven-year-old children were able to see similarity between source and target domains, but their ability to transfer information could be improved if they received explicit instruction about the transfer process. Similarly, Thiele and Treagust (1994b, 1995) reported that a broad range of analogies employed in Australian chemistry textbooks greatly varied in the extent of mapping.

Investigations into analogy use in the classroom have focused on the teacher's use of analogy during instruction where it is frequently idiosyncratic (Friedel et al., 1990; Thiele & Treagust, 1994a). Dagher (1995a) found analogy use covers diverse source domains such as actual life experience, observed life experience, science fiction, personalised stories, and common objects. Teachers use analogies mainly for descriptive and explanatory purposes, rather than for evaluation. Dagher went on to propose a typology of analogical models consisting of compound, narrative, procedural, peripheral and simple. Compound analogies involve drawing on more than one source domain, whereas narrative analogies rely on a sole domain source, but are dynamic in nature and take on the characteristics of a story. Procedural analogy comprises analogy for which there is a focus on the procedures associated with the way that the scientific inquiry is conducted. A peripheral analogy is a secondary or accidental analogy that is typically not developed extensively and is deeply embedded in the main analogy. Such analogies are employed for descriptive purposes, and are frequently created spontaneously, almost as an afterthought. Finally, simple analogy refers to analogy that is directly related to the target, but, like peripheral analogy, is not fully developed, often only involving a sole link to the target. Thiele and Treagust's (1994a) classroom study of Australian secondary school chemistry teachers' use of analogies is consistent with the work of Dagher (1995a) and revealed that teachers mainly used analogies for the purposes of explanation when learners were struggling to cope with the concepts. Similarly, according to

Jarman (1996) the greater proportion of the analogies used in the science classrooms were generated spontaneously (ca. 58% of the total observed) although some were adapted from prior exposure to instruction.

A number of studies have found that analogy in chemistry classrooms aids understanding for abstract concepts such as the conservation of matter. For example, Stavey (1991) and N. Taylor and Lucas (1997) found that the use of acetone and a highly coloured substance, elemental iodine (I_2) in water helped overcome the common alternative conception that vaporisation does not involve conservation of mass. Learners were able to offer a scientific explanation for the evaporation of acetone when they first encountered the evaporation of iodine. A similar study by N. Taylor and Coll (1997) found that the use of a highly coloured substance (potassium permanganate) acted as a bridging analogy and proved effective in remediation of alternative conceptions for Fijian and ethnic-Indian pre-service primary teachers (see also, Clement, 1987). However, research also has revealed that even senior-level learners retain realist views of analogue models (Ingham & Gilbert, 1991) which is consistent with secondary school learners' use of other models (Bent, 1984b; Gabel et al., 1992; Harrison & Treagust 1996; Pereira & Pestana, 1991). Likewise, use of verbal analogy and physical analogue models, evaluated using a Piagetian style test eliciting learners' explanations for the diffusion of coloured dye in water and oil, found that the analogies offered a useful conceptual model for the diffusion process (Lawson, Baker, DiDonato, Verdi, & Johnson, 1993).

Despite the highly abstract nature of chemical bonding theories, there have been few reports in the science education literature of investigations into classroom use of analogy for chemical bonding: the literature consists primarily of examples of appropriate analogies, and exhortations for their use (Licata, 1988; Taber, 1995a). For example, Licata (1988) provides an analogy for covalent bonding related to eating one's lunch. Sharing one's lunch is a non-polar covalent bond, unequal sharing of lunch is a polar covalent bond, and stealing someone's lunch is a co-ordinate covalent bond.

Interestingly, some research found that the use of analogies or analogue models does not necessarily aid conceptual understanding (e.g., Gabel & Samuel, 1986; Gick & Holyoak, 1983; Kaiser, Jonides, & Alexander, 1986; Stepich & Newby, 1988). For example, Friedel, Gabel, and Samuel (1990) found no improvement in college first-year chemistry learners' understanding of the conservation of matter when using real-world analogies. The authors concluded that "students' mathematical anxiety, spatial visualization skill, and proportional reasoning ability are more important aptitudes for determining chemistry achievement" (p. 679).

2.3 Alternative Conceptions in the Sciences

2.3.1 Recent Changes to Epistemological Beliefs

Basic beliefs about how individuals acquire knowledge have changed in recent times. In the traditional positivist belief system, learners were seen as blank slates, or possessing empty heads, to be filled by the teacher via the so-called transmissive or conduit approach. However, this view has largely been supplanted by the constructivist paradigm which holds as its general premise that individuals construct their own knowledge (see Chapter 3). This change in beliefs led some investigators to question the effectiveness of traditional teaching methods and resulted in a systematic attempt to learn about learners' views of scientific concepts. Surprisingly to many, this research revealed considerable mismatch between learners' views and the scientific view, thus calling into question whether conventional teaching approaches were appropriate for the teaching of abstract science concepts (Driver, 1989a, 1989b, 1989c; Driver & Easley, 1978; Driver, Guesne, & Tiberghien, 1985; Duit, 1994; Novak, 1987, 1993; Pfundt & Duit, 1997; Schwandt, 1994; Treagust, Duit, & Fraser, 1996).

Learners' concepts that are in disagreement with the scientific view have been referred to in the literature as misconceptions, children's science, world-

views, and alternative frameworks depending on the epistemological beliefs of the investigator (Driver, 1981; Driver & Easley, 1978; Gilbert, J.K., Watts, 1983; Nussbaum & Novick, 1982). Many researchers feel that labelling learners' world-views of scientific concepts as misconceptions is too dismissive of children's views—potentially undermining their confidence. Consequently, it is now more common to refer to learner's intuitive ideas as alternative concepts or children's alternative frameworks, rather than misconceptions. The term misconception is now usually reserved for alternative conceptions that arise as a result of instruction (Treagust, 1995). When a concept is used consistently over more than one context or event it is referred to as an alternative framework (Boo, 1998).

There are a number of patterns to learners' views about science (Gilbert, J. K., Osborne & Fensham, 1982). First, is the view that non-observable entities do not exist; for example, being unable to feel an electric current means it is not present. Second, learners have a self-centred viewpoint, for example, considering that the difference between ice and water is that ice floats and that you can drink water. Third, learners hold anthropomorphic beliefs, implying that inanimate objects have feelings or act with a purpose (Lawson et al., 1993). Finally, learners infer that objects possess properties, implying, for example, that heat is a physical entity. Being egocentric in outlook, learners focus on matters that arise from their personal everyday experiences which are fairly limited compared with those of teachers and scientists (Osborne, Bell, & Gilbert, 1982; Reif & Larkin, 1991). Specifically, learners are unlikely to encounter or think about contrived experimental situations such as the force of gravity on other planets, or water boiling under reduced pressure. Learners fail to see the necessity for mutually coherent or generalisable explanations, instead tending to focus on an explanation that will satisfy the immediate need to explain a specific situation or event. Finally, learners are typically unfamiliar with scientific terminology, frequently confusing such terminology with everyday usage (Brook & Driver, 1989).

Alternative conceptions may be environmentally derived from interaction with the physical environment or socially derived from interaction with family members, peers, or the media (Driver & Easley, 1978; Solomon, 1983). Some authors also believe that alternative conceptions are commonly generated as a consequence of instruction; that is, given a problem to solve, the learner may generate an alternative conception which seems to provide an appropriate solution (e.g., Bar, 1990; Bar & Travis, 1991; Osborne, & Cosgrove, 1983; Scott, Asoko, & Driver, 1992). Such a situation is perhaps more likely in the sciences, where learners frequently encounter abstract concepts and contrived situations. However, Ben-Zvi and Hofstein (1996) argue that no single aspect can account adequately for the whole "spectrum of learning difficulties and their underlying causes" (p. 117), and suggest that learners' difficulties arise from mismatch of their abilities in information-processing, inadequacies or deficiencies in knowledge structure, information overload, and communication difficulties such as inappropriate use of analogy or confusion of scientific terminology and the vernacular.

One of the most consistent and important findings in the science education literature is that alternative conceptions are robust and highly resistant to change (Banerjee, 1995; Barrow, G.M., 1994; Carmichael et al., 1990; Kogut, 1996; Nakhleh, 1992; Tobin & Roth, 1996; Viiri, 1996). Learners often are reluctant to change their views even in the face of incontrovertible evidence. Bodner (1991), for example, reported that tertiary-level learners asked to explain why both ice and the Titanic are able to float on water given that "ice is less dense than water, but steel is almost eight times as dense as water" (p. 388), explained that it was because "the Titanic was made from titanium, not steel" (p. 388). Aside from the erroneous notion that titanium ($\rho = 4.5 \text{ g cm}^{-3}$) is less dense than water, the fact that the learner changed the facts to suit his or her explanation is indicative of the lengths to which learners sometimes will go in order to make concepts fit their existing views. Interestingly, by way of contrast, Chi, Slotta and de Leeuw (1994) claim that learners' alternative conceptions in

the biological sciences are less resistant to change and that stable alternative conceptions were readily changed by instruction.

2.3.2 *Learners' Alternative Conceptions for Chemical Bonding*

There seems to be a wide-spread perception amongst researchers and instructors that many learners find chemistry difficult (see, e.g., Barrow, G.M., 1994; Carter & Brickhouse, 1987; Kirkwood & Symington, 1996; Nakhleh, 1992). The reason suggested is that chemistry is a complex subject possessing many abstract, frequently counter-intuitive concepts (Gabel, 1998). Furthermore, Hawkes (1996) and others (e.g., Fensham & Kass, 1988; Taber, 1995a) point out that there are many alternative conceptions in commonly used chemistry textbooks. Interestingly, Hawkes stated that "after writing an article on textbook errors I received a letter from a Nobel Laureate expressing disbelief in my statement that only 2% of aqueous CdI_2 exists as $\text{Cd}^{2+}(\text{aq.})$ " (p. 421).

One of the essential characteristics of chemistry is the constant interplay between the macroscopic and microscopic levels of thought, and it is this aspect of chemistry (and physics) learning that represents a significant challenge to novices (Bradley & Brand, 1985). Numerous reports support the view that the interplay between macroscopic and microscopic worlds is a source of difficulty for many chemistry learners. Examples include the mole concept (Gilbert, J.K. & Watts, 1983), atomic structure (Harrison & Treagust, 1996; Zoller, 1990), kinetic theory (Abraham, Grzybowski, Renner, & Marek, 1992; Stavy, 1995; Taylor, N., & Coll, 1997), thermodynamics (Abraham et al., 1992), electrochemistry (Garnett & Treagust, 1992; Sanger & Greenbowe, 1997), chemical change and reactivity (Abraham et al., 1992; Zoller, 1990), balancing redox equations (Zoller, 1990), and stereochemistry (Zoller, 1990).

Despite the importance and abstract nature of chemical bonding, there have been few reports in the science education literature into learners' understanding of the concept. Interestingly, what research does exist has revealed prevalent and consistent alternative conceptions across a range of ages and cultural settings.

There has been considerable attention placed on uncovering of learners' understanding of intermolecular bonding. While there is some evidence that learners appreciate the relationship between intermolecular bonding and physical properties such as boiling point (e.g., De Posada, 1997; Peterson & Treagust, 1989; Peterson, Treagust, & Garnett, 1989; Taber, 1995b, 1998; Taylor, N., & Lucas, 1997), research reveals that learners believe intermolecular bonding is stronger than intramolecular bonding (Goh, Khoo, & Chia, 1993; Peterson et al., 1989), that they invoke intramolecular bonding in inappropriate circumstances (e.g., in ionic compounds) (Taber, 1995b, 1998), or believe it is absent in polar molecular substances such as water (Birk & Kurtz, 1999; Griffiths & Preston, 1989).

A highly prevalent alternative conception for chemical bonding is that continuous covalent or ionic lattices contain molecular species (Birk & Kurtz, 1999; Butts & Smith, 1987; De Posada, 1997; Peterson et al., 1989; Taber, 1998). Butts and Smith (1987) suggest that the ubiquitous use of ball-and-stick models used to model ionic lattices may be instrumental in the generation of this alternative conception because learners mistake sticks for individual chemical bonds. The fact that other research revealed that learners believed ionic substances such as sodium chloride possessed covalent bonds adds some credence to this suggestion (Peterson et al., 1989; Taber, 1994, 1997). A related alternative conception, reported by Boo (1998), is that some learners believe that a chemical bond was a physical entity. She suggests that this arises from a worldview that building a structure requires energy input, whereas destruction involves release of energy—that is, learners believed that bond breaking releases energy and bond making involves energy input.

Confusion over the understanding of electronegativity is also widespread, resulting in a number of alternative conceptions for chemical bonding; inability to establish the correct polarity of polar-covalent bonds, the view that non-polar molecules are formed between atoms of similar electronegativity and that the number of valence electrons, the presence of lone pairs of electrons, or ionic

charge determine molecular polarity (Birk & Kurtz, 1999; Boo 1998; Harrison & Treagust, 1996; Peterson et al., 1989).

Learners appear to have little appreciation of the underlying electrostatic nature of chemical bonding (Boo, 1998; De Posada, 1997; Taber, 1995b). For example, attraction between two oppositely charged species was thought to result in neutralisation rather than bond formation, the likely source of confusion being the parallel with acid-base chemistry (Boo 1998; Schmidt, 1997). Similarly, learners have a poor understanding of the bonding in metals, seeing metallic bonding as unimportant or in some way inferior to other forms of bonding, despite being able to use the common sea of electrons model to explain the properties in metals (De Posada, 1997; Taber, 1995a, 1998). There are a number of other alternative conceptions about covalent bonding reported in the literature. Some learners believe that the number of valence electrons and number of covalent bonds were one and the same; other conceptions include confusing resonance forms with molecular structures and believing that covalent bond formation involves the transfer of electrons (Taber, 1994, 1997, 1998).

2.4 Summary

This chapter has provided a review of relevant studies in the science education literature to provide background for the principle research goal for this inquiry that concerns learners' mental models for chemical bonding. The first part of the review reported here considered the use of models and modelling in science and science education. The second part of the review considered the second research goal concerned learners' use of analogies for chemical bonding and the final section of this chapter comprised a review of the literature for learners' alternative conceptions in chemistry and chemical bonding, that is, the third research goal.

Chapter 3 represents a literature review on the theoretical perspectives for the inquiry. Basic metaphysical belief systems are described, followed by a description of the development and characteristics of the constructivist paradigm

and ending with a discussion of the relationship between paradigms and methodology, and a description of the relevance this paradigm holds for this inquiry.

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CHAPTER THREE
LITERATURE REVIEW:
THEORETICAL PERSPECTIVES FOR THE INQUIRY

Overview of the Chapter

The chapter comprises the second part of the literature review and provides the theoretical framework for the inquiry. The chapter begins with a description of the basic belief systems of conventional and constructivist paradigms based on ontological, epistemological, and methodological assumptions. The second section builds on the description of metaphysical beliefs and describes the foundations and development of the constructivist paradigm along with a discussion of its relevance to this inquiry. The chapter ends with a discussion of the relationship between paradigms and methodology along with a description of the researcher's metaphysical beliefs.

3.1 Paradigms as Basic Belief Systems

Paradigms are belief systems that are based on ontological, epistemological and methodological assumptions (Cohen & Manion, 1989; Lincoln & Guba, 1985; Patton, 1990). Guba and Lincoln (1994) state that a paradigm

May be viewed as a set of basic beliefs (or metaphysics) that deals with the ultimate or first principles. It represents a *worldview* [original italics] that defines, for the holder, the nature of the 'world', the individual's place in it, and the range of possible relationships to that world and its parts. (p. 107)

Alternative paradigms include positivism, post-positivism, critical theory and constructivism. These belief systems are essentially acts of faith and it is important to realise that no construction is or can be considered incontrovertibly right "advocates of any particular construction must rely on *persuasiveness* and

utility rather than *proof* in arguing their position [original italics]" (Guba & Lincoln, 1994, p. 108).

The question as to what is the form or nature of reality or what is there that can be known is referred to as ontology (Chinn & Brewer, 1993; Cohen & Manion, 1989; Leplin, 1994). Conventional or realist ontological beliefs assert that a single independent reality exists outside the reference frame of the observer, or as Boyd (1994a, p. 97) states "reality is prior to thought". This reality is immutable and conforms to natural laws—many of which possess the nature of cause and effect. The relativist ontology contrasts with the realist ontology in that it asserts that there exist multiple, socially-constructed realities. For the relativist view, there is no causal relationship and mental construction precedes observation (Boyd, 1994a, 1994b; Nussbaum, 1989). Truth is considered to be the construct that possess the greatest "power with which the information is understood and used" (Guba & Lincoln, 1989, p. 84).

The relationship between the knower and the known is the question of epistemology. In other words, epistemology is the pursuit of an answer to the question "how can we be sure we know what we know?" (Guba & Lincoln, 1989, p. 83). Guba and Lincoln believe that the "response to the epistemological question depends on the prior response given to the ontological question" (p. 88). For example, if one subscribes to a conventional realist ontology, one is likely to be a dualist-objectivist in epistemology (Linn, Songer, & Lewis, 1991). Constructivists ascribe to a transactional and subjectivist epistemology; that is, they believe that the findings of an inquiry are literally created by the investigator. In the words of Schwandt (1994, p. 125), "constructivists are deeply committed to the contrary view [of realists] that what we take to be objective knowledge and truth is the result of perspective. Knowledge and truth are created, not discovered by mind".

Methodology addresses the issue of how we go about finding out whatever it is that we believe we know or can come to know (Guba & Lincoln, 1989, 1994; Schwandt, 1994). The answer to the methodological question is

dependent upon an individual's stance on the ontological and epistemological questions. For example, positivists rely on inquiry that is experimental and manipulative, in which questions or hypotheses are stated and are evaluated by empirical testing. In this approach careful control of experimental conditions is necessary to prevent outcomes being subject to extraneous influences. In contrast, in the methodology used by constructivists, constructions under inquiry are elicited by interaction between the investigator and participants.

3.2 The Development of the Constructivist Paradigm

Classical scientific thought was based on the Aristotelian view of a passive observer. In this view, it was only by removing one's self from the phenomenon under investigation that one could see nature as it really was (Guba & Lincoln, 1989; Smargorinsky, 1995). In the seventeenth to nineteenth century, the empirical-positivist view gained ascendancy since science was seen almost universally as an empirical process. Adherents considered that the remarkable success of empiricism implied strong evidence for the belief that scientists have "latched on to the way things are" (Worrall, 1994a, p. xvi); in other words, empiricists believed that "at the level of empirical consequences, the success of presently accepted theories in 'mature' sciences like physics, is, while not quite total, nonetheless hugely impressive" (Worrall, 1994a, p. xv). Adherents to the empirical-positivist school of thought believe that scientific knowledge grows as a result of humans finding out true or confirmed knowledge, such knowledge being acquired primarily by the use of the senses. From an empirical-positivist view, these true facts and theories are able to be verified by external observation. Induction, the process of deriving valid generalisations from a collection of specific observations, is a major part of this approach (Millar, 1989).

There are three fundamental difficulties with a positivist paradigm (Guba & Lincoln, 1989, 1994). First, there is the phenomenon of reactivity; even if it is possible in physical experiments to overlook reactivity, it is impossible to remove it from human behaviour, since humans are not inert passive objects. The

second difficulty is the phenomenon of indeterminacy, summed up in Heisenberg's uncertainty principle which Guba and Lincoln (1989) contend applies equally well to social and human inquiry in that "the scientist who approaches human 'subjects' with a particular set of questions or hypotheses may set the stage for certain observations but may thereby be prevented from pursuing others" (p. 99). Finally, there is the phenomenon of interactivity, in which it is recognised that outcomes are not only indeterminate, they are formed during the course of an inquiry; that is, the very nature of inquiry necessitates interaction between the investigator and subject of his or her inquiry.

The beginning of the twentieth century was characterised by dramatic advances in modern physics, particularly in relation to atomic structure, the nature of electromagnetic radiation, and gravity (Jones, 1994; Redhead, 1994). New theories such as quantum mechanics and relativity assumed the nature of interpretative multiplicity; that is, the "failure of any one interpretation to provide an 'explanatorily satisfactory' link between the mathematic formalism and the world of laboratory experience" (Jones, 1994, p. 281). Hence, changes in the ideas of scientific thought began to undermine the conventional belief that science could make absolutist claims. Philosophical, psychological, and logical arguments began to accumulate against the possibility of ever confirming or proving knowledge, leading to the relativist view which proposed that knowledge is not discovered but is a subjective, human construction. As Nussbaum (1989) puts it:

Theory precedes observations, and that observations can be selected and conducted only through theoretical expectations...therefore our own constructed theories determine how we perceive the world. (p. 531)

It would be misleading to suggest that there is universal agreement with the constructivist paradigm, although there is consensus that a qualitative constructivist mode of inquiry is the most appropriate means of recognising the

context of individuals and groups (Good, Wandersee, & St Julien, 1993; Tobin & Tippins, 1993; Wheatley, 1991). There also is consensus about the fundamental basis of constructivism—that is, an individual's knowledge represents a mental construct, but there is considerable disagreement about some other aspects of the paradigm. Wheatley (1991) sums up the situation.

The theory of constructivism rests on two main principles. The first principle is readily agreed to by most persons but the second causes much controversy. Principle one states that knowledge is not passively received, but is actively built up by the cognizing subject. Ideas and thoughts cannot be communicated in the sense that meaning is packaged into words and 'sent' to another who unpacks the meaning from the sentences. That is, much as we would like to, we cannot put ideas in students' heads, they will and must construct their own meanings. Our attempts at communication do not result in conveying meaning but rather our expressions *evoke* [original italics] meaning in another, different meanings for each person. Principle two states that function of cognition is adaptive and serves the organisation of the experiential world, not the discovery of ontological reality...thus we do not find truth but construct viable explanations of our experiences. (p. 10)

Constructivists strove to bring about improvements to the learning environment by initially making in-depth investigations of learners' prior knowledge. Inherent in a constructivist approach to learning is a shift away from the conventional positivist proposition that science is a codified body of knowledge that can be transmitted to the learner. In a positivist view, learners are seen as blank slates, or possessing of empty heads, to be filled by the teacher, that is, via a transmissive or conduit approach (Cobern, 1993; Millar, 1989). Methodological constructivists, by way of contrast, attempt to foster active learning, guiding learners to create their own constructs using a process of peer and teacher-facilitated learning; learning through negotiation rather than by imposition (Driver, 1989a, 1989c Driver & Oldham, 1986; Wheatley, 1991).

Since the underlying and fundamental aspect of this view is that learners bring their own well formed constructs to the learning process, much research and classroom activity focused on the acquisition of an understanding of learners' prior knowledge (e.g., Driver et al., 1985; Fensham, 1994; Scott, Asoko, Driver, & Emberton, 1994). A major outcome of this research was the alternative conception or misconceptions movement (Solomon, 1994; Wheatley, 1991). Interestingly, in addition to the plethora of data gathered about learners' views of scientific concepts, this movement stimulated considerable debate about the status of learners' intuitive ideas, that is, the so-called ideological-based terminological controversies (Solomon, 1994). Many researchers feel that labelling learner's world-views of scientific concepts as misconceptions is unnecessarily dismissive of their views and it is now more common to refer to discrepant views as *alternative conceptions* or *alternative frameworks* rather than misconceptions (Millar, 1989). Solomon argues that this controversy represents a form of self-contradiction within the constructivist paradigm, that is, it may be indicating that there are some underlying flaws in the theoretical basis to constructivism and that as a paradigm, it may be on the wane.

In summary, the constructivist paradigm subscribes to relativist ontology—in which it is believed reality is of the form of multiple intangible mental constructs, a transactional/subjectivist epistemology—in which it is believed that findings are created rather than being discovered, and employs a methodology in which constructions are elicited and refined through interaction.

3.3 The Foundations of Constructivism

Inspection of Piaget's research work suggests that much of it is constructivist in origin since he was concerned with the way children construct knowledge (Flavell, 1963; Good et al., 1993; Johnson & Gott, 1996; von Glasersfeld, 1993). This has led some authors to suggest that Piaget was the founder of constructivism (e.g., Bliss, 1995; Johnson & Gott, 1996). However, Piaget's theory of knowing is a form of genetic epistemology, that is, it is limited

to "the problem of how knowledge is increased" (Good et al., 1993, p. 76). Piaget proposed that children increase in cognitive ability via a process of spontaneous maturation through four stages namely, sensory-motor (birth to 2 years), pre-operational (2 to 7 years), concrete-operational (7 to 11 years), and formal-operational (11 years plus) (Novak, 1978). Although Piaget, like many modern constructivists, used a recapitulation theory to categorise some children's ideas, he did this from a substantially different perspective, in relation to the child's cognitive development, rather than by relating its ideas to mature scientific thinking (Solomon, 1994). Furthermore, many view Piaget as too judgmental to be considered a constructivist, since he was dismissive of children's intuitive ideas (e.g., Johnson & Gott, 1996; Solomon, 1994). According to Solomon (1994), it is doubtful that Piaget would consider himself a constructivist. In Solomon's view, the development of constructivism is not due to Piaget, but to Driver and Easley (1978) who articulated much of the necessary language, thus producing the coherent set of tools necessary for the rise of constructivism in science education. Solomon's contention is that the very success of a new paradigm like constructivism is somewhat paradoxical in that the rapid acceptance of a new paradigm suggests that much of the framework was already in place. What has changed, and what Solomon asserts Driver and Easley achieved, is that the objects of study (i.e. aspects of learning and human nature) were already familiar, hence recognition and acceptance of the paradigm was correspondingly rapid.

3.4 Forms of Constructivism

The general acceptance that individuals construct their knowledge led to a systematic attempt to discover learner's views about scientific concepts, and to build upon knowledge of these views in the development of research and instructional strategies (Allender, 1986; Cohen & Manion, 1989; Guba & Lincoln, 1989, 1994). As mentioned previously, it was surprising to many that this research revealed that conventional instructional strategies were relatively

unsuccessful for the teaching of counter-intuitive scientific concepts. Consequently, considerable interest developed in teaching by a constructivist-informed approach which in turn led to many variants as each researcher or instructor sought to apply a constructivist-informed approach to their own setting (Bettencourt, 1993; Good et al., 1993; Nussbaum, 1989; Schwandt, 1994; Tobin & Tippins, 1993). As Schwandt (1994, p. 126) put it "the terrain of constructivist approaches is marked by multiple uses of the term". Good et al. (1993) identified a total of 15 different adjectives used to modify the term constructivism: the most widely used being contextual, methodological, radical, and social constructivism. Naturally there is considerable overlap between the different forms of constructivism; however, Good et al. caution that the persistent "lumping together of meanings under the heading constructivism in a way that obscures crucial differences amongst proponents" (p. 71) may be counter productive. Wheatley (1991) agrees with this view.

Frequently I am berated by my colleagues for being pedantic and abstruse when I take exception to certain words used in communication and when I raise epistemological issues. But the inherent process of knowing is the making of fine distinctions...I ask you to consider the distinctions made as more than mere quibbling. (p. 9)

Radical constructivism, espoused by Ernst von Glasersfeld and others, is perhaps the most contentious form of constructivism (Bettencourt, 1993; von Glasersfeld, 1988, 1993; Tobin & Tippins, 1993). von Glasersfeld (1988) describes radical constructivism as being radical "because it breaks with convention and develops a theory of knowledge in which knowledge does not reflect an 'objective' ontological reality, but exclusively an ordering and organization of a world constructed by our experience" (p. 201). Wheatley (1991) suggests that this view in which "we have no 'Gods eye' view of a 'real' world and thus can know the world only through our experiences" (p. 10) is

problematic for many scientists who most likely hold empirical-positivist beliefs. Whilst not all radical constructivists oppose the existence of an external reality, there is general agreement within the movement that radical constructivism "denies the possibility of knowledge transmission, even in principle" (Bettencourt, 1993, p. 40). That is, radical constructivists consider that "there is no way of checking reality against what it was supposed to represent. One can compare knowledge only with other knowledge" (von Glasersfeld, 1993, p. 24). According to von Glasersfeld, the confusion that arises about the nature of the real world lies in the relationship between viability and ontological beliefs.

For [radical] constructivism, the fact that something works (is 'viable') does not mean that it is therefore a representation of that 'real' world that prevents other things from working. The 'real' world remains unknowable no matter how well we manage in the domain of our experience. (p. 25)

Bettencourt (1993, p. 47) summarises the situation succinctly: "radical constructivism shows us that the relation between our knowledge and our experience is, at best, undetermined".

Contextual constructivists assert that a crucial feature of knowledge creation is that it is not carried out in isolation but is subject to influence by an individual's context; that is, his or her prior knowledge and experiential world (Cobern, 1993; Good et al., 1993; Wheatley, 1991). Contextual constructivism and the related social constructivism hold that personal constructivism is too limited since humans are social beings, and knowledge creation is influenced by the prior experiences and social environment of the learner. Wheatley (1991, p. 49) summarises the position by claiming that "we continually negotiate the meaning of events in our lives so that we can benefit from the experiences of others as well as our own". In Wheatley's view, scientific concepts are no different to other events in a learner's experiential world and similarly are subject

to negotiation. Culture represents an important part of an individual's context and can exert a significant influence on social interaction; that is, learners' views are rooted in a cultural milieu (Solomon, 1994). Cobern (1993) points out that subtle cultural factors often remain undetected, that is, apparent societal homogeneity may mask deep cultural differences.

Social constructivists believe that an important part of construction is social interaction through which we come to a common understanding of knowledge, including scientific concepts (Solomon, 1994; von Glasersfeld, 1993; Wheatley, 1991). Tobin and Tippins (1993) put it this way "the individual and social components [are seen as] being parts of a dialectical relationship where knowing is seen dualistically as both individual and social, never one alone, but always both" (p. 20). However, we may appear to have the same view of concepts as others, but our understanding is commonly discrepant, for example, when there is an undetected communication breakdown.

The social constructivist view addresses fundamental issues as a basis for instruction and inquiry. For example, some critics hold that constructivism provides a licence for learners to hold views at variance with the scientific view. Tobin and Tippins (1993) maintain that this assessment is flawed and that this issue can be addressed from the framework of a social constructivist.

An often misunderstood aspect of constructivism is that the theory incorporates a value position that any construction is as viable as another. Such a position is based on a belief that personal viability is the critical issue in constructivism. The position ignores the social component of knowledge, that is, that knowledge must be viable not only personally, but also in the social contexts in which actions are to occur. (p. 5)

von Glasersfeld (1993) agrees about the importance of social context because "individual meanings are constructs that have been through a certain amount of social adaptation" (p. 30), that is, it is important "to emphasize social construction of knowledge" (Guba & Lincoln, 1989, p. 131). According to Bliss

(1995), instruction involves not only actively exploring the physical world, but learning how science concepts are negotiated among scientists, not discovered, the negotiation being based on "communal standards of argument and evidence" (p. 156).

3.5 Constructivism: Methodology or Referent?

Methodology is the system employed as the means of inquiry, that is how we go about finding out things. An individual's methodological views stem from his or her ontological and epistemological beliefs; for example, an objectivist is likely to adopt an inquiry approach that "strip[s] the context of possible contaminating influences...so that 'the way things really are' and 'the way things really work' can emerge" (Guba & Lincoln, 1989, p.89). The ultimate goal of methodology for realists is to provide better means of predicting and controlling events. By way of contrast, a constructivist methodology seeks to

Expose the constructions of the variety of concerned parties, open each to critique in the terms of other constructions, and provide the opportunity for revised or entirely new constructions to emerge—a hermeneutic methodology. (Guba & Lincoln, 1989, p. 89)

The ultimate goal of a constructivist methodology is a process which results in a *successively* better understanding, that is, it is seen as a continual, iterative, process.

The act of [constructivist] inquiry begins with issues and/or concerns of participants and unfolds through a 'dialectic' of iteration, analysis, critique, reiteration, reanalysis, and so on that leads eventually to a joint (among inquirer and respondents) construction of a case. (Schwandt, 1994, pp. 128-129)

Von Glasersfeld and other radical constructivists refer to the use of a constructivist approach purely as a tool for investigation of learning as trivial, or methodological, constructivism (Bettencourt, 1993; Good et al., 1993; von Glasersfeld, 1988, 1993). Tobin and Tippins (1993) share these reservations believing that authors who use constructivism to represent a method of teaching present a view that is too simplistic and fails to recognise the contribution that constructivism can make to the myriad of learning opportunities open to learners. In their view, rather than being simply a method, constructivism should be viewed as a referent; that is, constructivism should be used to analyse the learning potential of *any* learning situation. For example, from a trivial or methodological constructivists' viewpoint, teaching practices such as lecturing are not cognitively challenging, and consequently of little value in assisting learners to make meaning of the concepts being addressed. Tobin and Tippins believe using constructivism to dismiss lecturing as a flawed or ineffective teaching approach is inappropriate. They assert that constructivism

Must have explanatory power in all situations where knowledge is constructed...similarly, constructivism ought to be useful in predicting how any given set of circumstances might be changed to improve the opportunities of persons who wish [or have] to learn in such situations. (p. 8)

von Glasersfeld (1993) agrees, suggesting that talking and lecturing can bring about conceptual change, since the instructor can challenge an audience to create "perturbation about conceptual structures that have been used unthinkingly" (p. 32). A similar view by Millar (1989) was espoused nearly a decade ago "a consequence of the constructivist model of learning is that science should be taught in whatever way is most likely to engage the active involvement of learners" (p. 589).

3.6 The Relevance of the Constructivist Paradigm to this Inquiry

3.6.1 Relevance of the Ontological and Epistemological Perspective of the Researcher

Cobern (1993) maintains that doing research is much more than just applying a particular method and Millar (1989) argues that the personal beliefs of an investigator need not relegate one to a particular school of epistemological thought, or predetermine his or her methodological approach. According to Millar, one can be an empiricist and yet carry research from a constructivist paradigm—a view shared by some realists (see, e.g., Boyd, 1994a, 1994b). To put this proposition into perspective, consider the most common difficulty encountered in the teaching of school science from a constructivist paradigm.

For good, understandable pedagogical reasons, constructivist science educationalists...acknowledge that science as a school subject poses a formidable challenge to the teacher in maintaining the involvement of many pupils simply because the science covered at school is, almost entirely, a consensually agreed body of knowledge. There is, therefore, a limited value in children taking away from science lessons ideas that diverge radically from the accepted ones. This means that science can come to look like the transmission of a body of knowledge that cannot be challenged by the learner, and whose learning leaves little scope for the creative involvement of the learner. (Millar, 1989, p. 590)

Instructors wanting to teach from a constructivist paradigm are faced with a dilemma, namely, the apparent realist ontological belief system of science at the school level. Perhaps in reaction to this dilemma, authors like Millar (1989) suggest teaching or conducting research from a constructivist paradigm, even whilst holding ontological beliefs that appear to be inconsistent with epistemological and methodological beliefs. In spite of Millar's comments, many authors believe that the personal beliefs of the investigator exert a pervasive

influence over all aspects of an inquiry (e.g., Cobern, 1993; Monk, 1995; Tobin & Tippins, 1993; von Glasersfeld, 1993; Wheatley, 1991). Indeed the use of constructivism as a referent for research has a number of important implications. First, according to Tobin and Tippins, because constructivism acknowledges the impossibility of realising an absolute truth, it is more appropriate to view the investigator as a co-learner rather than as a seeker of the truth. They state that it is "the role of the researcher to make personal sense of experience and, in a socially mediated way, to build knowledge in a given field" (p. 15). Thus, from a constructivist's viewpoint, data collection is not seen as the gathering up of facts—implying an objectivist outlook, rather data are "constructed from experience using personal theoretical frameworks that have greatest salience to the goals of the individual conducting the research" (Tobin & Tippins, 1993, p. 15). This view, that data are constructed rather than gathered, is supported also by Smargorinsky (1995) who like Johnson and Gott (1996) maintains that "the act of analysis is a construction of the researcher" (p. 198). Johnson and Gott further assert that what data are deemed incorrect or irrelevant depends on the researcher's ontological and epistemological beliefs as much as his or her domain knowledge.

The research design of many studies contains an implicit assumption that data collection is a straightforward process. However, a number of authors have pointed out that data collection is inherently problematic and that making sense of children's' views of science concepts is much more complex than it appears (Bell, B., Osborne, & Tasker, 1985; Guba & Lincoln, 1989; Johnson & Gott, 1996; Patton, 1990). For example, it is relatively easy for researchers to uncover a variety of alternative conceptions, but to understand how a learner arrived at his or her views is much more difficult, since "finding out what a child thinks rests on an *interpretation* [italics added] of a child's response to a researcher's question" (Johnson & Gott, 1996, p. 563). One means of facilitating the process of uncovering learners' views is via a *translation interface* (Figure 3.1) which recognises that "the researcher's frame constructs and gives meaning to the

question. It is then within the child's frame that a meaning to the question, in turn, is constructed " (Johnson & Gott, 1996, p. 564). This process is repeated when the learner responds to the researcher's question. Thus a constructivist researcher needs to be aware that it is not possible to construct another individual's constructs; the best means of addressing this difficulty is by the development of a *neutral ground* in which interactive and undistorted communication takes place, what is known as a hermeneutical and dialectical methodology.

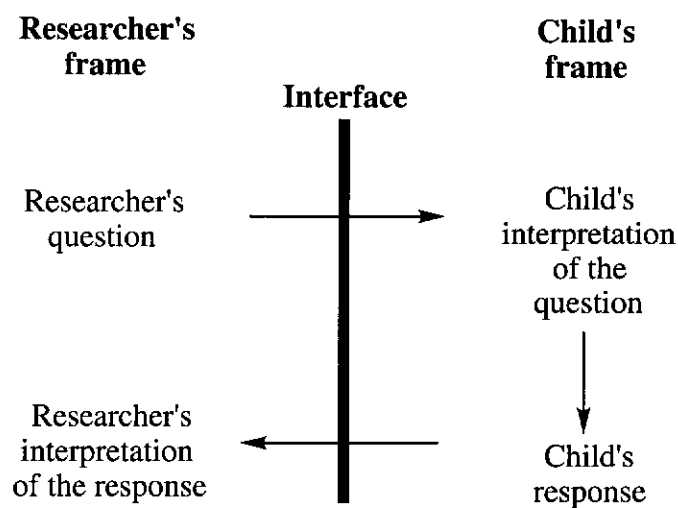


Figure 3.1 The translation interface in clinical interviewing (after Johnson & Gott, 1996)

As Johnson and Gott (1996) put it

The researcher must be alive to any number of possibilities of meaning in a child's response interpretation [of the response] must attempt to understand what a child is saying *on his or her own terms* [italics added] and the researcher must guard against imposing meanings from his or her reference frame. (p. 566)

Three basic methodological principles can be used to guide research efforts onto neutral ground. First, the task itself should be neutral, that is, it must

be accessible to both the learners' and researcher's frame. For example, leading questions should be avoided during clinical interviews as these may introduce unfamiliar verbiage or concepts resulting in misleading responses (Patton, 1990). Second, data interpretation also must be carried out on neutral ground, insofar as such neutral ground exists (Johnson & Gott, 1996). For example, words that have an established scientific meaning may only be ascribed meaning imparted to them in the conversation of the interviews (Bell, B., et al., 1985; Patton, 1990). This latter task is particularly challenging for researchers, many of whom automatically assume that the learners are familiar with scientific terms. Third, triangulation should be used because it "addresses not only the issue of reliability but also increases our confidence in the validity of the evidence" (Johnson & Gott, 1996, p. 567).

3.6.2 *Ontological and Epistemological Beliefs Held by the Researcher in this Inquiry*

The previous discussion has highlighted the fact that the term constructivism can have many different meanings and forms. Furthermore, there is reasonable consensus that the ontological and epistemological beliefs of the researcher exerts substantial influence on his or her methodological beliefs. This researcher agrees with the view of Wheatley (1991) that it is prudent rather than pedantic to state at the onset one's ontological and epistemological beliefs. As Wheatley and others (e.g., Good et al., 1993; Monk, 1995) suggest, it is important for investigators to make *explicit* their beliefs, rather than simply say they are constructivists, or that this investigation has been carried out based on a belief system that is constructivist in nature. Having said that, it is the belief of this investigator that as Tobin and Tippins (1993) point out, there is often considerable overlap between the different forms of constructivism. What follows is a subjective and retrospective analysis of this researcher's ontological, and epistemological beliefs, culminating in the present held beliefs.

I consider myself a contextual constructivist, and further, consider that social and cultural interactions are an important aspect of an individual's context.

I believe, despite my training under an empirical-positivist regime during my undergraduate and postgraduate studies in chemistry, that I have always held relativist, rather than realist, ontological beliefs. I believe that during my science career my epistemological beliefs were dualist-objectivist in nature. However, as a result of my studies into science education, I now subscribe to a transactional-subjectivist epistemology. That is to say, I believe that data are constructed rather than gathered and that data analysis is strongly influenced by the subjective metaphysical beliefs of the researcher. Consistent with these ontological and epistemological beliefs, I believe inquiries into science education such as that described in this work are best addressed using a hermeneutical and dialectical methodology; that is, the individual constructions of interest are best elicited by interactive dialogue between the researcher and the participants. Inherent in this view, is the stance that interactive dialogue must be conducted on neutral ground.

3.7 Summary

This chapter has provided the second phase of the review of relevant studies in the science education literature beginning with a discussion of the basic metaphysical belief systems used by scientists and science education researchers. The foundation and development of the constructivist paradigm were described along with their relevance for choice of methodology for the inquiry; the chapter ended with details of the epistemological and metaphysical beliefs of the researcher.

Chapter 4 draws on the theoretical framework detailed in Chapter 3 and describes the methodological development for the inquiry. It begins with a general description of methodological approaches used in science education inquiries, with particular emphasis on qualitative and naturalistic methodological approaches. A detailed description of the interview protocol follows, and the chapter ends with a discussion of the measures taken to ensure the trustworthiness of the inquiry and pertinent ethical issues.

CHAPTER FOUR

METHODOLOGY

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CHAPTER FOUR

METHODOLOGY

Overview of the Chapter

This chapter, which consists of a description of the methodology employed in this inquiry, begins with an overview of the methodological approaches used in science education inquiries, followed by a discussion of the nature of qualitative clinical interviewing—the principal data collection tool used in the inquiry. A detailed description of the development of the interview protocol is next, along with a description of the data analysis procedures used in the inquiry. The chapter concludes with a discussion of the measures taken to maintain trustworthiness, and a consideration of ethical issues.

4.1 Methodological Approaches in Science Education

Guba and Lincoln (1989) point out that it is common to confuse methods with methodologies, "that is, tools and techniques with overall guiding strategies" (p. 158). This confusion arises since some authors consider that the difference between paradigms is simply a difference in inquiry tools used rather than differences in their underlying belief systems, involving ontology, epistemology *and* methodology. But the methodology of the constructivist is very different to that of the conventional inquirer. Guba and Lincoln (1989) sum up the position:

Methodology is best understood as the overall strategy for resolving the complete set of choices or options available to the inquirer. Far from being merely a matter of making selections among methods, methodology involves the researcher utterly—from unconscious worldview to enactment of that worldview via the inquiry process. (p. 183)

Hence, while two researchers may utilise the same tools, their ontological and epistemological beliefs may be very different.

Research in science education since the turn of the century has been dominated by the use of a quantitative methodological approach (Denzin & Lincoln, 1998; Filstead, 1979; Jaeger, 1988; Porter, 1988; Rossman & Wilson, 1985) which is based on scientific empiricism and attempts to use the power of mathematical analysis to establish general laws and principles (Burns, 1994; Filstead, 1982; Mason, 1993). Gradual recognition of the differences between scientific and educational research led to increasing interest in a qualitative methodological approach with foundations in ethnography, borrowing data gathering tools such as unobtrusive observation, participant observation, and in-depth interviews (Bell, J., 1993; Gage, 1989; Hitchcock & Hughes, 1989; Keedy, 1992; Lythcott & Duschl, 1990; Stake, 1988, 1994). It is worthwhile to clarify the use of the terms qualitative and naturalistic here since some researchers use them to mean much the same thing (Guba & Lincoln, 1989, 1994; Lincoln & Guba, 1985). For example, some authors use the term qualitative to refer to a method of data collection, whereas others use it in a sense that "implies that the term *qualitative* is an umbrella term superior to *paradigm* [original italics] (Guba & Lincoln, 1994, p. 105). Guba and Lincoln (1994) state that they prefer the term, constructivism which they "earlier called 'naturalistic' inquiry" (p. 105). The term naturalistic inquiry is usually used to describe inquiries that involve an individual or individuals in their natural rather than contrived setting (Guba & Lincoln, 1994; Lincoln & Guba, 1985). Guba and Lincoln believe that "from our perspective both quantitative and qualitative methods may be used appropriately with any research paradigm" (p. 105). As Shulman (1988) points out, naturalistic inquiries typically utilise a variety of data gathering tools, and can include quantitative tools such as survey instruments. The principal difference between a naturalistic or phenomenological approach and a purely quantitative approach is that the former recognises the significance of subjective experience, and in general is characterised by greater depth (Wolcott, 1988b).

Quantitative and qualitative methodological approaches of inquiry each possess advantages and disadvantages and the choice of methodology often comes down to a trade-off between breadth and depth (Peshkin, 1993). Patton (1990) summarises the situation.

Qualitative methods permit the evaluation researcher to study selected issues in depth and detail; the fact that data collection is not constrained by predetermined categories of analysis contributes to the depth and detail of qualitative data. Quantitative methods, on the other hand, require the use of a standardised approach so that the experiences of people are limited to certain predetermined response categories. The advantage of the quantitative approach is that it is possible to measure the reactions of many subjects to a limited set of questions, thus facilitating comparison and statistical aggregation of data. By contrast, qualitative methods typically produce a wealth of detailed data about a much smaller number of people and cases. (p. 165)

Some researchers have called for the use of a combined methodological approach to research in science education (Denzin, 1970; Fraser, 1991, 1994; Patton, 1990; Reichardt & Cook, 1979). The two methodological approaches have their origins in different paradigms and are derived from opposing theoretical and philosophical perspectives: consequently, some researchers argue that they are incompatible and should not be combined (Burrell & Morgan, 1979; Smith, J.K., 1983). However, other researchers have argued against this stance, maintaining that the paradigm argument is essentially irrelevant (Goodwin & Goodwin, 1984; Mason, 1993). Cizek (1995) argues that qualitative and quantitative methodological approaches are investigating the same thing: a view supported by Goodwin and Goodwin (1984) who assert that the difference is one of choice of data collection tools, and that the choice of methodology should depend solely on the research question or questions.

There are a number of advantages of combining quantitative and qualitative methodologies (Fraser, 1991, 1995; Reichardt & Cook, 1979). First, much educational research has multiple purposes, being interested in both processes and outcomes. Thus, analysis of monitoring, impact assessment, and causal explanation represents a broad range of tasks most efficiently achieved by a combination of methods. Second, the two different approaches build upon each other. For example, choosing a statistical model to fit the data, interpreting the output results, and generalising the findings to their settings, all rely on qualitative knowledge; "quite simply, researchers cannot benefit from the use of numbers if they do not know, in common sense terms, what the numbers mean" (Reichardt & Cook, 1979, p. 23). Thus, qualitative data may prove valuable in establishing if statistically significant differences observed in a quantitative study are in fact meaningful, or simply indicating the presence of statistical rareness (Carver, 1978, 1993). Third, data triangulation, the gathering of data from different sources (Section 4.7.6, pp. 98-100) through convergence, affords more confidence in the interpretation of the data (Patton, 1990). Convergence resulting from triangulation is most convincing when the methods of data collection are at their most disparate, that is, quantitative and qualitative methodologies (Denzin & Lincoln, 1998).

In spite of the advantages of combining quantitative and qualitative methodologies described above, and a number of calls for such an approach in the science education literature, such inquiries are less common than pure quantitative or qualitative inquiries (Blumenfeld & Meece, 1988; Gogolin & Swartz, 1992). A number of reasons have been proffered. First, cost is often a major factor in science education research and one of the main advantages of using survey instruments is their cost-effectiveness. Second, the use of a combination of methodologies may prove too time consuming for many inquiries (Reichardt & Cook, 1979). Quantitative inquiries often involve studying the effect of an intervention, adding to the length of the inquiry (Maor & Fraser, 1996). Qualitative inquiries also are commonly of long duration especially if

lengthy enculturation is necessary. The fact that it is not always possible to carry out the two approaches of data collection concurrently further exacerbates this problem (Sieber, 1978). Qualitative research requires considerable expertise on the part of the researchers, for example, when conducting clinical interviews and classroom observation (Bell, B. et al., 1985). Clearly expertise is also necessary for quantitative work, and there are few researchers who possess a high level of expertise in both methodologies.

This issue of choice of methodology is best resolved by considering the more fundamental issue of research design (Shulman, 1988). Patton (1990) asserts that the research question or goal should dictate which methodology, or combination of methodologies, is appropriate.

Which research design is best? Which strategy will provide the most useful information to decision makers? There is no simple, immediate, and universal answer to that question. The answer in each case will depend on what intended users want to know, the purpose of the study, the funds available, the political context, and the interest/abilities/biases of the researchers. (pp. 95-96)

Thus, some research questions will be readily answered using qualitative means, others quantitative, and some will be best addressed using a combination of the two. As Patton (1990) puts it, "the challenge is to find out what information is most needed and most useful in a given situation, and then to employ those methods best suited to producing the needed information" (p. 96).

4.2 Cross-Age Inquiries in Science Education

Many inquiries into conceptual understanding in science education involve investigations of learning at particular points in time. Such inquiries provide little information about how learners' conceptual understanding changes with time or as a result of instruction. Two alternative ways of probing learners'

understanding are longitudinal and cross-age inquiries (Andersson & Karrquist, 1983; Boyes & Stanisstreet, 1991; Guesne, 1985; Novick & Naussbaum, 1981; Summers, & Kruger, 1994; Taber, 1997).

Longitudinal inquiries involve tracing the learning experiences of a learner or learners across a period of time whether over a relatively short period or many years (e.g., Abell & Roth, 1995; Driver et al., 1994; Mulkey & Ellis, 1990; Spradley & McCurdy, 1972; Welch, 1983; Wolcott, 1988b). Such inquiries are often, but not always, investigations into the learners' conceptual development with maturation or instruction (Pelto, 1970; Wolcott, 1988a). Because longitudinal inquiries are often carried out over many years, they frequently involve relatively few participants. Furthermore, as an individual's personal circumstances may change over a long period of time, high attrition rates are not uncommon. Longitudinal inquiries of individuals can be used to predict how an individual learner's reasoning skills, such as problem-solving, change as a result of changes associated with maturation, cognitive development, and learning experiences (Taber, 1995b; Driver, Leach, Scott, & Wood-Robinson, 1994).

Cross-age inquiries investigate cohorts of learners of different ages or age ranges (e.g., Birk & Kurtz, 1999; Ingham & Gilbert, 1991; Lawson, A., 1988; Wilson, 1998). Interestingly, a number of cross-age inquiries have revealed that learners' views are not idiosyncratic; rather, similar forms of reasoning have been observed (see, e.g., Brook, Briggs, & Driver, 1984; Guesne, 1985; Leach, Scott, Driver, & Wood-Robinson, 1995). Cross-age inquiries have an advantage over longitudinal inquiries in that they are able to be performed over a shorter duration, reducing attrition. However, cross-age inquiries cannot be used to provide information about individual learning development, since they do not evaluate conceptual progression. Nonetheless, cross-age inquiries can give clues to the changes in learning strategies and can, for example, be useful for curriculum development (Driver et al., 1994).

4.3 Qualitative Clinical Interviewing

4.3.1 *Clinical Interviews in Science Education Inquiries*

Clinical interviews have been used extensively in therapeutic situations, but it was Piaget who first used the technique to investigate the nature and extent of children's understanding (Erickson, 1979, 1980). The chief goal of clinical interviewing in science education research is to ascertain the nature and extent of an individual's knowledge about a particular subject or domain by identifying the relevant conceptions that the learner holds and the perceived relationships among these conceptions. The clinical procedure is well suited for investigations into learning and is a key tool for the qualitative researcher.

The rationale for the use of clinical interviewing for evaluating cognitive structure is essentially the same one Piaget offered for his clinical method. The method is highly flexible, allowing a skilful researcher both to probe the areas of the knowledge domain of particular interest and to let the subject speak freely, while constantly checking his or her spontaneous remarks for those that will prove genuinely revealing. (Posner & Gertzog, 1982, p. 197)

An important feature of interview technique is to check participant's spontaneous remarks and to cross-check responses to gain a deeper understanding of the perceptions held for the concept under investigation (Erickson, 1979; Patton, 1990). Interviewing is a complex and difficult task requiring care and skill on the part of the interviewer in order to obtain valid and reliable data (Bell, B. et al., 1985).

There are three approaches to conducting interviews; *the informal conversational interview*, *the general interview guide approach*, and *the standardised open-ended interview* (Patton, 1990). These approaches differ in the extent to which the interview questions are determined and standardised before the interview occurs.

The *informal conversational interview*, as the name implies, is relaxed in nature, and the generation of questions is spontaneous arising from natural conversational flow. This approach is common in ethnographic inquiries where it is usually combined with participant-observation and fieldwork (Wolcott, 1988b). Such inquiries frequently involve multiple interviews and are of long duration, months or even years (e.g., Wolcott, 1988a). The same participant may be interviewed on many different occasions, and for multiple participant inquiries the questions asked and data gathered will be different for each individual interviewed. The interviewer has the advantage of maximum flexibility, and can modify questions depending on the context of the investigation. The main advantage of the use of an informal interview approach is the depth of information gathered compared with other more structured approaches. There are, however, a number of disadvantages to the approach. In addition to the time requirements already mentioned, the interviewer must be able to establish a close and comfortable working relationship with participants. Since data collection is less systematic, analysis may prove problematic. In addition, because interviews are often conducted in the field, audio-taping may not be practical—thus it is usually necessary to take extensive field notes.

The *general interview guide approach*, also referred to as *partially-* or *semi-structured interview*, is more structured in nature than the informal conversational interview and involves outlining a set of issues that are to be explored before interviewing begins (Patton, 1990; Wiersma, 1986). There is not necessarily a set order to the questions, and the specific wording used varies from participant to participant. The interview guide serves as a form of checklist to ensure that all relevant topics are covered. There is still a considerable degree of flexibility retained in this approach, but the use of the interview guide helps to make the data gathering more systematic, facilitating analysis.

The *standardised open-ended interview* is the most structured of the three interview approaches and resembles a verbal questionnaire. Each participant is led through a defined sequence of questions using essentially the

same wording each time. There is little flexibility, the emphasis is on minimising interviewer influence—thus data analysis is more straightforward. Patton (1990) identifies three major reasons for the use of standardised open-ended interviews; the instrument is open to inspection by interested parties, variation among interviewers is minimised allowing for multiple interviewers, and because the interview is so highly focused, interview time is minimised. Such advantages are also realised by the use of written questionnaires (Fraser, 1991). The advantage a standardised open-ended interview holds over a self-completion questionnaire is that despite its relatively structured approach, some flexibility is retained, for example, participants have the opportunity to clarify ambiguity in questions.

A common characteristic of all three interview approaches is that they are more flexible than written questionnaires and afford the participants the opportunity to express their own views and perceptions in their own words, that is, the response is open-ended, and not confined to set predetermined categories. In practice, a given inquiry may employ a number of interview approaches.

4.3.2 *Interview Techniques*

Expert interviewers have identified a number of key techniques needed to obtain high quality data, chief among these as mentioned above, is the need to achieve a relaxed atmosphere in which the respondent is free to state his or her own views (Bell, B. et al., 1985; Posner & Gertzog, 1982; White & Gunstone, 1992). Good technique involves the interviewer saying as little as possible, just sufficient to keep the conversation moving, that is, "interested listening that rewards the respondent's participation but *does not evaluate* [italics added] the responses" (Fontana & Frey, 1994, p. 364). Any responses from the interviewer should be non-judgemental and non-committal—neither admonishing nor praising. The interview needs to proceed at an appropriate pace. If the questions are presented too slowly, the respondent may become flustered and feel that they are expected to know more than they have said—if questioning is too rapid, respondents may feel that their opinions are not valued and resort to

monosyllabic responses. Finally, the interviewer must follow up areas of uncertainty or ambiguity with appropriate exploratory questions.

An important part of good interview technique is good question design—"good questions should, at a minimum, be open-ended, neutral, singular, and clear" (Patton, 1990, p. 295). Genuinely open-ended questions are those that contain neither explicit nor implicit predetermined response categories, but allow the respondent to "select from among that person's full repertoire of possible responses" (Patton, 1990, p. 296). Dichotomous response questions, that is, questions indicating that a simple yes or no answer is required, are best avoided as they can turn the interview into an interrogation, inhibiting in-depth answers. Patton suggests caution in the use of presupposition questions, but points out that used properly they can add considerably to the depth of response—for example, by increasing the likelihood of gleaning more detail. One of the fundamental rules in qualitative interviewing is to ask clear, unambiguous questions, avoiding jargon and terminology that may be unfamiliar to the interviewee. One way of reducing ambiguity is to ask singular questions; in this way, the interviewee is not confused about which question to answer and the investigator will have much less difficulty in interpretation of interview data.

4.3.3 *Interviews About Instances and Interviews About Events*

The Interview About Instances (IAI) and Interview About Events (IAE) techniques have their origins in the work of Piaget who used drawings and physical objects to probe children's cognitive development. These techniques represent variations on the semi-structured interview approach and have been used extensively by J.K. Gilbert, Osborne and others to probe understanding in a number of disciplines especially physics (e.g., Bell, B. et al., 1985; Carr, 1991, 1996; Osborne, & Gilbert, 1980a, 1980b; White & Gunstone, 1992; Taylor, N. & Lucas, 1997). In this approach the interviewer employs objects or line drawings that depict an instance or event as a focus for questions to probe the learner's understanding of a concept.

In the IAI approach, the interviewer probes the learners' understanding of a single concept to determine if the learner is able to recognise instances in which the concept is either present or absent. Similarly, in the IAE approach the researcher probes the learner's ability to explain a phenomenon as opposed to a concept. A feature of the two approaches is that they employ objects or occurrences familiar to the participant, thus improving the likelihood of accessing each learner's worldviews about scientific concepts (Carr, 1996). An important part of the procedure is to probe effectively the learners' understanding of the concept under study by asking in-depth, penetrating questions. For instance, rather than just eliciting a dichotomous response, the interviewer would use follow-up questions such as, why do you say that? what sort of force is present? in what direction is the force acting?, intended to reveal how the participant arrived at his or her concept. The boundary between IAI and IAE is somewhat indistinct, since cards depicting instances often depict events. However, the distinction is not particularly important "since interviews about events will reveal the learners' understanding of associated concepts" (White & Gunstone, 1992, p. 74). The main difference is in the procedure; specifically the nature of the questions—those for IAE's are usually more open-ended in nature. Some caution is needed when conducting IAIs or IAE's since "there are dangers in interpretation of the interview-about-instances material when the respondents are mature and likely to play games" (Carr, 1991, p. 18). Hence, it is important that the questions and tasks are of an appropriate level for more able and senior learners, least the relaxed informal nature of the procedure trivialises the process.

The interview techniques described above were utilised in this inquiry and represent the means used to take cognisance of the translation interface described by Johnson and Gott (1996) (see, Section 3.6.1, pp. 56-59).

4.4 Conceptual Theme for the Inquiry

4.4.1 *Scientists' View of Bonding and Epistemological Beliefs of the Investigator*

In order to devise an appropriate methodology for this inquiry it is necessary to develop the conceptual theme for the inquiry, that is, to relate metaphysical beliefs and theoretical framework to concepts of chemical bonding. Inspection of common chemistry textbooks and curriculum material encountered by learners, including those involved in this inquiry, reveals that there is considerable discrepancy in treatment of the models used to explain theories of chemical bonding. For example, Gillespie, Humphreys, Baird, and Robinson (1986) offer one view of metallic bonding: "because of their small core charges, metals have little tendency to accept electrons to form negative ions. Covalent bonding is also not possible in solid metals, because a metal atom does not have enough valence electrons to form covalent bonds to all its 12 or 8 neighbouring atoms" (p. 491). Elsewhere metallic bonding is described as covalent in nature "metals are just covalently bonded solids with partially filled energy bands, and do not require any special bonding mechanism for their understanding" ("Metallic Bonding," 1994, p. 1965). How is it possible to reconcile such disparate views and have confidence that a description of mental models for chemical bonding represents the scientists' views? In this inquiry, the dilemma has been addressed from a social and contextual constructivist view of learning.

It is an illusion that there is knowledge in textbooks or documents. They contain language, which is a string of words, deposited in them by authors. The words have meaning for the authors and the readers and interpreters, each one of whom has built up [his or] her subjective meanings according to [his or] her individual experience. Though these individual meanings are constructs that have been through a certain amount of social adaptation (because their users have socially interacted with others), they remain subjective and to some extent idiosyncratic,

which never fails to come to the surface in a serious discussion.
(von Glasersfeld, 1993, p. 30)

That the learners' views have been built upon the scaffolding of the scientists' view of models of chemical bonding is a crucial issue. As this inquiry is based on a contextual and social constructivist standpoint, it is the view of this researcher that the scientists' view represents a social construction (Section 3.4, pp. 50-54). If it is accepted that learners construct meaning personally, it is hard to imagine that however idiosyncratic this process may be, that it can be done in isolation. Hence from a contextual constructivist standpoint, the context of learning is all important. The context for this inquiry is the personal lives, including the learning experiences, of the participants. Hence, from the perspective of the learners in this inquiry, the scientists' view is that described in curriculum material encountered during instruction and communicated to them by their instructors: this is the view with which their constructs will be compared. Consequently, the scientists' view of the models for chemical bonding have been negotiated between the author and the instructors who participated in this inquiry.

4.4.2 *Target Systems and Target Models for the Inquiry*

The theoretical framework for this inquiry is based on Norman's (1983) typology of mental models (Chapter 2, p. 24); that is, *the target system*, the *conceptual model of the target system*, the *user's mental model of the target system* and the *scientists' conceptualisation of the target system*. Based on Norman's typology, chemical bonding has been classified into a series of three target systems, namely, *metallic*, *ionic* and *covalent* bonding. Examination of curriculum material and interviews with instructors resulted in the identification of a series of *target models* for each of these target systems (Figure 4.1).

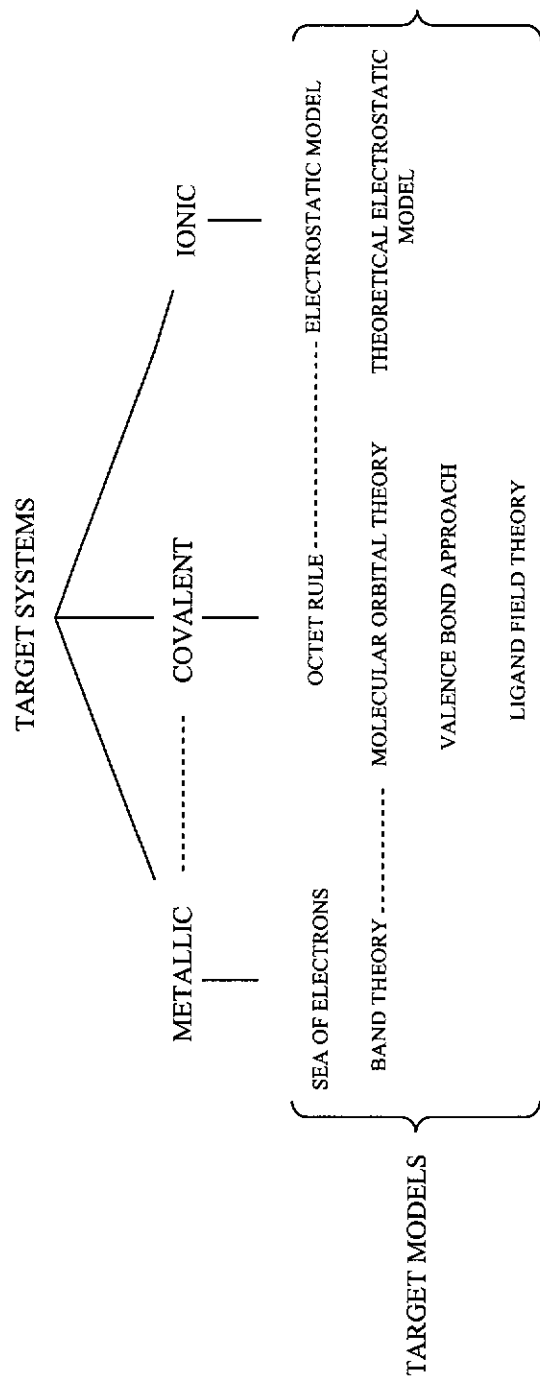


Figure 4.1 Target systems and target models for the inquiry

For metallic bonding, there are two target models—the *sea of electrons model*, and the *band theory*; the latter being derived from molecular orbital theory. For ionic bonding there are two models—a model based in part on the octet rule of full shell stability which has been termed the *electrostatic model*, and a theoretical model based on the calculation of the forces present in an ionic lattice, termed the *theoretical electrostatic model*. For covalent bonding, a total of four models were identified—the *octet rule*, the *valence bond approach*, the *molecular orbital theory*, and the *ligand field theory*. Whilst no specific models were identified for intermolecular or van der Waals forces or the bonding in covalent networks, learners' views of these also were probed during the interviews when discussing covalent bonding. This was deemed necessary after negotiation with the instructors as it was felt that in order to adequately understand covalent bonding, learners must be able to distinguish the bonding in molecular species from that of covalent networks and intermolecular forces.

4.5 Development of an Interview Protocol for the Inquiry

4.5.1 Interview Protocol

Data collection comprised two distinct stages. The first stage, summarised in Appendix A, involved a detailed examination of curriculum material combined with informal interviews with the instructors involved in the inquiry; lesson plans, lecture notes, textbooks, and workbooks used by learners. The second stage of data collection involved clinical interviews, including an IAE approach, and employed strategies of data collection developed from the research goals in Chapter 1 (p. 3).

The research goals for this inquiry are to:

1. Establish if there are preferred mental models for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.
2. Establish the prevalence of the use of analogies for the understanding of the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.
3. Establish the prevalence of alternative conceptions for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

These data consisted of participant-validated verbatim transcripts, together with drawings produced by the learners during clinical interviews. Reflection, and results from the pilot study (Chapter 5), indicated that it was unlikely that research goals could be adequately addressed solely by an IAE approach as was the original intention. Hence, an interview protocol was developed for each of the three target systems of chemical bonding (Table 4.1).

For each target system in turn, there were three phases to the interview. The interview began with phase one with the researcher showing the participant a familiar sample or object, for example, in the case of metallic bonding, aluminium foil and steel wool. The learner was then asked to explain the bonding in the substance in terms of his or her understanding of chemical bonding. Learners were encouraged to draw their models; however, some respondents preferred to describe the bonding verbally and were not pressurised. At the beginning of the interview, most learners indicated a preference for a given model, for example, the sea of electrons model or the octet rule. Once learners had indicated a preference, the researcher probed his or her familiarity with the model. If a learner did not identify a preferred model, the researcher simply probed his or her understanding of chemical bonding for that target system.

Table 4.1 Interview protocol for the inquiry

Target System: Metallic bonding	
<i>Phase 1</i>	Shown sample of aluminium foil— <i>please describe the bonding in this substance</i> Shown sample of steel wool— <i>please describe the bonding in this substance</i>
<i>Phase 2</i>	Shown focus card MB02— <i>please explain this process</i> Shown focus card MB03— <i>please explain this process</i>
<i>Phase 3</i>	Shown focus card MB01— <i>which of these models appeals most/least to you?</i>
Target System: Ionic bonding	
<i>Phase 1</i>	Shown sample of sodium chloride— <i>please describe the bonding in this substance</i> Shown sample of lithium chloride— <i>please describe the bonding in this substance</i>
<i>Phase 2</i>	Shown focus card IB02— <i>please explain this process</i> Shown focus card IB03A/B— <i>please explain this process</i>
<i>Phase 3</i>	Shown focus card IB01— <i>which of these models appeals most/least to you?</i>
Target System: Covalent bonding	
<i>Phase 1</i>	Shown sample of molecular iodine— <i>please describe the bonding in this substance</i> Shown sample of chloroform— <i>please describe the bonding in this substance</i>
<i>Phase 2</i>	Shown focus card CB02— <i>please explain this process</i> Shown focus card CB03A/B— <i>please explain this process</i>
<i>Phase 3</i>	Shown focus card CB01— <i>which of these models appeals most/least to you?</i>

The second phase of the interview involved the use of IAE focus cards depicting phenomena that involved the use of the target system (Figures 4.2-4.4, pp. 79-82); learners were asked to explain the process or event in terms of their understanding of chemical bonding. The events depicted on the IAE cards were devised to provide the interviewer with an opportunity to further probe familiarity of the models selected. As for the first phase, familiar objects or events were used, for example, the conductivity of copper wire (Figure 4.2, MB01, p. 79) and common table salt being crushed (Figure 4.3, IB01, p. 80). In cases for which there were no obvious worldview examples, events were chosen from curriculum material. There were slight variations to the IAE cards used for different levels of learner. For example, focus card IB03A (Figure 4.3, p. 80) was used for secondary school learners since it was felt that they would be more familiar with diamond compared with silica which was present in focus card IB03B (not shown) which, being more challenging, was deemed more appropriate for tertiary level learners. Similarly, secondary school learners were shown focus card CB03A (Figure 4.4, p. 81) since the experiment depicted was known to be a common teaching tool for this part of the Year-13 curriculum. In contrast tertiary level learners were shown focus card CB03B (Figure 4.4, p. 82) which depicted an example common in first-year chemistry.

The third phase of the interview protocol involved showing learners a card illustrating some ways in which the bonding in common substances had been depicted (MB01, p. 79; IB01, p. 80; CB01, p. 81). Respondents were asked to indicate which model they preferred; this was followed by questions that attempted to uncover reasons for their preference. Learners also were asked to indicate the model that had least appeal and again were probed as to reasons for their choice.

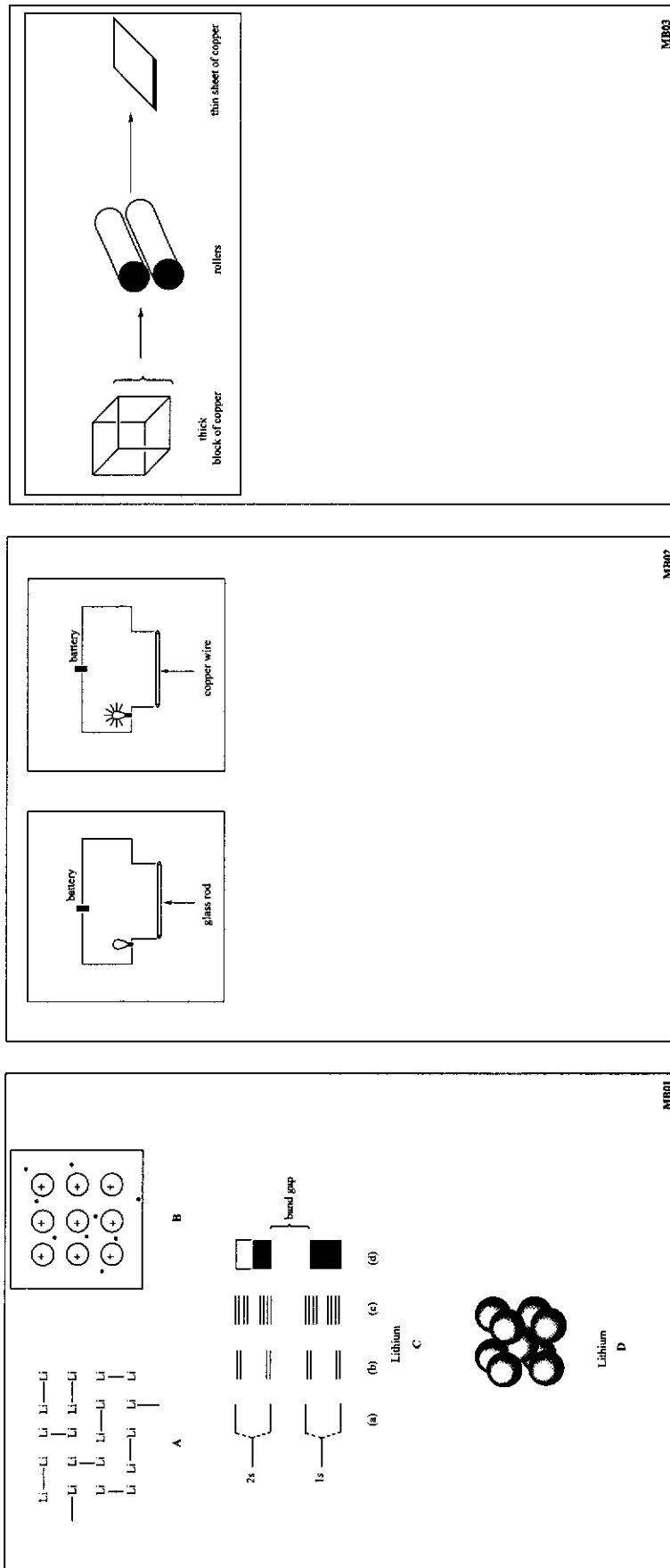


Figure 4.2 IAE focus cards for the target system metallic bonding

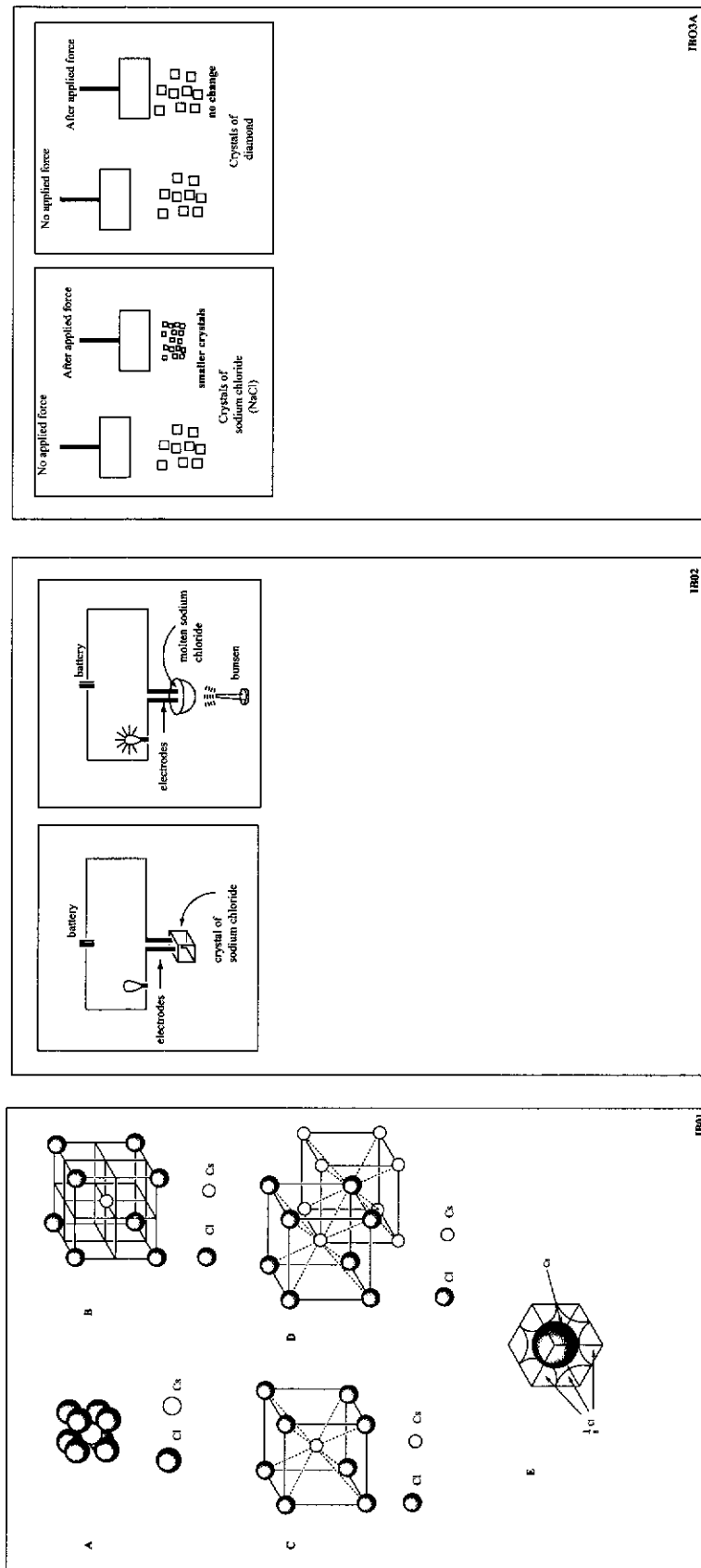


Figure 4.3 IAE focus cards for the target system ionic bonding (Note: Focus card IB03B is not shown. This card is identical to IB03A except that silica is replaced by diamond)

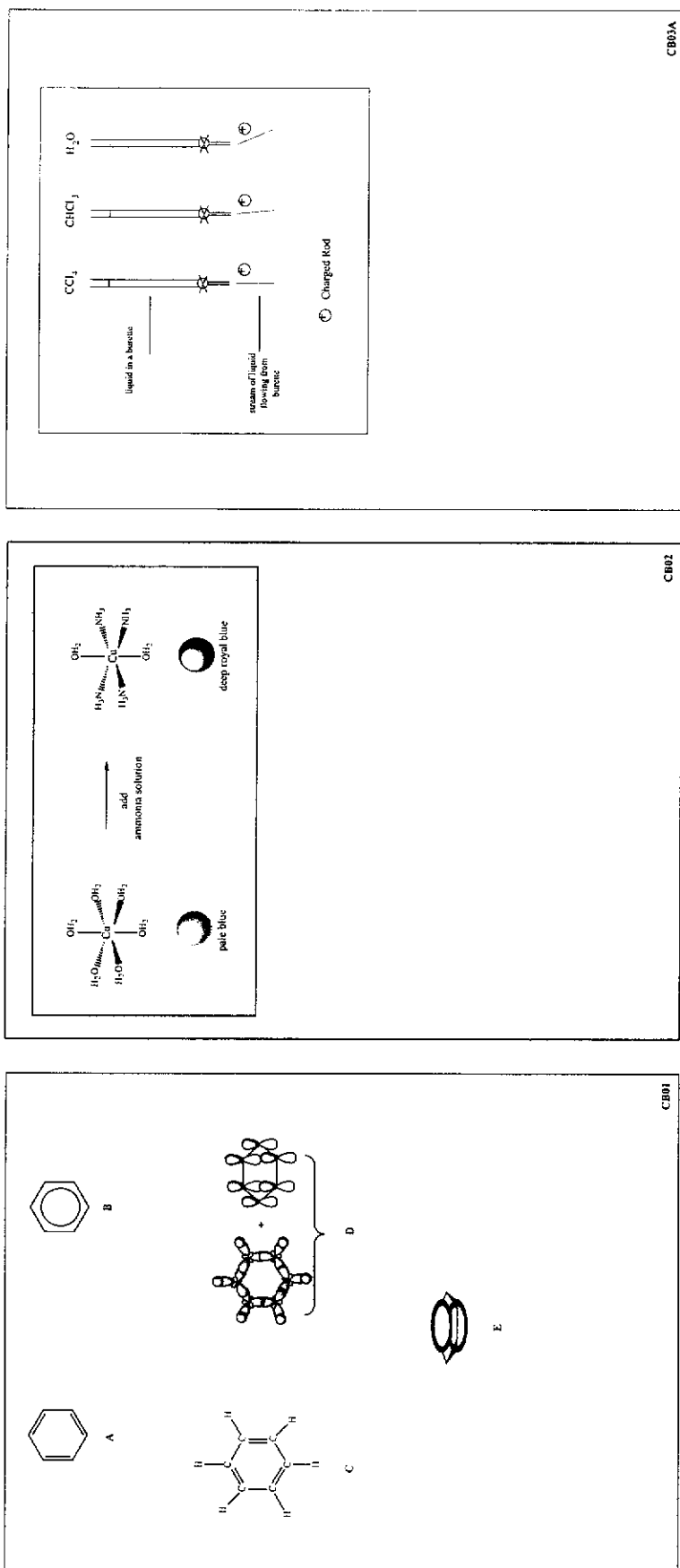


Figure 4.4 IAE focus cards for the target system covalent bonding

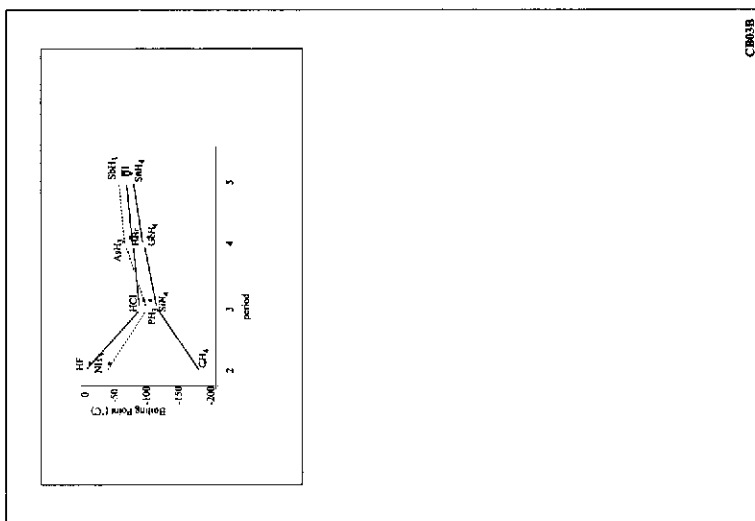


Figure 4.4 (continued) IAE focus cards for the target system covalent bonding

4.5.2 *Development of IAE Focus Cards for the Interviews*

Development of IAE focus cards was based on an eight-step algorithm developed by J.K. Gilbert, Watts, and Osborne (1985) (Table 4.2). The first step involved identification and analysis of the scientists' view of the target models used for chemical bonding, that is, identifying the scientists' science meaning of the model and producing a detailed description of its attributes/components. This was followed by an analysis of the scientists' science view (step 2), that is, an exploration of the accepted understanding of the concept, including its vagueness/ambiguity—for example, the extent to which the model has multiple equally legitimate meanings—along with any limitations of the model.

Table 4.2 Eight step algorithm for Interviews About Events focus card development (from Gilbert, J.K., et al., 1985)

-
1. Identify the scientists' science meaning of the word
 2. Analyze the scientists' science view
 3. Identify the criterial attributes of the word
 4. Identify the non-criterial attributes of the word
 5. Identify sources of obvious linguistic confusion
 6. Identify sources of invalid use of the scientists' science meaning
 7. Producing cards
 8. Ordering cards into a deck
-

The scientists' view reported in Appendix A represents a synthesis of the models and bonding theories that the learners in this study have been exposed to, that is, through curriculum material and learning experiences, and represents the scientific conceptualisation negotiated with the instructors (see, Section 4.7.8, p. 102). The third step of card development involved identification of criterial attributes. The principle research goal for this inquiry involves identifying learners' preferred mental models for chemical bonding; that is, their preferences for the array of target models that they had encountered during instruction. In order to ascertain learners' depth of knowledge about target models, criterial

attributes were developed for each target model at each academic level of learner (Tables 4.3 –4.10). Criterial attributes represent the essential qualities, all of which must be recognised if the model is used in a way that is acceptable to scientists. The criterial attributes were developed from the scientists' view for each of the target models, that is, from the detailed descriptions of each model reported in Appendix A. In a similar manner to the development of the scientists' conceptualisation, agreement of criterial attributes was negotiated with the instructors involved in the inquiry (see, Section 4.7.8, p. 102). Learners have been classified into three levels; level 1—postgraduates, level 2—undergraduates, and level 3—secondary school learners. The criterial attributes for a given target model vary depending on the level of the learner, as negotiated with instructors. Some target models (e.g., molecular orbital theory) did not form part of the secondary school curriculum. Hence, for level 3 learners (i.e., secondary school learners) no criterial attributes were provided for these target models. Nonetheless, because of the relatively open nature of the interview process, there was scope for learners to reveal their prior knowledge, as occurred during the pilot study (see, Chapter 5, p. 110).

Identification of criterial attributes was followed by the development of non-criterial attributes—statements that are sometimes made about situations or circumstances which involve the target model in some way. Non-criterial attributes were identified by examination of curriculum material and books on consumer chemistry and applied chemistry (Fieser & Williamson, 1992; Selinger, 1997; Stine, 1978). Examples include preparing structural models, identifying chemical hazards and interpreting consumer information. Sources of obvious linguistic confusion, antonyms, synonyms, and homonyms were obtained from a thesaurus, informal interviews with non-participants, and informal interviews of teaching staff.

Table 4.3 Algorithm for the development of Interviews About Events protocol for metallic bonding: *Sea of electrons model*

Critical Attributes		Non-Criterial Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
lattice structure	lattice structure	lattice structure	preparing structural models	<i>homonyms-sea:</i>	directional bond,
electron mobility	electron mobility	electron mobility	relating structure to physical properties	see, cee, cede, seed	molecular bond,
alloy-interstitial	alloy-interstitial	alloy-interstitial	distinguishing between compounds	<i>synonyms-sea:</i>	ion/nuclei confusion.
alloy-substitutional	alloy-substitutional	alloy-substitutional	investigating solubility	surf, ocean, beach	
			writing chemical formulae	<i>antonyms-sea:</i>	
			writing chemical equations	land, sand	
			performing thermochemical calculations	<i>homonyms-gas:</i>	
			performing syntheses-inorganic	gaze, gash,	
			selecting instrumental methods	<i>synonyms-gas:</i>	
			interpreting spectroscopic data	air, gasoline, fumes	
			explaining reactivity/stability	wind	
			analysing for environmental pollutants	<i>antonyms-gas:</i>	
			separating metallic ions	solid, hard, rock	
			predicting alloy formation		
			designing suitable protective coatings		
			interpreting consumer information		
			estimating chemical hazards		

Table 4.4 Algorithm for the development of Interviews About Events protocol for metallic bonding: *Band theory*

Critical Attributes		Non-Criterial Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
lattice structure	lattice structure		preparing structural models	<i>homonyms:</i> banned, bandage	bond purely electrostatic,
electron mobility	electron mobility		relating structure to physical properties	bairn, barn	molecular bond,
band formation	band formation		distinguishing between compounds	<i>synonyms:</i> hairband, band (together)	directional bond.
band gap	band gap		investigating solubility	join, co-operate, musical band	
band formation	band formation		writing chemical formulae	mark, identify, circle	
alloy-interstitial	alloy-interstitial		writing chemical equations	group, pack, company	
alloy-substitutional	alloy-substitutional		performing thermochemical calculations	belt, tie, bind, collaborate	
Aufbau Principle	Aufbau Principle		performing syntheses-inorganic	ribbon, strip, stripe	
			selecting instrumental methods	<i>antonyms:</i> continuum	
			interpreting spectroscopic data		
			explaining reactivity/stability		
			analysing for environmental pollutants		
			separating metallic ions		
			predicting alloy formation		
			designing suitable protective coatings		
			interpreting consumer information		
			estimating chemical hazards		

Table 4.5 Algorithm for the development of Interviews About Events protocol for ionic bonding: *Electrostatic model*

Critical Attributes		Non-Criterial Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
ion formation	ion formation	ion formation	preparing structural models	<i>homonyms:</i> iron (clothing)	bond purely electrostatic,
ion size	ion size	ion size	relating structure to physical properties	ironing, iron (Fe)	ignore polarisation
ion shape	ion shape	ion shape	distinguishing between compounds	<i>synonyms:</i> salt formation	
ion type/charge	ion type/charge	lattice formation	investigating solubility	ionic crystal	
lattice formation	lattice formation	radius ratio	writing chemical formulae	inert gas	
lattice structure	lattice structure	bond direction	writing chemical equations	<i>antonyms:</i> neutral	
ionic-coval. continuum	ionic-coval. continuum	ionic-coval. continuum	performing thermochemical calculations	uncharged	
ion polarisation	ion polarisation		performing syntheses-inorganic	non-polar	
			selecting instrumental methods		
			interpreting spectroscopic data		
			explaining reactivity/stability		
			analysing for environmental pollutants		
			separating metallic ions		
			predicting alloy formation		
			designing suitable protective coatings		
			interpreting consumer information		
			estimating chemical hazards		

Table 4.6 Algorithm for the development of Interviews About Events protocol for ionic bonding: *Theoretical electrostatic model*

Criterial Attributes	Level 2	Level 3	Non-Criterial Attributes	Potential Linguistic Confusion	Potential Invalid Model Use
Level 1					
ion formation	ion formation		preparing structural models		bond purely
ion size	ion size		relating structure to physical properties		electrostatic,
ion shape	ion shape		distinguishing between compounds		ignore polarisation
ion type/charge	ion type/charge		investigating solubility		
lattice formation	lattice formation		writing chemical formulae		
lattice structure/type	lattice structure/type		writing chemical equations		
bond direction	bond direction		performing thermochemical calculations		
ionic-coval. continuum	ionic-coval. continuum		performing syntheses-inorganic		
lattice energy	lattice energy		selecting instrumental methods		
Born-Haber	Born-Haber		interpreting spectroscopic data		
Madelung Constant	Madelung Constant		explaining reactivity/stability		
ion polarisation	ion polarisation		analysing for environmental pollutants		
			separating metallic ions		
			estimating chemical hazards		
			designing suitable protective coatings		
			interpreting consumer information		

Table 4.7 Algorithm for the development of Interviews About Events protocol for covalent bonding: *Octet rule*

Criteria Attributes		Non-Criterial Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
full-shell stability	full-shell stability	full-shell stability	preparing structural models	<i>homonyms:</i> octagon	incorrect electron count,
electron pair formation	electron pair formation	electron pair formation	relating structure to physical properties	octopus	incorrect central atom,
molecule formation	molecule formation	multiple structures	distinguishing between compounds	<i>synonyms:</i> octahedron,	inappropriate molecularity
bond directionality	bond directionality	bond directionality	investigating solubility	octahedral	resonance same
unequal sharing	unequal sharing	unequal sharing	writing chemical formulae	octogenarian	equilibria
non-bonded pairs	non-bonded pairs	non-bonded pairs	writing chemical equations		
multiple structures	multiple structures	non-bonded pairs	performing thermochemical calculations		
resonance	resonance	resonance	performing syntheses- inorganic		
			performing syntheses- organic		
			performing syntheses- organometallic		
			selecting instrumental methods		
			interpreting spectroscopic data		
			constructing reaction mechanisms		
			explaining reactivity/stability		
			relating structure to biological function		
			analysing for environmental pollutants		
			analysing for unsaturation		
			analysing essential oils		
			separating/extracting organic compounds		
			interpreting consumer information		
			interpreting catalytic cycles		
			estimating chemical hazards		

Table 4.8 Algorithm for the development of Interviews About Events protocol for covalent bonding: *Valence bond approach*

Critical Attributes		Non-Criterial Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
electron pair formation	electron pair formation	preparing structural models		<i>homonyms:</i>	using full orbitals,
non-bonded pairs	non-bonded pairs	relating structure to physical properties		valence valiance	not allowing for
electron localisation	electron localisation	distinguishing between compounds		dalliance	phase of
bond direction	bond direction	investigating solubility		bondage	wavefunction,
orbital	orbital	writing structural formulae		<i>synonyms:</i>	confusing hybridised
orbital geometry	orbital geometry	writing chemical equations		bond (personal)	& nonhybridised
orbital size/shape	orbital size/shape	performing thermochemical calculations		bonding (personal)	orbitals.
orbital overlap	orbital overlap	performing syntheses-organic		bind, binding	
orbital hybridisation	orbital hybridisation	performing syntheses-inorganic		outer shell	
Aufbau Principle	Aufbau Principle	performing syntheses-organometallic		<i>antonyms:</i>	
Resonance	Resonance	selecting instrumental methods		core shell	
		interpreting spectroscopic data		inner shell	
		constructing reaction mechanisms		antibonding	
		explaining reactivity/stability			
		relating structure to biological function			
		analysing for environmental pollutants			
		analysing for unsaturation			
		analysing for essential oils			
		separating/extracting organic compounds			
		interpreting consumer information			
		estimating chemical hazards			

Table 4.9 Algorithm for the development of Interviews About Events protocol for covalent bonding: *Molecular orbital theory*

Criteria Attributes		Non-Criteria Attributes		Potential Linguistic Confusion	Potential Invalid Model Use
Level 1	Level 2	Level 3			
LCAO*	LCAO*	preparing structural models	relating structure to physical properties	<i>homonyms:</i> mole (animal), orbs	not allowing for <i>s-p</i> mixing,
electron delocalisation	electron delocalisation	distinguishing between compounds	investigating solubility	mole (number)	not allowing for phase of
boundary surface	boundary surface	writing structural formulae	writing chemical formulae	orbital bones	wavefunction,
orbital geometry	orbital geometry	writing chemical equations	writing thermochemical calculations	<i>synonyms:</i> satellite orbit	confusing hybridised & non-hybridised orbitals,
orbital size/shape	orbital size/shape	performing syntheses-organic	performing syntheses-inorganic	eyes, circuit	assuming positive electron density at nuclei,
Aufbau Principle	Aufbau Principle	performing syntheses-organometallic	selecting instrumental methods	small	not allowing for orbital symmetry,
bond order	bond order	interpreting spectroscopic data	constructing reaction mechanisms		incorrect order for energy levels.
relative energy level	relative energy level	explaining reactivity/stability	relating structure to biological function		
group theory	group theory	relating structure to environmental pollutants	analysing for unsaturation		
		analysing for essential oils	separating/extracting organic compounds		
		interpreting consumer information	estimating chemical hazards		

*Linear Combination of Atomic Orbitals.

Table 4.10 Algorithm for the development of Interviews About Events protocol for covalent bonding: *Ligand field theory*

Criterial Attributes Level 1	Level 2	Level 3	Non-Criterial Attributes	Potential Linguistic Confusion	Potential Invalid Model Use
Degeneracy electrostatic field orbital shape orbital orientation orbital splitting relative energy level orbital occupancy spectrochemical series group theory	Degeneracy electrostatic field orbital shape orbital orientation orbital splitting relative energy level orbital occupancy spectrochemical series		preparing structural models relating structure to physical properties distinguishing between compounds writing structural formulae performing syntheses-organometallic selecting instrumental methods interpreting spectroscopic data interpreting magnetic data constructing reaction mechanisms explaining reactivity/stability relating structure to biological function analysing for environmental pollutants interpreting consumer information interpreting catalytic cycles estimating chemical hazards	<i>homonyms:</i> legend <i>synonyms:</i> field, farm, and, paddock <i>antonyms:</i> metal centre central atom transition metal	confuse <i>d</i> -orbitals, confuse energy level order, confuse tetrahedral & octahedral.

Sources of invalid use of the scientists' science meaning followed identification of linguistic confusion. Usually this involves common usage meanings and clear misuse of the target models. Potential sources of invalid model use were obtained from informal interviews with teaching staff, a survey of the literature on alternative conceptions (Section 2.3, pp. 37-42), and the results of the pilot study (Chapter 5, pp. 121-127). Further invalid model use was identified during the interviews; the use of the semi-structured approach allowed the researcher to follow up invalid model use as part of the interactive interview process.

Card production for IAI and IAE focus cards usually consists of producing examples and non-examples; each non-example has one or more of the criterial attributes absent but also includes some of the non-criterial attributes. In the present inquiry, the focus cards were used in a slightly different manner to that employed by other researchers in that the cards were designed to depict events which involved the target model in some way. The intention was to allow respondents to make choices about which of the target models, if any, they employed to make sense of the phenomena depicted on the cards. As recommended, the card sequence began with simple examples, finishing with more challenging examples (Gilbert, J.K., et al., 1985).

4.6 Data Analysis

Participant-validated transcripts were inspected for statements that revealed learners' views for each of the target systems, namely metallic, ionic and covalent bonding. These statements were compiled to form an inventory for a given target system, for example, metallic bonding: these data were combined with learners' drawings to develop a view of their mental models. When learners identified a specific target model, their views were compared with the scientists' conceptualisation by reference to the criterial attributes for that target model at the appropriate level (Tables 4.3 – 4.10). In this way learners' familiarity with a given model could be adjudged.

The second research goal has as its main focus learners' use of analogy to aid understanding. Because it was not concerned with the use of analogy during instruction, this interview-based inquiry did not involve classroom observation. Consequently, to address the second research goal, interview transcripts were analysed for statements revealing use of analogy; analogies were classified using Dagher's (1995a) typology, namely, compound, narrative, procedural, peripheral and simple (Chapter 2, p. 35).

Learners' alternative conceptions for chemical bonding were identified by inspection of interview transcripts and drawings produced by participants. Data were analysed using a concept profile inventory (CPI) based on that employed by Erickson (1979, 1980) and Rollnick and Rutherford (1990). The CPI procedure consists of examination of interview transcripts for expressions and statements that could be construed as evidence for learners' views, in this instance, their alternative conceptions for the target models of chemical bonding. These expressions were summarised and formed the unit of analysis. By examining the entire set of expressions in the transcripts, it was possible to gain a global perspective of the learners' views of what represents an alternative concept. These views were then organised into a series of categories which formed the *Conceptual Inventory* for an individual alternative conception. Commonality of views was deduced from examination of the inventories and used to summarise the research findings.

It was noteworthy that inspection of interview transcripts revealed considerable use of anthropomorphic language by learners across all academic levels. However, restrictions on the size of this thesis precluded the inclusion of any in-depth analysis of the data in this respect, although brief mention is made in the pilot study (see, pp. 123-124).

4.7 Validity and Reliability in Qualitative Research: The Trustworthiness of an Inquiry

4.7.1 Establishing the Trustworthiness of a Naturalistic Inquiry

The traditional means of judging the quality or rigor of a research inquiry is by reference to the four criteria of internal validity, external validity, reliability, and objectivity (Altheide & Johnson, 1994; Guba & Lincoln, 1989; Lincoln & Guba, 1985; Merriam, 1988). The internal validity of an inquiry is the extent to which variations in outcomes can be ascribed to controlled variation in dependent variables—in other words, how well the research findings match reality. Guba and Lincoln (1989) identify a number of threats to internal validity—history, maturation, testing, instrumentation, statistical regression, differential selection, experimental mortality and selection. External validity has its focus on the ability to generalise the findings of the inquiry to a target population. Just as there are threats to internal validity, there are a number of threats to external validity including non-random selection, setting effects, history effects, and construction effects. Reliability, a precondition for internal and external validity, refers to an inquiry's consistency, predictability, dependability, stability and accuracy. In other words, the question asked is, how can we be sure that if this measurement was repeated we would get the same results? Objectivity addresses the desire for neutrality, that is, freedom from the biases, prejudices, and personal perspectives of the investigator; put simply, how much are the findings of the inquiry influenced or determined by the participants, particularly the investigator?

These traditional criteria for judging the quality of an inquiry are consistent with the ontological and epistemological beliefs systems of an empirical-positivist paradigm (Altheide & Johnson, 1994; Guba & Lincoln, 1989; Janesick, 1994; Lincoln & Guba, 1985; Lincoln & Denzin, 1994). However, serious objections have been raised as to their suitability for judging the quality of inquiries carried out within a constructivist paradigm (Altheide & Johnson, 1994). Hence, different criteria have been proposed for constructivist inquiries, to judge the *trustworthiness* of the inquiry, that is "considering the unique

contribution made to the goodness or quality by the *nature of the hermeneutic process itself* [original italics]" (Guba & Lincoln, 1989, p. 233). Guba and Lincoln (1989) propose that credibility replace internal validity, dependability replace reliability, confirmability replace objectivity, and transferability replace external validity.

4.7.2 *Credibility*

Credibility can be judged from a position consistent with a constructivist paradigm, in which isomorphism between an objective reality and the research findings is replaced by isomorphism between reconstructed realities, that is, the ontological basis has changed from realist to relativist. The match between the constructed realities (i.e., reality in the relativist sense) is enhanced by a number of factors including prolonged engagement, persistent observation, peer debriefing, negative case analysis, member checks, and progressive subjectivity. The purpose of prolonged engagement is to provide the opportunity to establish good rapport and trust with participants, allowing the researcher to overcome the effects of misinformation, distortion or presented fronts (Guba & Lincoln, 1989). Persistent observation allows the researcher to identify the characteristics and elements in the inquiry that are most relevant to the issue under inquiry. Peer debriefing, with a disinterested peer, that is, someone who has no contractual interest helps the investigator to "understand his or her own posture and values and their role in the inquiry" (Guba & Lincoln, 1989, p. 237). Negative case analysis involves revising the "working hypothesis" in the light of hindsight; in other words, an inquiry is seen as a dynamic rather than static process. Member checks, that is, the process of negotiation with stakeholders, provides participants with the opportunity to offer additional information to that gained from, for example, interviews, and allows participants the opportunity to confirm individual data. Finally, progressive subjectivity, the "the process of monitoring the evaluator's (or any inquirer's) own developing construction" (Guba & Lincoln, 1989, p. 238), serves to remind the inquirer that in a constructivist inquiry the researcher's construction should not be afforded a

higher status than that of another. As Guba and Lincoln put it, "any construction that emerges from an inquiry must, to be true to constructivist principles, be a *joint one* [original italics]" (p. 238).

4.7.3 *Dependability*

Dependability is concerned with the stability of data over time. It is perhaps on the issue of dependability that constructivist inquiries differ most from their positivist equivalents—that is, reliability. Guba and Lincoln (1989) point out that methodological changes and shifts in construction are the very lifeblood of naturalistic inquiries, and do not impact adversely on dependability. For conventional inquiries alterations in research design are "thought to expose inquiries to unreliability" (Guba & Lincoln, 1989, p. 242). In naturalistic inquiries, these changes are seen as an integral part of the inquiry process and, rather than representing flawed methodology, indicate increasing maturity of the inquiry. What is critical, is that the changes and shifts in constructions be clearly identified and fully described: as Guba and Lincoln put it they should be "tracked and trackable" (p. 242).

4.7.4 *Confirmability*

Like its positivist equivalent, objectivity, confirmability seeks to ensure that the results of an inquiry have not been subject to influence by the investigator. The usual means of ensuring objectivity in conventional inquiries is via strict adherence to method, that is, "follow the process correctly and you will have findings that are divorced from the values, motives, biases, or political persuasions of the inquirer" (Guba & Lincoln, 1989, p. 243). However, in constructivist inquiries, the confirmability of an inquiry rests on the data themselves. Hence, the raw data and process used to compress them are made available to scrutiny by the reader (Cronbach & Suppes, 1969). This provides an audit trail which is intimately linked with the tracking process necessary to assure dependability.

4.7.5 *Transferability*

Transferability is the constructivist equivalent to external validity or generalisability—Merriam (1988) describes it as "the extent to which the findings of one study can be applied to other situations" (p. 173). In conventional inquiries, generalisability is strongly dependant on sample selection, specifically on the randomness of the sample (Merriam, 1988; Patton 1990; Wiersma, 1986). Typically a target population is identified and a selection of participants made via a random sampling procedure or some more efficient variation such as stratified random sampling. Guba and Lincoln (1989) point out that for constructivist inquiries the onus is shifted from the inquirer to receiver. Geertz (1973) suggests that the nature of ethnographic and naturalistic inquiries is such that they are "rather more of an observational and rather less of an interpretative activity" (p. 9). Thus the constructivist inquirer describes the context of the inquiry and provides detailed descriptions of methodology and interpretation: it is then up to the reader to decide if the findings are relevant or pertinent to their own situation. The normal means for facilitating the process of transferability is via so-called *thick description* (Geertz, 1973; Merriam, 1988). In this process, the inquirer provides a full and highly detailed description, commonly incorporating extensive portions of verbatim transcript in order to "facilitate transferability judgements on the part of others" (Guba & Lincoln, 1989, p. 242). The quotes provided in Chapter 5, 6 & 7 have undergone some light editing (e.g., removal of repeated words or phrases, changes of tense, removal of neutral interviewer prompts, etc.) to make them more readable.

4.7.6 *Triangulation*

Patton (1990) agrees with the views expressed by Guba and Lincoln (1989), and along with Janesick (1994) and others (e.g., Altheide & Johnson, 1994; Cohen & Manion, 1989; Merriam, 1988; Stake, 1994) suggests that triangulation is the most effective means of enhancing the credibility of research findings for naturalistic inquires. Triangulation involves the gathering of

information from a number of sources to cross-check and to assess the authenticity of individual accounts (Bell, J., 1993; Mathison, 1988; Shulman, 1988; Welch, 1983; Wolcott, 1988b; Fielding & Fielding, 1986). By comparing and contrasting one source of information with another the researcher is able to produce a more comprehensive and balanced study in response to the research question. This approach not only provides more information about the validity of a study but aids in interpretation in that it affords the investigators an opportunity to "solve the problem of rival causal factors" (Denzin, 1970, p. 26).

There are three forms of triangulation used in practice; data triangulation, investigator triangulation, and methodological triangulation (Denzin, 1970; Fielding & Fielding, 1986; Mathison, 1988). Data triangulation involves the use of different data sources for the study and this can take a variety of *types*—time, space (i.e., situation), person, and *levels*—aggregate (i.e. individual person), interactive (i.e., the individual's immediate neighbours in the social setting), and collectivity (the larger group, for example, a company or institution, in the individual's social setting). The *types* and *levels* of data sources allow the investigator to explore such things as temporal influences (e.g., by a longitudinal study) and to conduct comparative research. Investigator triangulation involves the use of different investigative staff during the data collection. This is common in quantitative and large ethnographic inquiries that frequently involve research assistants (Denzin, 1970; Sieber, 1978; Gall et al., 1988). One function of this type of triangulation is to identify subjective bias that is frequently an issue of concern in naturalistic inquiries (Webb, Campbell, Schwartz, & Sechrest, 1966; Welch, 1983). However, group dynamics play an important part in successful multiple-investigator inquiries and the different language or research perspectives of researchers may lead to conflict during interpretation (Fielding & Fielding, 1986).

Methodological triangulation comes in two forms: within-method triangulation, that is, using the same method (e.g., a survey) and employing multiple strategies, and across-methods (or between-methods) triangulation, that

is, applying different methods (e.g., observation and interviews) to the same research question. Some researchers hold the view that qualitative inquiries are impaired unless they involve across-methods triangulation that attempts to relate different sorts of data in such a way as to counteract various possible threats to the validity of a study that would come from the use of a single method (Denzin, 1970; Fielding & Fielding, 1986). The overall purpose of triangulation is to ensure that the bias inherent in any data, investigator, or method will be cancelled out, thus resulting in a convergence upon the social phenomenon under investigation (Denzin, 1970; Mathison, 1988).

There are three possible outcomes of triangulation in educational research—convergence, inconsistency, and contradiction (Denzin, 1970; Mathison, 1988; Fielding & Fielding, 1986). The historical goal of triangulation has been convergence, that is, the data provide consistent evidence for a particular conclusion. Inconsistency occurs when one data set does not confirm the findings of another set, but does not completely contradict it either. Contradiction occurs when the data disagree to such an extent that it is not possible to provide a plausible explanation. These latter two outcomes are often not perceived favourably since sometimes researchers feel that they cast doubt on the validity of the study or require greater imagination to devise plausible explanations for contrary data. However, lack of convergence provides different perspectives that may ultimately produce a deeper understanding of the research questions or goals. Because of this, each of the three outcomes of triangulation can have real value in science education research.

4.7.7 Measures Taken to Maintain Trustworthiness in the Inquiry

Credibility was maintained following the means described in Section 4.7.2 above (pp. 96-97). Although interview data were obtained over a comparatively short time span (five months) data collection did involve prolonged engagement and persistent inquiry. This occurred since the researcher was known to most of the participants for several years prior to the inquiry. Hence, prolonged engagement did occur in this inquiry and the researcher was able to establish good

rapport and trust with participants who were relaxed during interviews and spoke freely. To further aid in producing a relaxed atmosphere, almost all interviews were conducted outside working hours. Peer debriefing occurred with two disinterested peers—this proved invaluable, enabling the researcher to maintain perspective reducing the likelihood of subjective bias. Negative case analysis also proved beneficial and, for example, each interview was transcribed and read soon after completion. This enabled the researcher to continually examine the goal of the inquiry to understand the learners' preferred mental models for chemical bonding in light of the methodology. The instance described in the pilot study (see, Chapter 5, pp. 125-126), in which part of the interview protocol was altered, is consistent with the constructivist nature of this inquiry, being dynamic rather than static; this responsive approach has likely improved the credibility of the interview data. Member checks were monitored by participant validation of transcripts by inspection of written transcripts, writing clarifying notes where appropriate, and additional informal interviews with participants to seek clarification where ambiguity in interview transcripts was detected. Field notes were compiled while interviews were in progress and in a number of instances brief informal interviews were conducted to clarify field notes and statements made during interviews. Achieving progressive subjectivity is more difficult to ascertain. In this inquiry the researcher continually examined his own stance in relation to the research goals and methodology. The intimate involvement of participants, both learners and instructors, in all phases of data collection means that this is genuinely a joint inquiry.

Dependability as it relates to this inquiry is determined by an audit trail; that is, the provision of a detailed description of methodology. No significant changes were made to the methodology for the duration of the inquiry. In a similar manner, confirmability was achieved by the provision of detailed descriptions, in this instance of the data themselves. An appropriate audit trail is provided in the results and discussion presented in Chapters 5, 6 and 7.

Triangulation of the first phase of data collection, that is, the production of scientists' view of the target systems and models presented in Appendix A, was achieved by examining a wide variety of curriculum materials comprising textbooks, lecture notes, and lesson plans. These data were further triangulated with informal interviews of the instructors, along with their inspection of the descriptions of target models (i.e., Appendix A). Investigator triangulation involved consultation with instructors and participants throughout the inquiry, and along with peer debriefing (see, Section 4.7.8, p. 102), served to address the issue of subjective bias. Methodological triangulation involved cross-checking learners' views as elicited from interview data with the descriptions of target models produced from the analysis of curriculum material.

4.7.8 *Validation of Data by Peer Review*

Validation of data and the researchers' interpretation of the research findings involved participation of eight peers. Four of these were instructors from the learning institutions involved in the inquiry whose principal contribution consisted of the provision of validation of the description of target models reported in Appendix A. Other contributions consisted of validation of the *Concept Profile Inventories* for alternative conceptions provided in Appendix B, and the criterial attributes detailed in Tables 4.3-4.10 (pp. 85-92). The researchers' construction and interpretation of the learners' mental models for chemical bonding reported in Chapters 6 and 7 were similarly validated by two of these individuals along with two further instructors from institutions not involved in the inquiry—one a secondary school teacher, the other a tertiary level instructor/research chemist. Two further individuals, neither chemists, but both involved in tertiary level science education, acted as disinterested peers and provided regular informal feedback regarding methodology and the construction and interpretation of the research findings.

4.8 Ethical Considerations

There were a number of ethical issues to be addressed before commencement of the main study of this inquiry. The issues of concern identified were; participants feeling coerced into participation, the confidentiality of the participants' identity and opinions expressed during the study, and a potential conflict of interest since the investigator was required to act as an examiner for some of the undergraduate learners. These ethical concerns were addressed in the following manner.

Individuals were approached regarding their participation in the study via a written, rather than face-to-face approach (Appendix C, p. 371). It was intended that participants would feel free to decline involvement with this less confrontational approach. The purpose of the inquiry was explained to potential participants via a brief summary and their participation formally requested in writing. It was made clear to potential participants that they had the right to withdraw from the inquiry at any stage they wished. Participants were identified only by code numbers in the recording of the research data. Field notes and data records were secured and will be destroyed five years after the completion of the inquiry. Participants were given the right to request that part or all of the research findings be not reported in the literature and the report of the research findings employed the use of pseudonyms. Interview data were collected June 1998 - Dec. 1998. Only undergraduate learners who had completed their studies and examinations involving the researcher prior to being involved in the study were interviewed.

4.9 Summary

This chapter provided a description of the methodology for the inquiry. Building on the literature review of Chapter 2 and the theoretical perspective detailed in Chapter 3, a conceptual theme for the inquiry was developed. The methodology based in a constructivist paradigm comprised a three-phase

interview protocol for each target system of chemical bonding, including the use of IAE focus cards.

Chapter 5 reports the results of the pilot study which was conducted in Perth, Australia, during the researcher's on-campus residency period.

CHAPTER FIVE

PILOT STUDY

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CHAPTER FIVE

PILOT STUDY

Overview of the Chapter

This chapter consists of a description of the pilot study conducted during the researcher's residency at Curtin University of Technology, Perth, Australia, in June-July 1998. Variations to the three-phase protocol were investigated during the pilot study and the results along with a discussion of the implications for the main investigation are reported herein.

5.1 Sample Description

The sample chosen for the pilot study comprised six learners, two learners from each educational level, namely, secondary school, undergraduate, and postgraduate. All participants were of European extraction and were self-selected after approval was given by senior administrators of the learning institutions involved. Pseudonyms have been used to protect learners' identities.

The secondary school learners were from a single-sex private school in a middle-class suburb in the Perth Metropolitan area. The two learners, females aged 16 (Natalie) and 17 (Linda), were Year-12 learners in the final year of their secondary schooling. Both learners enjoyed chemistry and saw it as a promising career path. Natalie was quite confident, whereas Linda, although quite relaxed, was less outspoken.

The undergraduate learners were chemistry majors in the Department of Applied Chemistry at Curtin University of Technology. One learner, Rosalie a female aged 25, was very keen on chemistry, also enjoyed mathematics, but was proceeding with chemistry as she felt the career prospects were better. She was in the second year of her undergraduate degree and had taken the previous year off for personal reasons. Rosalie possessed a bright, out-going personality and spoke freely at length with little prompting. She was a confident, mature person, with few inhibitions and seemed particularly keen to be involved in the inquiry.

The second undergraduate learner Mike, a 20 year old male, was also confident and performed well in his first year at university, but less well in his second year due to ill health. He was very keen on chemistry, mainly as a result of childhood experiences and an on-going fascination with pyrotechnics. Mike also enjoyed physics, but like Rosalie felt that the career prospects for chemistry were better.

The two postgraduate learners were male PhD candidates. John, in the first year of his PhD, was a confident out-going individual who was relaxed and communicative. He enjoyed chemistry and his thesis topic was concerned with applied chemistry in the organic environmental area. His interest in chemistry was stimulated as a child by the gift of a chemistry set by an elderly relative. He had no real preference for a field of chemistry, other than an inclination towards organic chemistry. In contrast to John, Nigel, a 24 year old, was reserved and hesitant and appeared to be rather under-confident despite being in the final year of his doctorate. He was stimulated to study chemistry because of an inspiring high school teacher; his thesis topic was concerned with the use of activated carbon in the absorption of gold from solution.

5.2 Results from the Pilot Study

5.2.1 Learners' Mental Models of Target Systems

The interview protocol employed in the pilot study was based on the three phases described in Chapter 4 (Table 4.1, p. 77). Each learner was presented with samples of metallic, ionic and covalent substances, and asked to describe the bonding in the substance. Second, they were shown prompts in the form of IAE focus cards depicting events which involved the use of models of chemical bonding. Finally, each was shown prompts in the form of focus cards that showed ways in which the bonding in specific metallic, ionic and covalent substances had been depicted.

The main results from the pilot study are discussed here and are presented in the same sequence as the research goals detailed in Chapter 1 (p. 3).

A brief description of learners' preferred models is provided first, followed by a description of their use of analogy and alternative conceptions.

Learners' mental models for the target systems comprised a description of their choice when prompted with samples of metallic, ionic and covalent compounds, followed by their choice from the focus cards that contained depicted models (i.e., MB01, p. 79; IB01, p. 80; and CB01, p. 81). The preferred models described by learners, when given free choice were those they had encountered during instruction, namely, the target models for this inquiry (Figure 4.1, p. 74).

5.2.2 *Learners' Mental Models of Metallic Bonding*

For metallic bonding, the preferred model for all learners' was the sea of electrons model, for which they showed a good understanding. Linda stated that the ions would be "in a three dimensional lattice" which she was reluctant to draw, but extended her explanation upon probing to "it's in a definite arrangement of ions". Aluminium in Linda's view is held together by "attractions between different charge, ions and electrons" and the electrons were seen by Linda as "detached from the actual ions". Natalie provided a similar description of the sea of electrons model and stated that "bonding in metals [consists of] a metal surrounded by a sea of delocalised electrons" and "the electron cloud would be moving". In contrast to Linda, Natalie readily drew a representation of her mental model (Figure 5.1) illustrating the metal arrangement and delocalised electrons.

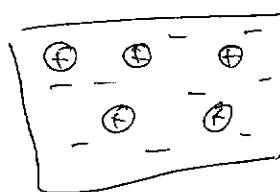


Figure 5.1 Natalie's drawing illustrating the bonding in aluminium foil

Natalie was able to use the sea of electrons model to explain the phenomenon depicted on the IAE focus card MB02 (p. 79) in which the conductivity of copper wire and a glass rod are compared "the copper wire has got metallic bonding, its got like electrons in a sea of electrons and they can carry the charge from the battery so the circuit is complete". Similarly, Natalie offered a reasonable explanation for the malleability of metallic copper (MB03, p. 79) based on the sea of electrons model.

The ions wouldn't like be getting bigger the atoms, I think they are going to, are gradually, like, let's think about it. Oh, OK, I've got it. The ions would like slide, because the electrons, they're like between the layers, and there's no attraction so they can slide over each other like without breaking, um, yeah without like shattering.

Interestingly, undergraduate and postgraduate learners, whilst also expressing a preference for the sea of electrons model, were rather more vague than the secondary school learners. Undergraduates explanations were more brief and, for example, John simply stated that "it's just a whole pile of aluminium atoms that share their electrons and, um, the sharing of all the electrons holds it together". This vagueness in descriptions for undergraduates and postgraduates for the sea of electrons model may simply be because the model was fresher in the minds of the secondary school learners. An informal interview with the school teacher revealed these learners had received instruction about the sea of electrons model immediately preceding their interviews.

In contrast to their younger colleagues, undergraduate and postgraduate learners placed more importance on the packing arrangements of metallic lattices than the bonding between metal atoms or ions. However, they tended to use concepts from other models when unable to explain some aspect of bonding using the sea of electrons model. Nigel, for example, stated that metals comprise an array of close-packed atoms, but also introduced the idea of orbitals; although he seemed uncertain if orbitals are actually present in metallic bonding.

Nigel. I suppose yeah I think of metallic bonding, I just think of a whole lot of atoms that are sort of in close, real close together in a sort of ordered array, ah that's pretty much how I think of it, a whole lot of spheres just like closely packed.

Interviewer. What's actually holding those spheres or atoms together?

Nigel. It's pretty much just the electrons and that's pretty much it.

Interviewer. Do you want to tell a bit more about the electrons how you see them in the structure?

Nigel. Mm...ah...I don't really visualise them too much you know, um, it's probably a bit different when you come to types of bonding. I can sort of see them as orbitals but probably not with metallic bonding.

Interviewer. Do you think there are orbitals in metallic bonding?

Nigel. Ah...well there would have to be because the electrons have to be in some region.

Interviewer. When you say they'd have to be in some region do you want to just sort of expand on that a bit.

Nigel. Well an orbital is defined as a region in space in which the electrons exist.

Interviewer. So you think the metals will have orbitals that like that?

Nigel. Well they must do if that definition is true.

Whilst the undergraduates and postgraduates were less clear about some details of the sea of electrons model, they were able to use the model to explain events depicted on the IAE focus cards. John, here explaining the malleability of copper metal (MB03, p. 79), produced a fairly coherent explanation.

The copper can be, I don't know like the copper is basically malle, malleable I think is the right the right term for that. Because it's like a rigid structure, because you've got the electrons again which can flow through the entire structure, the atoms aren't fixed. They can vibrate, they can move around, 'cos your not actually breaking any really strong bonds. You're just squeezing it out and making it longer. It doesn't change it, just you know, I wouldn't say you would be compressing the copper atoms closer together, it just makes it longer. You're changing the form, and you can change the form because like there isn't any rigid bonds which you'd find in a salt crystal or something like that.

Responses to the prompt card showing depictions of metallic bonding (MB01, p. 79) revealed that learners' choice was consistent with their open-ended response (i.e., when shown aluminium foil). Although some choose more than one model, four out of the six learners choose B, a simple depiction of the

sea of electrons model. In addition, there was some evidence that learners possessed realist notions about bonding and structure, with two learners also indicating that D, a depiction consisting of close-packed spheres, held some appeal. Nigel indicated that the depiction of metallic lithium which appealed least to him was depiction C (MB01, p. 79) because such a model was unlike lithium on an atomic scale "that sort of doesn't give you that three dimensional view, you can't actually, looking at that you can't see what lithium looks like at the atomic level". Natalie was more explicit and stated her preference clearly for a model that she perceived as realistic—"it's like a three-D model, so you can see it's like a more realistic sort of model of the bonding in a metal". Only one learner, Linda, indicated that C, the band theory model, held some appeal. It is somewhat surprising that Linda, a secondary school level learner, employed the more sophisticated molecular orbital-based band theory, whereas the postgraduates and undergraduates preferred the simple sea of electrons model. Band theory is not part of the Year-11 or Year-12 curriculum, but Linda indicated that a sibling was studying university physics, and had described the model to her.

5.2.3 *Learners' Mental Models of Ionic Bonding*

In a similar fashion, learners preferred the *electrostatic model* for the bonding in ionic substances. Learners viewed the bonding as an interaction between opposite charged species formed by the transfer of electrons. However, the secondary school learners, Natalie and Linda, were more interested in the lattice structure of the ionic compound, making only brief mention of the attraction between ions as evidenced by Linda's comment that "there's maybe an attraction between the negative and positive ions".

The tertiary level learners provided more detailed explanations. John, for example, described the bonding in Epsom's salt (MgSO_4) in terms of electron transfer.

Basically this is ionic bonding this time and it occurs because the sulfate component basically takes the electrons off the magnesium.

So you are left with SO_4^{2-} with two extra electrons, and Mg^{2+} deficient in two electrons and they are attracted to each other.

Nigel placed some emphasis on ionic size, although like John, he related ionic bonding to the loss and gain of electrons.

Well there is a cation and there is an anion, the anion is much larger than the cation 'cos it's got an extra electron or electrons. So it's, be bigger, and the cation's much smaller 'cos it doesn't, it doesn't have, well it's missing electrons, and when the sulfate gives up a couple of electrons to form a bond, that's pretty much it.

In contrast to metallic bonding, learners across all three academic levels placed emphasis on the structure, readily drawing three-dimensional structures when prompted. Linda talked about a "lattice of positive and negative ions" in a "rigid position" and Natalie likewise showed an appreciation of the three-dimensional nature of the structure—"like I mean it's like each ion is like surrounded on every side". John viewed the bonding and structure of Epsom's salt (MgSO_4) similarly drawing Figure 5.2, but upon prompting provided a more detailed description than either Natalie or Linda.

You have say [drawing], um, say an Mg^{2+} , and surrounding that, I can't remember the exact crystal structure, but basically you have got Mg^{2+} , and you'll have adjacent sort of an SO_4^{2-} enabling them to sort of hold together. I'd say there is a very regular pattern, like with your, unlike your metallic bonding, the way it is, there's not actually a lot of movement between the different ions.

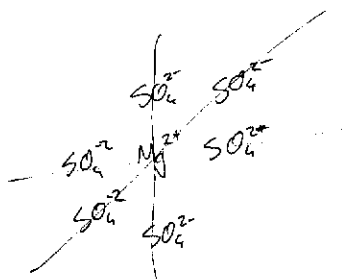


Figure 5.2 John's drawing illustrating the structure of magnesium sulfate (MgSO_4)

In a similar way Rosalie described sodium chloride as consisting of a continuous, three-dimensional arrangement (Figure 5.3) in which "Na⁺, chlorine [drawing], it's a sort of pattern, where the sodium's close to the other sodium, and the chloride is close to the other chloride, and that's a continuation in three dimensions".

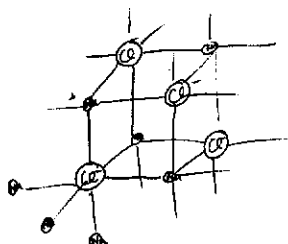


Figure 5.3 Rosalie's drawing illustrating the structure of sodium chloride (NaCl)

Responses to the prompt card showing depictions of ionic bonding (IB01, p. 80) revealed that learners' choice was consistent with their open-ended responses, with four learners choosing A, a space-filling depiction. Whilst some learners stated that this depiction appealed because it was more familiar, others explicitly stated that this model seemed more real. The data seems to suggest that learners may see such depictions as copies of reality, as typified by Natalie's statement that "A is like showing you a more realistic model" and Nigel who commented " it's more of an indication of how it would look on an atomic scale".

Secondary school learners were able to use the electrostatic model for ionic compounds to explain events depicted on the IAE focus cards for ionic bonding (IB02, IB03A, IB03B, p. 80). Natalie provided an explanation for the friability of sodium chloride (IB03A, p. 80) that was consistent with her model of ionic bonding.

It's like ionic bonds are very strong between ions. But if a force is applied, it breaks those bonds, and the compound shatters, and forms smaller crystals, 'cos like in sodium chloride, they can't move over each other like in metals. So they don't, in the lattice, when one layer tries to move, you are forcing the particles from this layer, so

the two positives go together, and they repel each other and they like shatter.

Linda provided a similar explanation for the same event, citing the repulsion of like-charged species as the reason sodium chloride crystals shatter upon application of an external force (IB03A, p. 80).

In the ionic lattice the sodium chloride one the layers will try and move when the force is applied. But like charges will be put next to each other together and they will repel and they will break into small pieces.

However, undergraduate and postgraduate learners struggled to use their models to explain events. A typical case, John, discussed the conductivity of molten sodium chloride and non-conductivity of solid sodium chloride (IB02, p. 80) and related the conductivity to the loss of rigidity of the structure.

OK the light does not, it's not illuminated with the crystal sodium chloride, because the electrons can't travel through the solid block of an inorganic compound. I mean in an ionic compound it just doesn't happen. When it becomes molten, what I think that means is the electrons introduced to it from the battery are able to transfer through the molten sodium chloride, because there are no there's no fixed rigid structure preventing the transfer of electrons through it. How it actually works I not sure. I am not sure if one of the atoms picks up an electron and an atom just passes it on like that, or if it actually, or if the actual electrons goes through. But basically you're breaking down the structure so it allows the transfer of electrons through.

5.2.4 *Learners' Mental Models of Covalent Bonding*

The interview data revealed that learners' view covalent bonding as the sharing of electrons, with secondary school and undergraduate learners relating this specifically to the octet rule of full-shell stability. However, postgraduates used a number of concepts from other bonding or atomic models, typically describing the octet rule, but drawing on concepts from other models when their explanations broke down. Natalie did not describe the bonding in molecular

iodine (I_2), choosing instead to draw a picture of the bonding in molecular chlorine (Cl_2) (Figure 5.4) because it was more familiar.

Interviewer. I just wondered if you could explain how you understand the bonding in iodine.

Natalie. Covalent bonding is between elements. Each one atom is bonded to another iodine because it's a diatomic molecule. So iodine is bonded to iodine.

Interviewer. In what way is it bonded?

Natalie. They share electrons, covalent bonding is like where instead of one atom like giving up its electrons to the other and the electrons being free, they share the electrons. So that they will have the electron configuration of the of the nearest atom.

Interviewer. Would you like to draw how you see the bonding between the iodines?

Natalie. Between iodines? [respondent laughs, begins drawing] Oh it's easier with chlorine [respondent laughs]. There's two chlorines, and you have their electrons in each atom so they, share one of their electrons with the other so that they each have, they are stable when they are sharing the electrons.

Interviewer. You have drawn those electrons differently, or you have indicated them differently. Is there any difference between them?

Natalie. No there's no difference. It's just distinguishing them each one belongs to the other one so the electrons can be like in any position at any time, but each one has eight, so that makes the bond sharing electrons.

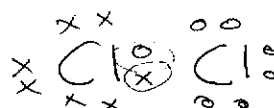


Figure 5.4 Natalie's drawing illustrating the bonding in molecular chlorine (Cl_2).

Natalie's description revealed a good appreciation of the octet rule. Furthermore, she used symbols (i.e., small circles and crosses) to identify the origin of electrons as an aid for electron counting, but realises that they are not different. It appears that Natalie felt more comfortable explaining the bonding in Cl_2 because this element was already familiar to her. However, this does not seem to have impacted negatively on her understanding, and her explanation is equally consistent with I_2 . Perhaps this instance emphasises how learners like to relate unknown concepts to existing mental models.

Mike was more explicit in his model description and drawing (see Figure 5.5), specifically relating the bonding in I₂ to the octet rule.

I know they are a bond, but I have to generally I think of it just in terms of the octet rule. I know it doesn't fit, oh yes it does sorry. Where you have got an iodine with the electrons you don't just draw an iodine nucleus just represented by the iodine [drawing I], with the valence electrons surrounding it. You've got one unpaired electron, and then you've got another iodine with seven electrons, valence electrons, surrounding it.

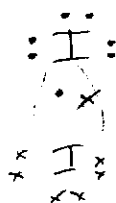


Figure 5.5 Mike's drawing illustrating the bonding in molecular iodine (I₂)

Rosalie, despite showing some uncertainty over terminology, also preferred using the octet rule as indicated by her statements and drawing (Figure 5.6).

Rosalie. This is the outer shell, I am just drawing the electron pair, shares, it's the same as the chlorine outer shell. It wants to contain one more electron in terms of electron pairs. It can share it with another iodine.

Interviewer. Can you tell me how many electrons?

Rosalie. Eight. There's eight each. Eight because that's what we were told [respondent laughs]. Eight because it creates the, I don't know the right terminology. It's creating a balanced type of formation, the electron formation. That's why there's eight. But in this case, if one iodine nucleus gets close enough to another iodine nucleus, they can actually share electron from each, creating a balanced outer type shell, a stable type configuration...I mean you've all your inner shells here as well [draws circles around I symbols].

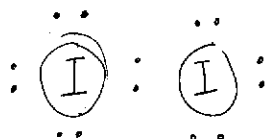


Figure 5.6 Rosalie's drawing illustrating the bonding in molecular iodine (I₂)

Nigel also stated that covalent bonding results from the sharing of electrons. However, his drawing of the bonding in I_2 appeared to indicate that he has confused molecular orbitals and shells. Nigel was comparatively unresponsive about covalent bonding, but seemed to believe that the valence or outer shell electrons were important as illustrated by his response and drawing (Figure 5.7).

Nigel. Yeah I just again see it as two iodines, sort of spheres [drawing] and each is just contributing electrons so you get an overall sort of shape, so each of the outer shell electrons is just interacting with each other.

Interviewer. OK. In the model you have drawn here, what's actually holding the iodines together?

Nigel. It's the electrons [draws two crosses between I symbols].

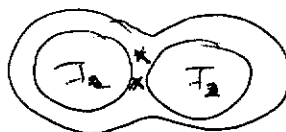


Figure 5.7 Nigel's drawing illustrating the bonding in molecular iodine (I_2)

John did not identify with the octet rule in any way. He seemed to hold a mental model that comprised a mixture of a simple model like the octet rule in which bonding occurred by sharing of electrons, with aspects of molecular orbital theory such as the delocalisation of electrons (Figure 5.8).

If you were to say look at two individual iodine atoms that were adjacent to each other. Because they've got a whole lot of electrons, you've got big electron clouds the further you get away from the nucleus. The weaker electrons are attracted to the nucleus, and the attractive the attraction of the adjacent nucleus is enough to basically pull the electron off the adjacent iodine. So if they are all next to each other, they will actually start to share the electrons from each other and that just basically forms a big cloud of electrons around it [draws circle around I—I]. You'll have say two electrons in it say [draws e^- and dots]. But in general the two electrons, one from each iodine will be almost likewise between the two iodine atoms. They can be anywhere within that localised area at any one particular time [indicates between iodine atoms in Figure 5.8].

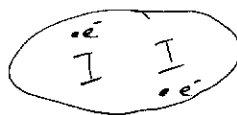


Figure 5.8 John's drawing illustrating the bonding in molecular iodine (I_2)

Model choice for covalent bonding given the prompt of focus card CB01 (p. 81), was uniform; four learners indicated a preference for B, a representation of the Lewis structure for the hydrocarbon benzene (C_6H_6). Unlike the metallic and ionic bonding focus cards (MB01, p. 79 & IB01, p. 80), for covalent bonding the focus card (CB01) did not contain depictions that were particularly realist in appearance—the closest being D which comprised a diagram based on the molecular orbital model boundary surface representation (see, e.g., Appendix A, Figure A28, p. 352). In this instance, learners did not chose depiction B because it was a more accurate representation for benzene; rather they simply considered it was familiar or more convenient to draw. Although learners expressed greater preference for depiction B, their explanation and understanding of this representation was incomplete as seen in Mike's response.

Mike. You've got six carbons in a hexagonal planar formation with six electrons whizzing around in the middle with an electron cloud in the middle. Each one has contributed one electron to it.

Interviewer. To what?

Mike. Carbons each one of the carbons.

Interviewer. The circle on that diagram B what does that mean to you?

Mike. Just indicates that there's, the circle just represents the fact that there's no specific bonds. Each of them forms a sort of half bond with the other carbons so each of them is uniform. So its not like two bonds up there, and two bonds down there. It's like a sort of hazy one and a half bonds up there and down there.

Rosalie also used multiple models for the bonding in benzene and, like Mike, her explanation was somewhat informal (see Figure 5.9). She introduced the term "resonating bonds" from Lewis theory, but her explanation of resonating bonds was drawn from molecular orbital theory.

Interviewer. What does B indicate to you about the structure?

Rosalie. The resonating bonds.

Interviewer. What do you mean by resonating bonds?

Rosalie. You see, in inverted commas, only one σ bond, and half a π bond between them. I can remember, the single line [drawing part of benzene structure], and like the dotted line [adding dotted line]. I think the single one is the σ and the dotted one is the π bond.

Interviewer. What do you mean by the dotted one?

Rosalie. It's only a half, it is only a half bond in between any two particular C's. But this half type bond can resonate backwards and forwards creating a full bond, so therefore still creating a, I don't know how to say it. It's still keeping the C happy [respondent laughs]. It's still got its four bonds [respondent laughs] with the hydrogen included. Does that make sense? [respondent laughs]. The C is really happy now [respondent laughs].

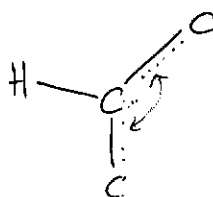


Figure 5.9 Rosalie's drawing of a portion of the benzene ring

Depiction B in CB01 (p. 81) appealed to John, and he related this depiction to molecular orbital theory.

Interviewer. What does B indicate to you about the bonding in benzene?

John. Adjacent carbon atoms, and to a hydrogen atom, and that's just basically a shared electron thing. So carbon A will share one electron with carbon B, and that carbon B will re-share one electron with him. So each bond has two electrons in it. What the actual ring in the structure tells me, is that you've got the π -electrons and these π -electrons are all equally shared between all six carbon atoms. The electron cloud, or the donut, or whatever you want to call it, consists of six electrons, and they are equally shared, there's no favouritism.

Natalie was the sole learner to prefer depiction C, chosen because, in her view, it provided more detail.

I prefer C. When I'm trying to figure out the bonds in between atoms. A I prefer, if I just had to draw it simply. But if I had to figure out what where the double bonds and where the hydrogens are, then I use C, 'cos it shows where the bonds are, what's connected to what.

It is interesting to consider why, in particular, the undergraduate and postgraduate learners overall retain simple mental models for chemical bonding. In one statement John, one of the PhD learners, related his views to a desire to gain what he perceived as practical skills from his university studies.

Interviewer. What stimulated you to come to Curtin?

John. Because it was a more hands-on course, Curtin is a lot more practical.

John reinforced this view in later conversation when prompted about the term antibonding which he introduced during a discussion regarding the bonding in benzene.

Interviewer. You mentioned before antibonding. Would you just like to tell me what you mean by that?

John. All I remember is that they are silly things that stick out either side. I couldn't really understand or fathom them. That's just how it is. That's how I remember the antibonding things. I mean just drawing your diagrams you've just got to remember your antibonding. You have your bonding and you have antibonding orbitals. Antibonding orbitals are just there because they are there. That's all it is. I didn't really understand why they are there, just there so the numbers balance.

It seems that John at least is interested in theoretical aspects of bonding models, only if they have a practical application.

5.2.5 *Learners' Use of Analogy*

Learners made surprisingly little use of analogy during their explanations possibly as a result of the relatively structured interview protocol. Such a structured protocol may have meant that learners first response was to rely on memory recall of target models that they had encountered during instruction. However, the use of common substances and events as prompts was intended to reduce the likelihood of learners viewing the interviews as a form of oral examination. The sea of electrons model is analogical in nature and so learners choice of this model does represent an example of analogy use. The preference

shown for this model may be related to the advantages of analogy use detailed in Chapter 2 (pp. 36-37). Learners only generated analogies to explain chemical bonding when they were struggling to explain a particular target model.

Natalie generated two analogies to help her explain the lattice structure of sodium chloride. As shown by her explanation and drawing (Figure 5.10) she likened the ionic lattice of sodium chloride to compass points and noughts-and-crosses.

Natalie. OK it's like this, with ions sort of arranged in rows and they will be attracted to those [indicating positive and negative symbols]. It's like noughts and crosses [respondent laughs, draws two rows of alternating noughts and crosses], and that continues in three-D. There are really strong bonds, 'cos the electric charges are attracted to each other.

Interviewer. You said in three dimensions. Would you just like to expand on that a little bit, tell me a little more about that?

Natalie. I mean it's [drawing double-headed arrow at an angle through lattice] like each ion is surrounded on every side like a compass point.

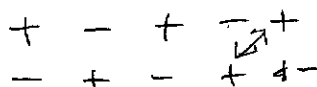


Figure 5.10 Natalie's noughts and crosses analogy for the bonding in sodium chloride (NaCl)

Mike also drew an analogy during his explanation of the conductivity of molten sodium chloride (IB02, p. 80), where he introduced the ball-and-stick model, and "clumps" of electrons.

Mike. With the crystal, I tend to go into the ball-and-stick thing again.

Interviewer. Alright.

Mike. The idea that I have got is clumps. That's where I get the idea that the electrons would be very tightly bound.

Interviewer. Right.

Mike. Because I do view them as separate balls generally with a crystal structure it makes it easier to visualise.

Interviewer. Can you just tell me what you mean by clumps?

Mike. Just like identifiable atoms. I know that the electrons are in a very close. The electrons are shared, and they are very close

together. I just tend to think of them as separate balls. As individual atoms with a single bond just between them. The bonds are just a line effectively.

John generated an analogy during his explanation of the difference in conductivity between solid and molten sodium chloride (IB02, p. 80).

Interviewer. Why do you think it's not conducting in the crystal, the solid crystal?

John. There's nothing to carry the electrons. The atoms are already in there. They are already fixed. They need some pathway for the electrons to transfer. So it's a fixed solid structure. It's like trying to walk through a door when it's locked. You just can't do it, but if the lock's busted you can go through.

Overall learners across all academic levels made use of analogy to aid their explanations of their mental models and to explain events depicting model use.

5.2.6 *Learners' Alternative Conceptions for Chemical Bonding*

A number of alternative conceptions were revealed in the pilot study. Despite having drawn reasonable three-dimensional lattices when discussing ionic bonding, a number of learners appeared to hold the alternative conception that metals or ionic compounds were molecular in nature. Rosalie described the bonding in aluminium foil and seemed confused about the continuous nature of metallic lattices as illustrated by her drawing (see Figure 5.11) and her statement that "my mind tells me the bonds exist internuclear, so between the intermolecular is between the molecules the electrons are flowing fairly freely through the system".

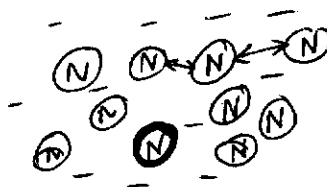


Figure 5.11 Rosalie's drawing illustrating the bonding in aluminium foil

Again Rosalie, comparing the bonding of an ionic compound sodium chloride (NaCl) with the giant covalent network silica (SiO₂), seemed to be confused about the bonding. Her explanation seems to indicate that she views sodium chloride as molecular in nature, because when asked " why do you think then the sodium chloride is crushed and the silica isn't?", she responded "because the intermolecular forces between the bonds of sodium are less than that of the silica". It is possible that this statement by Rosalie about intermolecular bonding in a giant covalent network, and her similar statements about the bonding in aluminium, simply represents semantic confusion. Mike also seems confused about the continuous nature of the bonding in ionic and giant molecular covalent substances. Mike's statement seems to confirm this alternative conception when comparing the bonding in molecular iodine with that of the ionic compound sodium chloride "with sodium chloride there is a specific sodium to chlorine bond". Mike also seemed to confuse the bonding in aluminium co-ordination compounds with metallic aluminium. He stated "I think of aluminium with three bonds" and his initial drawing (upper part of Figure 5.12) also suggested he considered there was a directional component to the bonding. Upon reflection he produced a second diagram which was more in accord with the sea of electrons model (lower part of Figure 5.12). However, he introduced as second alternative conception confusing aluminium ions with nuclei "for the metallic bonding I think of nuclei".

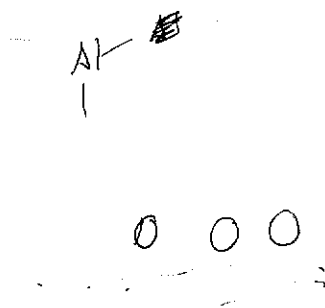


Figure 5.12 Mike's drawing illustrating the bonding in aluminium foil

Confusion about nature of the bonding in some covalent substances was also evident in learners' responses. Rosalie, for example, when describing the bonding in chloroform (CHCl_3), seemed to think that the bonding involved the transfer of electrons.

The covalent bond between the carbon atom or ion, means there is one electron from the carbon atom going to the chlorine. I mean it doesn't it doesn't actually go to the chlorine. The chlorine is attracted to the carbon to form a stable outer shell. The carbon is going to donate it by giving it up.

Linda also was confused about the nature of the bonding in chloroform, and, like Rosalie, seemed to believe that covalent bonding involves electron transfer. In response to a question about single lines between carbon and chlorine in her drawing she stated " they are just an indication of a bond. Rather than indicating that all the electrons are transferred, it's just indicating that there is a bond between the chlorine and the carbon and the hydrogen".

Confusion about the nature of charged species also was evident when Rosalie (Figure 5.11, p. 121), like Mike, described the bonding in aluminium and appeared to confuse nuclei with ions.

Well obviously the nuclei are charged. To me that defies the law of how it should work. You would think that one nuclei which would have a positive charge is bound to a nuclei which would have a positive charge as well [drawing]. Why should positive attract positive? Positive can attract positive because of the delocalised electrons, so therefore the bonds can occur between the two nuclei.

Confusion regarding the relative size of cations and anions also was evident. When discussing the bonding in lithium chloride (LiCl), Rosalie seemed unsure about ionic size of lithium and stated that "lithium would be larger".

There was some evidence that learners held anthropomorphic beliefs about aspects of chemical bonding. The ubiquitous use of the terms such as shell, shells, share, and sharing, in relation to, covalent bonding particularly, may mean that it is inappropriate to consider their use as evidence of anthropomorphic

beliefs. Nonetheless, the target system covalent bonding engendered the most anthropomorphic language as illustrated in the following responses.

Linda. Chlorine is in group seven. It will want to want to give an electron to chlorine. In ionic bonding lithium will want to give an electron to chlorine, it will just give it away [respondent laughs].

Nigel. Each of the outer shell electrons is just interacting with each other. One sort of grabbing onto each other.

John. Methane carbon doesn't want to give his, he doesn't have a big electron cloud, he's not going to share it around. So he's going to keep it to himself. Therefore there is going to be less interaction between individual methane molecules because there is, there is none of this sharing of electrons sort of thing. Whereas like say the tin, he plays more friendly with his mates. So he'll share it around.

John. Well they won't come right up close to each other 'cos they will repel. But they can get to a certain distance where they're happy at that distance apart. There's no repulsion, they're attracted to each other they can only get so close before the repulsion of the electron clouds kicks in. They just hold each other basically at a set distance.

5.3 Implications of the Pilot Study for the Main Inquiry

The purpose of the pilot study was three-fold. First, it was intended to see if the interview protocol would adequately address the research goals. Part of this aim was to see if it was feasible to evaluate learners' understanding of target models using the criterial attributes. Second, it was desirable for the researcher to trial the qualitative clinical interview. Finally, it was of interest to establish the duration of the interviews, least they be too long causing stress for learners and interviewer.

There were a number of beneficial outcomes from the pilot study for the main inquiry. Some simple practical changes were found to be necessary. For example, the pilot study revealed that one sample of an ionic compound magnesium sulfate (MgSO_4), was unfamiliar to some learners. This substance was chosen deliberately, as it was thought that a common household material, also known as Epsom's salt, could potentially provide access to learners' worldviews. However, as a result of the pilot study, lithium chloride was used in

the main inquiry, which whilst not a common household chemical, was found to be more familiar to these learners of chemistry.

The interview protocol comprised three phases for each of the three target systems, metallic bonding, ionic bonding, covalent bonding (Table 4.1, p. 77). Variations within the three-phase protocol were trialed during the pilot study. The first protocol used comprised the following overall sequence:

- | | |
|----------------|---|
| <i>Phase 1</i> | Shown focus card showing ways in which the bonding has been depicted— <i>which of these models appeals most/least to you?</i> |
| <i>Phase 2</i> | Shown sample of metallic, ionic or covalent substance— <i>please describe the bonding in this substance</i> |
| <i>Phase 3</i> | Shown IAE focus cards depicting events relating to model use— <i>please explain this process</i> |

On reflection and examination of transcripts, it was felt that this protocol which offered learners a choice of models prior to eliciting their views, could influence later responses, for example, when they responded to IAE cards. Hence, the order of presentation of the three-phase protocol was altered to:

- | | |
|----------------|---|
| <i>Phase 1</i> | Shown sample of metallic, ionic or covalent substance— <i>please describe the bonding in this substance</i> |
| <i>Phase 2</i> | Shown IAE focus cards depicting events relating to model use— <i>please explain this process</i> |
| <i>Phase 3</i> | Shown focus card showing ways in which the bonding has been depicted— <i>which of these models appeals most/least to you?</i> |

The principle difference between these two protocols is that in the second, the learners' views were elicited in a more open-ended fashion *before* any of the target models were introduced. This appeared to be a more effective strategy; however, some flexibility was still necessary. For example, it was evident in some interviews that learners possessed no clear mental model for a given target system. On occasions when this occurred, some learners became slightly distressed. Hence, in the main inquiry, an alternative strategy was adopted. If the

learner did not appear to possess a mental model for a particular system, the protocol was varied; typically this involved reverting to the initial protocol which entailed prompting learners with the card showing *Ways in which the bonding has been depicted* (i.e., MB01, or IB01, CB01). If this failed to stimulate recall, the interviewer simply moved onto the next target system. It is evident that this may have influenced later choices or answers to IAE probes. However, on balance it was decided that it was more important to reduce stress on participants.

The second major purpose of the pilot study was to see how practical it was to refer to the criterial attributes as the interviews were in progress. As described in Chapter 4 (pp. 93-94), once learners had identified a particular target model, the intention was to probe their understanding of these models in depth using the criterial attributes. To facilitate this, an interviewer prompt-sheet was prepared. This prompt sheet contained lists of criterial attributes of all of the target models on one sheet. For example, for the target system covalent bonding, the original prompt sheet contained lists of criterial attributes for the octet rule, the valence bond approach, the molecular orbital theory, and the ligand field theory. This procedure proved too complex, as it was difficult to easily locate the desired set of criterial attributes while the interview was in progress. Hence, a simpler system was developed in which an individual prompt sheet was prepared for each target model. Thus, when a learner began to describe a given model, for example, the octet rule for covalent bonding, this sheet was retrieved and the criterial attributes for model were checked off as the interview progressed. The latter interviews in the pilot study were conducted using this revised protocol and proceeded more smoothly. Because learners sometimes changed their target models during the interview, some flexibility was necessary. If learners introduced a second target model, the interviewer then retrieved the criterial attributes for this model and attempted to evaluate the learners' understanding of the second model. On occasions, a learner introduced a further

model late in the interview. In these instances, typically no further probing was conducted due to time constraints.

Repetition of interviews enabled the interviewer to become more organised in the presentation of samples and IAE cards. This proved highly beneficial and the value of this experience should not be underestimated. When the logistics of the protocol ran smoothly, the interviewer was able to concentrate on probing learners' views—a task much facilitated when not interrupted by trying to locate prompt cards or samples. In addition, as more interview experience was gained, better concentration was maintained, and there were fewer incidences of inappropriate questioning, for example, the use of leading or dichotomous questions.

The duration of the interviews was also of interest. The three-phase interview protocol for each of the three target systems is quite complex and it was possible that, for example, for secondary school learners long interviews may prove too demanding. This did not occur to any significant extent. The interviews ranged in duration from 30 to 90 minutes. There did not appear to be any link between the educational level and the duration of the interview. The main factor influencing duration of interviews was the verbosity, or otherwise, of the individual learner. This appeared to be mostly related to their personalities, for example, the interview with Rosalie, the most confident and out-going of all participants in the pilot study, was by far the longest. The only implication of long duration interviews, was for the interviewer—it became difficult to concentrate if the interview went beyond 90 minutes.

5.4 Summary

This chapter provided a description of the pilot study. A discussion of the results was followed by a discussion of the implications of the pilot study for the main inquiry.

Chapter 6 comprises a description of the first part of the data collection for the main inquiry and addresses the first research goal for the inquiry—learners' preferred mental models for chemical bonding.

CHAPTER SIX

RESULTS AND DISCUSSION:

LEARNERS' MENTAL MODELS OF CHEMICAL BONDING

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CHAPTER SIX
RESULTS AND DISCUSSION:
LEARNERS' MENTAL MODELS OF CHEMICAL BONDING

Overview of the Chapter

This chapter comprises a description and discussion of learners' preferred mental models for the target systems of chemical bonding. The chapter begins with a detailed description of the sample followed by the results of the data collection for the three target systems, namely, metallic, ionic, and covalent bonding. Each target system is described in turn beginning with a summary of the learners' mental models, followed by an analysis of their mental models by reference to the criterial attributes.

6.1 Sample Description

6.1.1 Sample Selection Procedure

The sample chosen for the inquiry comprised eight learners from each of secondary, undergraduate and postgraduate educational levels. All learners were approached only after approval was obtained from senior administrators of the learning institutions involved by written, rather than verbal, means (see, Chapter 4, p. 103). Learners were chosen purposefully to ensure an even gender mix and spread of academic abilities.

6.1.2 Secondary School Learners

The secondary school learners formed two cohorts—four females and four males. From the females' school, Anne was a 17 year-old female of Samoan-European ethnicity. She enjoyed chemistry, was a better than average chemistry achiever in her school, and contemplated a career in medicine or the sciences. She had conducted some peer-tutoring for Year-12 chemistry and science students. Anita, a 17 year-old European, was an academically low-achiever. She described

herself rather disparagingly and appeared to have quite low self-esteem. Nonetheless, she enjoyed chemistry as well as physics and biology. Anita's future career plans were rather uncertain, but options considered included food technology and primary science teaching. Claire, a mature 17 year-old European, was confident and outspoken with a strong academic record in chemistry and the sciences. She had carried out some peer-tutoring, although not in the sciences. Her future plans included a career in engineering, applied science, or a technology-oriented field such as biotechnology. Frances also had a confident outgoing personality, was an 18 year-old high achiever of European extraction, who had definite plans to take up a career in medicine as a first preference, followed by forensic science. She had done no peer tutoring.

The male secondary school learners were, in general, less confident and outspoken than their female counterparts. Neil, an 18 year-old European, was the most confident of the male secondary school level learners and was the top chemistry student in his school for Year-12. Neil enjoyed chemistry, found it easy, and was active in youth group support activities including peer-tutoring in science and mathematics. However, he did not contemplate a career in the sciences; rather his career aspirations were in the humanities or media studies. Keith, a less confident 17 year-old European, was an average academically achieving performer in the sciences and chemistry. He was not keen on chemistry, was interested in a career in law or commerce and had done no peer-tutoring. David was a quiet 18 year-old European male, and an average academically achieving performer in chemistry and the sciences. He enjoyed chemistry and anticipated taking up a career in engineering. He had conducted some informal tutoring of a sibling for Year-11 science and mathematics. Richard, also 18 years old and reasonably outgoing in nature, described himself as a New Zealander and did not identify with any ethnic group. A below average academically achieving performer in chemistry and science, Richard, did not enjoy the quantitative side of science. He expressed interest in environmental resource planning and contemplated a career in the resource

management area. Richard, like David, had conducted some informal science tutoring, in his case for a Year-11 sibling.

6.1.3 Undergraduate Learners

The undergraduate learners were BSc (Technology) chemistry majors in the Department of Chemistry at The University of Waikato based in Hamilton. Because the interviews for undergraduates were conducted late in the year after the completion of lectures, undergraduate learners had, at a minimum, completed two years of tertiary chemistry instruction. The BSc (Technology) degree is a co-operative education degree that integrates industrial work experience with academic study (Coll, 1997b). Learners universally indicated that they were committed to a career in chemistry and had chosen to study chemistry via this degree in particular, because they perceived their career prospects would be enhanced.

There were two male and two female second-year undergraduate participants in the inquiry. Bob and Steve were both 19 year-old New Zealanders of European extraction. Bob described himself as *Pakeha*, a somewhat ill-defined Maori term, generally taken to mean a white New Zealander, namely an individual of European origins. A little below average academic ability, Bob was talkative, although lacking in confidence, he was keen to be involved in the inquiry and was interested to know "how he had done" during the interviews. Steve, by way of contrast, a much more reserved individual and an outstanding academic achiever, was very measured and thoughtful in his responses. Both learners stated that they enjoyed chemistry and Bob indicated that he had done some peer-tutoring. Whilst not ruling out postgraduate studies, he intended taking up a career in industry. Steve indicated he had done no tutoring and intended pursuing postgraduate studies to the doctoral-level. Reneé, 20, and Kim, 19, were second generation New Zealanders that were ethnic-Chinese females with no obvious English language difficulties. Reneé was a highly academically gifted student with an out-going and talkative personality. On the other hand, Kim, was of average academic ability and was more reserved and hesitant. Reneé was completing a chemistry-biology double major and had not ruled out postgraduate studies, whereas Kim contemplated a

career in a chemical industry. Neither had conducted any tutoring to any extent though both reported conducting some informal high school tutoring in non-science topics.

There were two male and two female third-year undergraduate participants in the inquiry. Alan and Phill, 21 year-olds of average academic ability, both described themselves as Pakeha, were a little reserved, and claimed that they enjoyed chemistry. Alan, but not Phill, had done some informal peer-tutoring in science at high school. Jane and Mary, both 21 year-old females, described themselves as European. Jane, a student of high, though not outstanding, academic ability, was less confident although she spoke freely enough. Mary, a student of average academic ability, was more outgoing but lacking in confidence. Mary had not been involved in any tutoring, whereas Jane had been involved in informal peer-tutoring in science at high school.

6.1.4 Postgraduate Learners

The postgraduate learners, four PhD candidates and four MSc level candidates, were high academic achievers—a reflection of the entry requirements for postgraduate study at Waikato. In spite of this, there was a considerable spread in academic ability within this cohort, with some learners possessing outstanding academic records in their Masters level examination results. Like the undergraduates, these postgraduates enjoyed chemistry and were committed to careers in chemistry. All MSc candidates were purposefully chosen from the second-year class. The intention was to distinguish these postgraduates from final-year BSc learners: this selection criteria ensured that the learners had completed all of their MSc papers.

There were two male and two female MSc candidates involved in the inquiry. James, a 24 year-old European MSc candidate, had an outstanding academic record. He was a late starter in his chemistry career as a result of nearly completing an undergraduate degree in the humanities at another New Zealand tertiary institution. James was in the final stages of the write-up stage of his MSc at the time of interview. His research topic was concerned with organometallic

syntheses and aspects of theoretical chemistry pertaining to chemical bonding. This research involved performing sophisticated quantum mechanical calculations of electronic structure. In addition to undergraduate laboratory supervision common to all MSc candidates, James had conducted first-year and third-year tutorials in chemistry along with some private tutoring. James appeared quite relaxed and despite his extraordinary academic record, he came across as rather diffident; his responses were often limited and it proved rather difficult to probe his understanding. Brian, a 23 year-old European second-year MSc candidate, possessed a good academic record having completed his BSc (Technology) degree at Waikato, and spent his industrial placement at a pesticide manufacturing plant in Great Britain. His MSc research topic was concerned with an investigation of components of red wine. Brian, although a fairly quiet individual, proved a thoughtful respondent. Jenny, a 22 year-old European female, completed her BSc (Technology) degree at Waikato, was of average academic ability and possessed a bright out-going personality. She had carried out an industrial placement in the wood chemistry area and continued on with this work into her postgraduate studies, enrolling in an MSc (Technology) degree. Jenny seemed a little under-confident at times, often speaking quickly, only to modify her statements later. Rose, a 21 year-old European MSc candidate, completed her BSc at Waikato, had a good academic record, and a quiet personality. Her MSc research topic was concerned with mass spectromeric investigation of bismuth anti-ulcer drugs.

There were two male and two female PhD candidates involved in the inquiry. Jason, a 26 year-old European, was a student of high academic ability who graduated with BSc and MSc (Hons) from Waikato. At the time of interview, he had just secured a post-doctoral research fellowship at a prestigious British university. His research area was concerned with organometallic syntheses and the mass spectromeric investigation of organometallic complexes. He was a relaxed and confident individual, with considerable chemistry tutoring experience, particularly at the first-year level. Kevin, a 23 year-old European, had just begun the first year of his PhD at the time of the interview. Kevin had completed a BSc (Technology)

degree at Waikato and had carried out a twelve-month industrial placement in Britain. His Waikato-based MSc (Hons) research topic was concerned with organometallic syntheses along with mass spectromeric investigations of a variety of organic and organometallic substances. Kevin's PhD topic was similar to his MSc study, but unlike other PhD learners, he had only helped out in second-year laboratories and had not conducted any tutorial sessions. Kevin possessed an outstanding academic record, achieving an MSc (Hons), and was a cheerful outgoing individual. Although he was sometimes hesitant, he seldom seemed at a loss for ideas and typically provided lengthy responses to questions and prompt cards.

Christine, a 27 year-old European PhD candidate, was in the final year of her PhD studies in forensic chemistry which involved the development of new fingerprinting substances. Her MSc (Hons) from Waikato involved the development of environmentally-friendly cleaning solutions for the dairy industry. Christine had a cheerful out-going personality, was somewhat under-confident, and seemed rather unhappy with some of her responses; she was one of the few participants to make significant further contributions to her transcript upon validation. Like James and Jason, Christine had extensive experience in first-year chemistry tutoring, particularly with *Chem-Help* tutorials, a bridging pre-entry course offered to students with a weak chemistry background. Grace, a 25 female year-old second-year PhD candidate, described herself as European; however, she had in the past expressed interest in applying for a *Tainui* Scholarship which is only available to students identifying themselves as of Maori ethnicity. She possessed a good, rather than outstanding, academic record, completing her BSc at Waikato, but her MSc in marine natural products chemistry at a tertiary institution in Japan. Her PhD research topic was concerned with the analysis of surfactants of importance to the agricultural chemical industry. Like the other PhD candidates, she had considerable chemistry tutoring experience and like, Christine, had been involved in *Chem-Help* tutorials. Normally a talkative out-going individual, she appeared somewhat subdued during her interview.

6.2 Learners' Mental Models for Metallic Bonding

The overall aim of this inquiry was to gain an understanding of learners' mental models for chemical bonding. The principal research goal for this inquiry as reported in Chapter 1 is:

To investigate if there are preferred mental models for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

Learners' preferred mental models for metallic bonding were probed using the semi-structured interview protocol described in Chapter 4 (Table 4.1, p. 77). For metallic bonding elicitation of learners' views comprised five tasks (Table 6.1).

Table 6.1 Interview protocol for the target system metallic bonding

-
1. Shown sample of aluminium foil—*please describe the bonding in this substance*
 2. Shown sample of steel wool—*please describe the bonding in this substance*
 3. Shown focus card MB02—*please explain this process*
 4. Shown focus card MB03—*please explain this process*
 5. Shown focus card MB01—*which of these models appeals most/least to you?*
-

Learners were presented with a sample of aluminium foil and steel wool and asked to describe the bonding in these substances. Subsequently, learners were shown focus cards MB02 and MB03 (p. 79) and asked to explain the event depicted on these cards. Finally, learners were shown focus card MB01 (p. 79) which contained depictions of the bonding for the metal lithium and were asked which depiction they preferred and which appealed least.

6.2.1 Secondary School Learners

The data for secondary school learners showed that six preferred the sea of electrons model, the remaining two learners possessed no single mental model. Neither Anne nor Anita appeared to possess any coherent mental model for metallic bonding, their descriptions consisting of listing macroscopic physical properties of metals rather than a description of metallic bonding. This aspect is illustrated by Anne's description of the bonding in aluminium foil, claiming that "it's held together quite strongly" but when asked if she had a model in mind of the way it would be held together she replied "Um...not really". In contrast, describing his mental model for the bonding in aluminium foil, Keith appeared to utilise the octet rule invoking the formation of covalent bonds. Having drawn two aluminium atoms (Figure 6.1) and describing the dots and crosses as electrons, he went on to state "the aluminium ion there needs three more electrons to satisfy its full outer shell so it's bonding with that which has got three full ones".

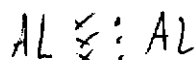


Figure 6.1 Keith's drawing illustrating the bonding in aluminium foil

The remaining learners described, or specifically referred to, the sea of electrons model. Claire, for example, whilst not explicitly identifying the sea of electrons model, drew and described a model that possessed the key elements, namely metal atoms or ions in layers and free electrons.

Claire: The electrons are all free, but the, nuclei are together.

Interviewer: Right.

Claire: I don't know, in layers or not, and the electrons are free between [drawing row of circles with + signs inside them, and surrounded by an ellipsoid] those sort of move around [draws curved lines from top to bottom of ellipse, Figure 6.2] which is why they conduct because the electrons are free to move and that's the current.

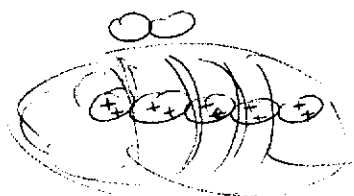


Figure 6.2 Claire's drawing illustrating the bonding in aluminium foil

Neil also viewed metals as containing "free electrons which can flow around metal atoms", but did not elaborate, claiming "it's like you have got like your little atoms in there, and the electrons they can flow around". However, the other secondary school learners specifically identified the sea of electrons model when describing the bonding in aluminium foil.

Frances. Mm...that's metallic, a sea of electrons.

Interviewer. Do just want to tell me what that means to you?

Frances. Um, what a sea of electrons really means to me? Well you can't really see, it's like they are all delocalised you can't really see where the electrons are.

David. The way I think of it is as metallic bonding 'cos we learnt it in chemistry, and I think the image I have got of that is just the metal with a sea of electrons, it's just how I think of it.

Interviewer. I am just trying to get an idea of what that actually means to you when you say sea of electrons. What picture do you have of that?

David. Oh just like, the sort of mental image I would have is like, sort of sandwich type thing.

Interviewer. Do you want to draw that, just so I am clear on what you mean.

David. Yeah sure [draws Figure 6.3]. I don't think I know if there is any stuff between the atoms.



Figure 6.3 David's drawing illustrating the bonding in aluminium foil

Secondary school learners were given the opportunity to choose a depiction of the bonding for the metal lithium (MB01, p. 79). Their choices of depicted models for lithium were overall consistent with their choice of model for the

aluminium foil prompt, with six learners choosing depiction B, a simple depiction of the sea of electrons model. It is interesting to note that learners like Anita who held no clear mental model for metallic bonding chose depiction B, whereas other learners like David who specified the sea of electrons model when describing the bonding in aluminium foil, did not choose B. Reasons for choice B were its familiarity and depiction of free electrons as summarised by Anita saying "that's how we normally see it textbooks, and the others basically look totally confusing". Two learners preferred choice D, with five learners in total indicating that D held some appeal. Choice D was seen as more realistic, showing the atom or ion arrangement more effectively with a three-dimensional image.

Claire. Because you can see that the electrons are all moving around, and they are not attached, and you have got the nuclei there. That one D is a good 3-D representation of how I sort of think the nuclei are arranged.

David. D, you can see the atoms there and how they are arranged.

Frances. You can really see the structure, whereas these [indicating A, B, and C on MB01, p. 79] are two dimensional and you can't understand the lines.

Learners' responses when probed as to the depiction that held least appeal were more brief. Depiction C was, perhaps not surprisingly, the least appealing, typically because it was unfamiliar or considered unclear, as stated by Richard—"I don't know what's going on there. It's just not clear", and David, "it doesn't have any resemblance to what I think an atom would be".

6.2.2 Undergraduate Learners

Undergraduate learners shared similar views to their secondary school counterparts, with four learners, Steve, Alan, Reneé, and Jane, specifying the sea of electrons model for metallic bonding. In contrast to the secondary school learners, as might be anticipated, undergraduates who chose the sea of electrons model, provided relatively detailed explanations as illustrated by Steve's verbal and written response (Figure 6.4).

I will just draw this [draws rows of Al^+ inside circles with negative signs also inside circles in other rows]. So you have got a system. This is a row of monovalent cations, cations in a delocalised sea of electrons [around it, and that's the metal bonding [drawing lines linking negative charges with Al^+]]. Metallic bonding you get from metals like aluminium.

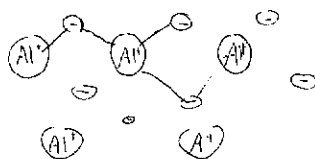


Figure 6.4 Steve's drawing illustrating the bonding in aluminium foil

In his drawing of his model shown in Figure 6.4, Steve appears to indicate that there are bonds between electrons and aluminium atoms. However, upon probing he was able to explain the origins of the attractive forces within the metallic substance in a manner consistent with the scientific view (Appendix A, p. 319).

Interviewer. What's actually holding that together?

Steve. Well it's the electrostatic forces of attraction between cations, the aluminium cations and the electrons. So they form a sort of network of attraction.

The remaining undergraduates held a variety of mental models for metallic bonding. Kim, like the secondary school learner Keith, viewed the bonding in aluminium as covalent in nature, although she seemed rather uncertain about her explanation.

Kim. It would be like Al sort of thing [drawing Figure 6.5].

Interviewer. So you have just drawn some Als there with a couple of dots between them.

Kim. Yeah.

Interviewer. Do you just want to tell me what that's meaning to you.

Kim. Well the bonding between them, that covalent sort of thing metallic bonding actually. I dunno [respondent laughs].

Interviewer. OK you said covalent, and you said you see these as covalently bonded together. Is that what you are saying here?

Kim. Yeah [respondent laughs].

Interviewer. OK, you also said metallic bonding. Are they the same here?

Kim. Um, isn't metallic bonding the same as covalent?



Figure 6.5 Kim's drawing illustrating the bonding in aluminium foil

Three learners, Phill, Bob, and Mary, had no clear picture of the bonding in metals, as typified by Bob's response.

Um, I honestly don't have much of an idea except that, in some way I see the atoms of the metal as being close together in regular fashion, they are bonded together, I don't know whether it's been that well explained to me.

Undergraduate learners' choice of depicted models (i.e., MB01, p. 79) were different to that of secondary school learners with five learners choosing depiction D, three B, and one A. Reasons for choices, likewise to secondary school learners, were the simplicity and familiarity of B, and the aesthetically appealing three-dimensional nature of D.

Interviewer. What's most appealing about B or what aspects of B do you like?

Phill. Just 'cos you can see it all quite simply.

Reneé. Ah because it looks more familiar to what we've read and seen at school, yeah.

Interviewer. Can you tell me what appeals to you most about D?

Bob. The packing together of the molecules in a regular fashion.

Steve. Well it's showing the lithium in a regular arrangement.

Depiction A was most disliked by five learners, because they saw it as inferring a molecular, rather than continuous structure.

Bob. Well it shows molecules, Li_2 molecules, which has been told to us don't exist.

Alan. It's showing like lithium-lithium type bonds and it's arranged as a diatomic crystal structure.

Interviewer. So why is that unappealing to you?

Alan. Um...well it's sort of like the sodium chloride pattern. I see the sodium chloride molecule as NaCl, but there's actually no such thing.

Interviewer. Oh yeah, OK. So that's sort of inferring?

Alan. Yeah. That you have an individual lithium-lithium molecule.

Choice C was disliked by two learners, and again, the reason given was its complexity, although it was evident that undergraduate learners, unlike secondary school learners, recognised that depiction C involved the molecular orbital theory. One learner, Mary, disliked depiction B, indicating that she found the diagram difficult to understand.

Mary. I don't really understand B [respondent laughs].

Interviewer. OK that's fine. Well I was just going to ask you which one of those appeals to you least?

Mary. Yeah probably B.

Interviewer. B is it?

Mary. Yeah I don't quite ah, yeah I can, I guess I take this as being lithium plus [taps circles enclosing crosses in depiction B of MB01] and I guess this is the electrons [indicates dots in depiction B of MB01], but I don't know why [respondent laughs], why they are all different.

Hence, overall undergraduates like secondary school learners preferred the sea of electrons model but differed in their choice of depicted models.

6.2.3 Postgraduate Learners

The preferred mental model for postgraduates was the sea of electrons model. Interestingly, whilst postgraduates in general provided more complete descriptions of their mental models than did their secondary school counterparts, two struggled. Grace appeared to possess no model for metallic bonding stating "I don't know" and Christine provided a rather vague description.

Christine. I think I don't actually think of them as being bonded.

Interviewer. OK.

Christine. I think of them as being just, I know they are not distinct species. I mean there is obviously a lot more than one atom.

Interviewer. Right, OK.

Christine. And I guess...I guess that's where the sharing of electrons comes back to. I prefer not, I wouldn't actually think of them as being strongly bonded together.

Although Christine was unable to produce a clear description of the lattice structure of aluminium during her interview, upon reflection she produced a diagram (Figure 6.6) during transcript validation reminiscent of the sea of electrons model.



Figure 6.6 Christine's drawing illustrating the structure of the aluminium lattice

Notwithstanding the comments about Christine and Grace, postgraduates descriptions of their preferred model more commonly incorporated less terminology from the analog domain, that is, the sea of electrons model. Postgraduates made greater use of nomenclature from instruction in chemical bonding, using concepts from other target models, such as electron cloud, molecular orbital as well as delocalisation, as illustrated by the following responses.

James. I think of metals as having lots of little positive centres, with delocalised electrons sort of flowing around.

Brian. OK well, the bonding in aluminium like all metals is, um, it doesn't involve direct bonds between atoms as such it just involves a collection of atoms held together with their own electrons being delocalised around and shared amongst the entire group.

Kevin. OK, the way I'd see aluminium anyway, would be metallic, well officially anyway. Metallic sort of bonding in which case the electrons are shared. You get electron clouds covering which help and also make it a metal as in the conductivity and that sort of stuff. So the way I'd really see it the, what makes it metallic is the fact that you have got

this, electron cloud. The electrons aren't specifically associated with atoms as such, they are generally shared around through the whole the entire system sort of thing that's the way I see the metals.

Jenny. The electrons from each atom are sort of surrounding the atom and then also like in way in a molecular orbital type way which they are surrounding the whole sort of cluster.

Postgraduate learners' choice of depicted models (MB01, p. 79) were similar to undergraduate learners. Six learners preferred choice D, one choice B and the other choice C. The usual justification for choice D was that the depiction was more useful in showing the arrangement of atoms in aluminium.

Kevin. As in the lithium, the metal side of the planes of the atoms. You have got the planes of atoms, the lattice sort of arrangement, which is what I automatically think of when I think of a metal, that sort of arrangement of atoms.

Although most learners chose D, the postgraduates were much more ambivalent about their choice, often changing their minds, typically evaluating the strengths and weaknesses of all choices extensively before settling on a final choice. Christine's response exemplifies this aspect of model selection for postgraduates.

Christine. Yeah, yeah, I don't like that sort of thing.

Interviewer. That's A?

Christine. I don't like A....I probably don't think of it as being like B either.

Interviewer. OK.

Christine. ...I probably yeah, I think I, aesthetically like D as well but I think C is, I don't really, I don't think of bonding because I know about orbitals and stuff like that.

Interviewer. OK.

Christine. I don't know if it's just a familiarity.

Interviewer. That's in relation to C. Is that what you mean?

Christine. Yeah. Like I wouldn't pick those two.

Interviewer. So you wouldn't pick A or B. Which one appeals to you most? It is D, is that right?

Christine. If I am looking at them straight, I'd say D and C. Like I see discrete atoms, but I know that's not, I'd probably think of that as single atoms, how they are packing.

Interviewer. Right, yep.

Christine. But C would be the actual bonding interaction in it.

Interviewer. Right, right sure. I understand what you are saying. So can you just tell me why you like D then? Start with D. D if I understand

what you said, you like D because it appeals to you, and you said that's how you see them packing is that right?

Christine. Yeah.

Interviewer. OK. So C, can you tell me what appeals to you about C?

Christine. Because it's to do with energy. Like you can see that, for instance, you've got your orbital for one lithium atom and you could have another one over this side [indicating RHS part of depiction C in MB01], and then you would combine to bring the energy down so that you would actually get an orbital where the electrons would go in.

Depictions A and C were most disliked for similar reasons as the secondary school and undergraduate learners, namely, the inference of molecularity in A and the complexity of C. It was, however, notable that dislikes, as for preferences, were more mixed, with learners overall more critical of the diagrams as typified by Jenny's response.

Interviewer. OK. Is there any one of those that particularly doesn't appeal to you?

*Jenny....*Ah I guess the first one, part A where they have two lithium atoms joined by a single bond it doesn't really appeal to me at all.

Interviewer. What aspects of that doesn't appeal to you?

Jenny. Well, it shows lithium as being two lithium's together, to be a discrete molecule which is, I know it doesn't happen. So it's showing definite bonds between atoms and that's not how I envisage lithium.

Here, rather than merely expressing preferences, postgraduate learners are clearly evaluating the depictions of bonding, indicating what they perceive to be limitations or alternative conceptions.

6.3 Learners' Understanding of Mental Models for Metallic Bonding

Learners' views of various aspects of their mental models were elicited during interviews and used to construct a description of their understanding of their mental models. Specifically learners' understanding of their mental models was probed by reference to criterial attributes for the sole target model identified, namely, the sea of electrons model. The criterial attributes for the sea of electrons model described in Chapter 4 (Table 4.3, p. 85) are reproduced in Table 6.2.

Table 6.2 Criterial attributes for the *sea of electrons* model for metallic bonding

-
- | | |
|----|----------------------|
| 1. | lattice structure |
| 2. | electron mobility |
| 3. | alloy-interstitial |
| 4. | alloy-substitutional |
-

The researcher monitored learners' descriptions of their mental model as the interview progressed. In many instances, learners made specific reference to criterial attributes spontaneously; if they did not, the researcher probed their views with specific prompt questions. For criterial attributes 1 and 2, most learners offered spontaneous responses, the results of which have been described above. For the remaining criterial attributes, 3 and 4, respondents were shown a sample of steel wool in order to probe their understanding of alloys.

6.3.1 *Learners' Views of Lattice Structure for Metals*

In addition to the more detailed explanations regarding their choice of mental model described in Section 6.2, undergraduate and postgraduate learners evidenced an understanding of the lattice structure and continuous nature of the bonding in metallic substances. Unlike secondary school learners, they typically drew diagrams showing lattice structures with little or no prompting. In contrast, some secondary school learners when questioned about the structure of the metallic lattice confused this with the electronic structure of aluminium, for example; to the question about what aluminium would be like on a very small scale Anne's response was "what do you mean, like the nucleus and the shells?". It appeared here that Anne has misunderstood the question. However, an attempt at clarification was no more illuminating. Keith likewise seemed confused by the question, again thinking of the electronic structure of the aluminium atom, rather than the lattice structure.

Interviewer. Do you have a picture in your mind of how the aluminiums would be arranged at all? Do you have a picture of that?

Keith. In the Periodic Table?

Interviewer. No sorry. If you are thinking of the atom as such.

Keith. Yes how they would be arranged like sort of the make-up?

Interviewer. Yes or organised or, no sorry I don't mean in terms of the atomic structure. I mean in terms of one aluminium atom next to another if you like.

Keith. Oh OK, I am not sure I imagine they are sort of...um...there must be something linking them together, some sort of bonding. It's probably metallic bonding, it must be metallic bonding.

Interviewer. OK that's fine. What does metallic bonding mean to you?

Keith. I am not sure [respondent laughs].

In response to the interviewer's question about what sort of picture in her mind she held for aluminium, Anita appeared to have no appreciation of the regularity of the metallic lattice, describing the lattice structure of aluminium as "a big mess". Some secondary school learners did show an appreciation of the structure and continuous nature of metallic lattices. Claire described the drawing she produced for aluminium, Figure 6.2 (p. 137), as containing layers.

Interviewer. Just looking at those rows you have drawn there, can you just tell me how you would expand that into three dimensions if you like. How would you see that being arranged in space.

Claire. Um...don't know, unless it's like layers on top of the other, like the graphite is sometimes drawn with the layers of carbon atoms but it'd have to be somehow so that the electrons can move around all the nuclei of the atoms.

Likewise, Neil stated that the lattice structure consisted of "just rows". Although these learners described the structure using terms such as row or layer, this does not necessarily mean they lack an appreciation of the three dimensional nature as evidenced by Claire's additional comment that the "layers [are] on top of each other".

Some undergraduates were rather vague in their descriptions of lattice structure. Kim for example, expressed a view of the structure (Figure 6.7) similar to that of secondary school learners describing the arrangement as consisting of layers.

Kim. Well aren't they structured in layers like [draws 4 circles in square pattern with lines linking them] that sort of structure?

Interviewer. OK so that's that cubic structure you have drawn there.

Kim. Yeah cubic.

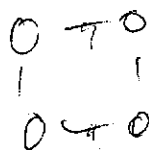


Figure 6.7 Kim's drawing illustrating the structure of the aluminium lattice

However, the descriptions of metallic bonding provided by undergraduate learners were more typically characterised by the spontaneous introduction of domain-specific terminology used for the lattice structure including close-packed, cubic close-packed, and hexagonal close-packed (Appendix A., p. 318).

Interviewer. So you see them [the aluminium ions] being arranged together somehow?

Bob. I know they are arranged because we have been told that anyway. Like close-packed, cubic-close-packed those type, those types of things.

Steve. Ah...well I suppose I picture them as being in a relatively regular sort of array. But I suppose it may depend upon probably the metal in question, but in a sort regular repeating unit of atoms, cubic or something like that.

Interviewer. OK so the atoms or nuclei you mentioned. Can you tell me how you see them organised in space?

Alan. Um, sort like the close-packed arrangement. Just a, layers.

Interviewer. So what does close-packing mean to you.

Alan. There's cubic close-packing, hexagonal close-packed, spheres.

Some undergraduate learners provided highly detailed descriptions, including discussion of lattice holes, and a description of the build-up of layers that results in the close-packed structures. The most comprehensive explanation was provided by Jane who went into considerable detail.

Jane. I mean you look at it and so you have got close-packed and like one series [draws three rows of circles, Top LHS Figure 6.8].

Interviewer. OK those circles what are they representing here?

Jane. I think of them as being like atoms, and then they are hard to draw that way...mm, and then you have got like the lattices and stuff [draws cluster of circles, top RHS Figure 6.8], and you have got octahedral holes and tetrahedral holes.

Interviewer. Just looking at those two diagrams you have drawn. On the left side you have got three rows and on the other side to that you have got, you have got something else, what's the difference between those two?

Jane. Yeah that's kind of like I was trying to show, that's looking up from the top or something and you have got like the hole [draws arrow pointing to circles, top RHS Figure 6.8].

Interviewer. OK so the one on the right is looking from the top is it?

Jane. Yeah, and then like you might have another layer underneath, but that's like hard to see and then you find that in the hole you like could have [draws four circles in diamond pattern and dotted circles overlying this, lower, RHS Figure 6.8], like you could have it, OK [respondent laughs].

Interviewer. I see that's those dotted ones you have drawn, that's the next layer underneath is it?

Jane. Yeah, and then there's like, you can imagine the hole being in there or something.

Interviewer. Right, what's the relationship of the hole, what's the significance of that?

Jane. It'd be like you sort of have another ion in there, or atom in there. I think, say like if you have like, I can't remember from last year, I think it's cubic close-packed, or what is it like [draws two rows of circles, lower LHS Figure 6.8], one, two, one, one, I've forgotten really.

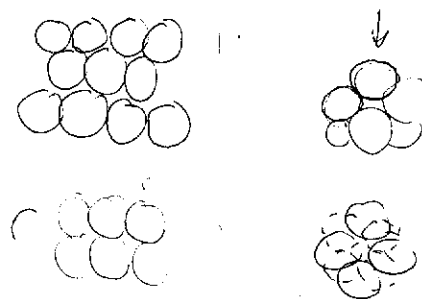


Figure 6.8 Jane's drawing illustrating the structure of the aluminium lattice

Similar to the undergraduates, postgraduates' explanations contained spontaneously introduced terminology specific to chemical bonding instruction such as cubic-close packing and hexagonal-close packing, as exemplified by Jason's explanation and drawing (Figure 6.9).

Jason. A whole lot of metal atoms basically all stacked as closely as possible together. There's a bunch of different metal structures like cubic and hexagonal close-packing and then the body-centred cubic, so basically all the metal atoms are as close together as they can possibly be.

Jason. I know that for example that you can have structures such as hexagonal close-packed and cubic close-packed which I am not sure I can describe. It's not until you get an actual model yourself and you can show that they are different and you can actually see they are different, but metals will hold to one structure or another.



Figure 6.9 Jason's drawing illustrating the structure of the aluminium lattice

Undergraduate and postgraduate learners' choice of models (MB01, p. 79) with structures that depicted three-dimensional lattices is consistent with their spontaneous descriptions discussed here and supports the view that they possess a greater appreciation of the continuous nature of ionic lattices. However, the greater aesthetic appeal of the space-filling type depictions also may have been a factor in model choice.

6.3.2 *Learners' Views of the Structure and Bonding in Alloys*

Across all three levels of learners, it was stated that the bonding in steel wool was essentially the same as in the pure metallic substance aluminium. Secondary school learners mostly failed to recognise that steel was an alloy containing iron as a base metal, with a variety of other metals substituted into the lattice, and also containing interstitial carbon as a hardening agent (Appendix A, p. 319).

Claire. It's metallic again. I don't see how it's different no.

Interviewer. So you wouldn't see that as different.

Claire. No, no.

Frances. It would be the same bonding because they are both metals so that still would have a sea electrons I am sure.

Interviewer. OK so you would see the bonding as much the same in the two?

Frances. Yeah, because they are both metals. So that's what comes to mind it would still have metallic type bonding.

Keith and David did identify steel as an alloy, and one form of alloy—a substitutional alloy, but failed to provide significant detail.

Keith. Yeah it'd have like different kinds of atoms in it I suppose, I dunno.

Interviewer. Do you have any thoughts in your mind what sort of atoms they might be?

Keith. I have no idea.

Interviewer. OK. You mentioned some other metals or other atoms present. Do you have a picture in your mind of what they might be?

David. ...Steel...you call them alloys, eh? Or something.

Interviewer. OK.

David. I think, I don't really know. They are not atoms themselves.

Interviewer. What does an alloy mean to you?

David. Um, like a mixture of metals.

More undergraduates than secondary school learners identified steel as an alloy but they were often vague about details. René and Steve both showed an appreciation of the interstitial nature of the alloy steel, René indicating that carbon is "in the middle" of the metallic lattice and Steve providing a little more detail

It being steel wool, I expect you would get an iron metal bonding system similar to the aluminium. But there would also be a certain amount of carbon in there as well mixed into the structure. So you would have [drawing Figure 6.10] sort of carbon atoms and the delocalised sea, sort of like that.

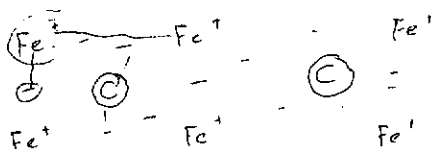


Figure 6.10 Steve's drawing illustrating the structure and bonding in steel wool

Alan showed an appreciation of the nature of alloys describing steel as a mixture of metals reminiscent of substitutional alloys. However, in his subsequent description he seems to have confused substitutional alloys with interstitial alloys, failing to appreciate that interstitial atoms are more commonly non-metals like carbon.

Interviewer. You mentioned an alloy here, can you just tell me what that means to you?

Alan. It'd be made up of two separate metals, that's in the steel.

Interviewer. How would you see the atoms of those different metals organised?

Alan. Oh, um, alternating...matrix I guess you could say, of the different metals.

Interviewer. OK, do you see any sort of order to that?

Alan. I suppose it would depend on the ratio of the two metals and the different sizes of the molecules, ah, the atoms.

Interviewer. Of the atoms, OK. So perhaps just think, if you had a big atom and a small atom do you have any views how you would see that organised?

Alan. Um, well you'd probably have the larger atoms surrounded by the smaller ones in a...it'd depend on the ratio of the smaller atoms.

Interviewer. So the ratio is that in terms of the amount of them is it [i.e., % composition], or the organisation?

Alan. No the organisation, I would say. Oh I suppose it would have to be the same wouldn't it?

Interviewer. I didn't automatically assume what you meant by ratio numbers. So can you just tell me a bit more about that?

Alan. Yeah. If you have the big one [draws two large circles and a series of smaller circles surrounding them, Figure 6.11] not necessarily two to one, but the smaller one's surrounding it and then the next one and so on.



Figure 6.11 Alan's drawing illustrating the structure and bonding in steel wool

Postgraduate learners, like undergraduates, routinely identified steel as an alloy but several learners who did not possess clear mental models for metallic bonding—Christine, Grace and Rose, were unable to provide much detail about the bonding in the alloy steel. Christine, for example, struggled to explain the bonding in steel in a similar way to that for aluminium, but she did recognise that it was a mixture of metals. Brian identified the sea of electrons model in his description of the bonding in aluminium, but for steel wool failed to identify steel as an alloy (in his comparison provided here, he mistakenly calls the aluminium foil, tin foil).

Brian. I'd say it would be exactly the same as the tin foil, well the metals just been drawn into strands rather than sheets.

Interviewer. In both these examples we are interested in what they would look like on a microscopic level rather than their physical appearance.

Brian. Yeah, the bonding would be identical.

Interviewer. Do you see it as being different in any way at all or not?

Brian. Um...well I mean I think as far as they're different metals and their overall bulk properties would be different. But apart from that, I don't really see any major difference.

Interviewer. OK so at the bonding level...

Brian. Yeah it's all effectively the same I'd say.

Jason was able to provide the most comprehensive picture of the bonding and structure for steel wool, although in his focus on interstitial carbon he neglected to mention substitutional metal atoms.

Jason. How I would see the bonding, the bonding would be fairly similar to the previous sample [i.e., aluminium foil]. The only difference is that this is actually steel, and the only difference is that it has got some interstitial carbon in it.

Interviewer. OK, could you just tell me what you mean by interstitial carbon?

Jason. Well when you pack the iron spheres together there's still space you can't, they're not cubes, so they can't pack completely, so there's no space at all.

Interviewer. So they are not cubes?

Jason. The atoms, no. I am sort of regarding them as spheres. So there's space and if you do the sort of geometric modelling, there's about twenty-four percent or so I think.

Interviewer. Twenty-four percent?

Jason. Space, and so the rest of this can be filled up by other smaller atoms and steel is, um, carbon and iron all mixed together in a certain percentage. Those carbon atoms are incorporated in the lattice, so the carbon atoms almost take on a, they help to lock the structure in place and that's why that why sort of steel is harder than iron.

Again like learners' mental models of metallic bonding, it seems that undergraduate and postgraduates show increasing sophistication in their explanations of material attributes compared with their secondary school counterparts; albeit possessing a similarity in preference for simple models like the sea of electrons.

6.4 Learners' Use of Mental Models for Metallic Bonding

Conventional instruction in relation to metallic bonding consists of describing their unusual physical properties, followed by a discussion of models for bonding, and subsequent use of the model to explain physical properties (see, e.g., Chang, 1991; Zumdahl, 1989). Hence in the present inquiry, learners were given the opportunity to use their mental models to explain some of the physical properties of metals (see, Appendix A, p. 317) by the use of two IAE focus cards; one which depicted the conductivity of copper wire (MB02, p. 79) and the other which depicted the malleability of copper (MB03, p. 79).

6.4.1 Learners' Explanations for the Conductivity of Copper Wire

In focus card MB02, the conductivity of copper wire was compared with that of a glass rod. Secondary school learners typically used concepts from the sea of electrons model to explain the conductivity of copper, namely, free or mobile, electrons, whereas the non-conduction of glass was typically attributed to fixed electrons.

The copper because it is metallically bonded, it's got lots more electrons going around the nuclei. So the electrons are free to move and carry the current which makes the circuit complete.

Here, Claire, although consistent with her description of the bonding in aluminium foil (pp. 136-137), inappropriately associates metallic bonding with "more electrons" in the aluminium foil. Neil and Richard viewed conductivity as associated with free electrons and David specifically related this to the sea of electrons model.

Neil. There's no free electrons in the glass rod and there is in the copper wire.

Richard. Well um, it's because of the copper wire, the electrons are free to move, like, it moves through, carries the current through, but the glass rod doesn't do it.

Interviewer. OK, OK. Can you just tell me why you believe the electrons are able to move in the copper wire?

Richard:...um...because the way they are bonded, just allows the electrons to flow through them, that's it.

David. Well the copper wire has got the sea of electrons around it, so that it'll conduct, help conduct, the flow of electrons around the circuit.

Interviewer. How would that happen? Or how do you see that happening?

David. Well it creates a, it gives the electrons something to flow through from the positive to the negative, positive negative throughout the whole thing.

Two secondary school learners, Anne and Anita, introduced other ideas to explain the conductivity of copper wire, in Jane's case she referred to ions, and Anita referred to the spacing of atoms in the metallic lattice.

Anne. Well copper's got ions that can allow a flow of electrons to go through it.

Anita. OK, it's how I see it, in the glass rod the bonds are not close enough together to have the electrons flowing through, or not through, or let them go through it. Whereas in the copper wire, really sort of close enough together to let them go through it.

It might seem reasonable to expect learners who chose the sea of electrons model as their preferred model for metallic bonding to then use this model to explain the physical properties of metals. However, for undergraduates there was no obvious correlation between model choice and model use (Norman, 1983). Undergraduates did refer to mobile and free electrons, but often introduced ideas from other target models such as the molecular orbital theory. In instances for which there was no clear model choice in the first place, learners typically borrowed terms and concepts from other models. Bob, for example, appeared to possess no clear mental model for metallic bonding (p. 140). He began his explanation of the conductivity of copper wire with the introduction of the molecular orbital theory and introduced the idea of delocalised electrons. However, he did not relate the concept of delocalisation to bands consistent with the molecular orbital-based band theory; rather his explanation is more consistent with the sea of electrons model.

It'd be to do with the electrons in molecular orbitals holding, well it wouldn't be a molecule, because it's not really a molecule obviously. But there is some sort of um...the electron doesn't seem to have any particular, or the electrons don't seem to have any particular individual

nucleuses. It sort of moves over them. So you have, if you had a potential across, it'll migrate across. As some come in one end, they'll be pushed off the other, and the glass rod not being crystalline for a start, is more metallic um...um...you know amorphous type thing I guess. There's no electrons to be, covalent bonding rather than metallic bonding.

Undergraduates who specified the sea of electrons model explicitly offered more coherent explanations as illustrated by Steve's explanation and drawing (Figure 6.12).

Steve. OK with the glass rod you have got, it is basically a silica structure inside the glass, and that's silicon covalently bonded in a sort of silica structure with oxygens [drawing SiO_4 unit, LHS Figure 6.12], sort of units like so. Whereas in the copper wire, you have got the metal bonding that we talked of before, with a delocalised sea of electrons [draws two Cu^+ with negative signs around them, RHS Figure 6.12] and so when you apply a potential to the copper wire, it enables the electrons to flow freely in the delocalised sea from one side to another [draws arrow].

Interviewer. Oh yeah, I see.

Steve. Setting up a current and that's why you get your light glowing. But because you have got covalent bonding, and electron sharing rather than the electrostatic sort of bonding that you have got with the metal bonding, it's not possible for the electrons to move through the system freely [draws arrow under SiO_4 unit].

Interviewer. Why is that not possible in that case?

Steve. Because the electrons are tied into this covalent bond here [draws line enclosing one Si—O], where they are shared between the silicon and the oxygen rather than being in a sea of delocalised electrons.

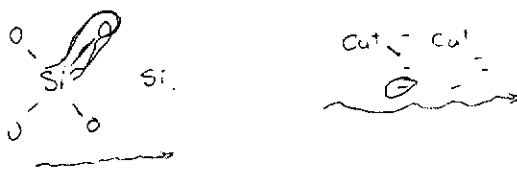


Figure 6.12 Steve's drawing illustrating the conductivity of copper metal and non-conductivity of glass

In a similar manner, Renéé provided a reasonable explanation for the conductivity of copper wire.

OK, the copper is a metal once again, like the aluminium, and so they're, the copper atoms are actually in a lattice, and they have got electrons that can that can be mobile and carry current through. The battery's pushing current through. You move the electrons which will, however, light the bulb and complete the circuit, and glass rod won't 'cos it's silicon dioxide. It'll actually be a covalent structure, and the electrons are not mobile in that structure, and like won't carry the current like, so the bulb won't work.

However, this type of explanation did not occur in every interview. For example, despite clearly preferring the sea of electrons model, Alan did not attempt to use this model to explain the conductivity of copper. The difference in conductivity, according to Alan, was due to the ionic nature of the bonding in silica and the covalent bonding in metals.

Interviewer. In what way is that different in terms of the conductivity?

Alan. The way I consider it, it is in the way the electrons are held, I would consider it to be more ionic.

Interviewer. Which one is that?

Alan. The glass.

Interviewer. The glass. OK the glass is more ionic, OK, and then the metal one you said you saw?

Alan. Um, sort of more covalent.

Despite the sea of electrons model being a common choice for postgraduates (Section 6.2.3, p. 141), in a similar way to the undergraduate learners, there was no particular correlation between their choice of model and how they explained the events depicted in MB02 (p. 79). For example, Jason's preferred model for metallic bonding was the sea of electrons model, however, his explanation of the conductivity of copper wire was inconsistent with his model choice, perhaps as a result of his focus on the nature of the bonding in the glass rod.

Jason. OK well the glass rod is, well an insulator it's very difficult for electrons to pass through the glass. As far as the copper wire is concerned [drawing two parallel lines enclosing large spheres, Figure 6.13], you've got a very, very narrow piece of copper wire so it'll see the electrons which are getting pushed along if you like by the battery or dragged along depends which...

Interviewer. Right, so you have just drawn a couple of lines with some spheres in it. The spheres are the atoms are they?

Jason. Yep they're not very well packed.

Interviewer. That's alright [interviewer laughs].

Jason. OK and so an electron, for example, experiences a general force in that direction [drawing arrow] and so it sort of transverses along through, and eventually you get a net flow of electrons in one way or the other.

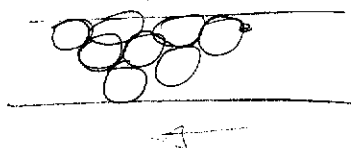


Figure 6.13 Jason's drawing illustrating the conductivity of copper metal

In Jason's explanation, there is no attempt to relate the conductivity to the presence of free or mobile electrons that form a crucial part of the sea of electrons (see, Appendix A, pp. 318-319). Three postgraduates, Brian, James, and Christine, however, related conductivity to the mobility of electrons.

James. It's the delocalised electrons are able to sort flow around over these positive centres so it can conduct the electricity.

Interviewer. OK so it's just the delocalisation?

James. Yeah, yeah. They are sort of not too strongly held by individual sort of centres, so they can move around yeah....

Christine. Because you have got loose electrons that will transmit.

Interviewer. In which one?

Christine. In the copper one that is why the light is on, Because it's got the electrons to move around.

Brian. The copper wire is a conductor because of the delocalised electrons. As I mentioned before the electrons are free to move. They are not restricted to bonds so as the battery exerts a voltage, a potential difference across the copper wire, the electrons move and are replaced by new electrons coming along the wire. So they are able to move through there.

However, the other postgraduates were rather confused. Kevin's description is not dissimilar to the sea of electrons model, except that he used the term cloud rather than sea (or gas). Jenny's description was less clear; she talked about "airy fairy" bonds.

Kevin. OK in terms of the electrical circuit, you are looking at a flow of electrons round the circuit which supplies the current. In the case of the

copper wire you have got a cloud of electrons, rather than the electrons being associated with specific atoms. That cloud of electrons, they interact with the circuit itself so you have got a free movement of the electrons through the entire circuit.

Jenny. [draws Figure 6.14]

Interviewer. OK so that's sort three coppers in a row, OK.

Jenny. Yes coppers. OK, and the electrons sort of jump [draws curved arrows from one sphere to the next] between like that, and the copper which means it's conductive. And the glass is sort of [draws planar SiO₄ units linked by O]. So they are not actually distinct. Like these are still distinct where these are actually like these [that] have got physical bonds whereas in the metallic being sort like airy fairy bonds [respondent laughs].

Interviewer. Airy fairy bonds [respondent laughs] so sorry, the fairy bonds are which?

Jenny. That in the copper.

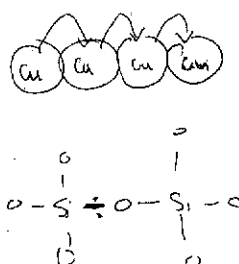


Figure 6.14 Jenny's drawing illustrating the conductivity of copper metal and non-conductivity of glass

6.4.2 *Learners' Explanations for the Malleability of Copper*

Learners' use of their mental models for metallic bonding also was probed by asking them to explain the malleability of copper metal (MB03, p. 79) which for all learners proved more problematic than the conductivity of copper wire. Anne, for example, was unable to offer any explanation, repeatedly saying "I don't know" when interviewed. Secondary school learners used a number of terms such as squished, squashed and flattened to describe the event, as was illustrated by Anita who changed her terminology upon probing.

Anita. When it goes through the rollers it's going to get flattened out more.

Interviewer. Flattened out, OK.

Anita. Instead of a big block it's a flat sort of a bit.

Interviewer. OK yeah that's fine. Why do you think they [the copper atoms] are able to flatten out in this case?

Anita. 'cos they are always moving. They are always just moving and the pressure of the rollers just sort of squashes them and they move.

Interviewer. OK so you see them as moving, and then when they come to that roller?

Anita. Yeah they squash.

Interviewer. Squash OK. If you think back to, say let's start with the thick block. Are they moving in the thick block at all?

Anita. Yeah I think they are moving.

Interviewer. OK

Anita. They are always moving I think.

Anita was likewise unable to provide a reason for the process in terms of the bonding, instead she stated that the copper atoms move because they have been placed "under pressure" and so have "gotta go" when subjected to this pressure. For some learners, the malleability of copper was explained in terms of changes to the size and/or shape of atomic species, be they ions or atoms, and rearrangement of lattices as illustrated by Neil who claimed that the copper atoms "would be just sort of reshaped". Others were familiar with the term malleability, indicating that they had encountered it during instruction, but likewise were unable to clearly explain the event depicted on focus card MB03 (p. 79). Frances, for example, although recognising that metals are malleable and change shape, seemed to have confused the mobility of electrons with the movement of atomic species stating that "the whole atom structure will be moved around". However, deeper probing revealed a different view; and it appears that Frances believes that the malleability is related to spacing of particles in the metallic lattice.

Interviewer. OK perhaps think about it on a small scale if you like. On an atomic scale. How do you see the change in arrangement, if you like with the atoms in the thick block, compared with the atoms in the thin sheet? Do you see any changes occurring there?

Frances. Well that would have more lattices going across [indicates thick block in MB03, p. 79], whereas that [indicates thin sheet in MB03, p. 79] would flatten to just one lattice so they are more compacted here, whereas they have got more space in the middle here, so...

Interviewer. Can you just tell me what you are meaning by lattice in this context?

Frances. OK the electrons, the whole nucleus within an atom is arranged in sort of lattices and so in the other structure where it's got more of a, um, say...um, um...

Interviewer. Would you like to draw it perhaps?

Frances. Um, you'd have, they all get [drawing small spheres, LHS Figure 6.15]. OK, well when they are in this they are close together like they are all sort of [drawing smaller spheres closer together, RHS Figure 6.15] squashed up.

Interviewer. So those spheres you have drawn there what are they?

Frances. The little, I dunno little molecules, and so you have got more space over here. They have sort of got this space.

Interviewer. Oh yeah I have got you. So in the case of the thick block you see those spheres you have drawn there as being more spaced out?

Frances. Yeah.

Interviewer. OK, OK and when they go through the rollers?

Frances. Yeah they are more compact.



Figure 6.15 Frances's drawing illustrating the malleability of copper metal

Undergraduates offered more detailed explanations for the malleability of copper than did secondary school learners and commonly related their explanations to their mental model for metallic bonding. Some, like Bob, struggled to explain the event but, like his explanation of conductivity of copper wire, he attempted to explain this event using molecular orbital theory.

Bob. Don't really have much idea, um...

Interviewer. OK that's fine. If nothing really springs to mind, that's fine.

Bob. I guess if the electrons were in a molecular type orbital, although there is no molecules in it, it's a metal, they would have a slight tendency to be slightly pliable sort of move around each other maybe. I don't know.

Alan used his mental model of sea of electrons to explain malleability—"I see copper or a metal bonding, it's just like a sea of electrons where, I don't sort of think the bonding would change a lot"—in contrast to his explanation of the conductivity for copper wire (p. 156) he used covalent bonding.

Steve used his mental model of sea of electrons to explain the event, and was the only learner able to relate his explanation clearly to the bonding in the metallic substance.

OK, well once again you have got the copper metal bonding in the same sort of system as I had before [draws row of Cu^+ with negative signs inside circles between rows, Figure 6.16], with the delocalised electrons, where you have a sea of delocalised electrons that are relatively free to move throughout the whole structure. Then the structure is relatively free to sort of move whenever a pressure is applied to it. It's easy for it to sort of be pressed down as it were, to change it's shape, so there is a freedom of compression so these can come in closer to each other [draws arrows towards the centre of rows], and therefore it presses the rod down into a sheet which would be denser.

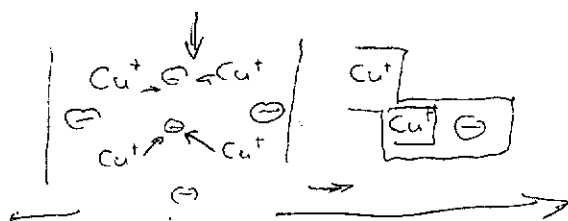


Figure 6.16 Steve's drawing illustrating malleability of copper metal

Interestingly, here Steve made the assumption that the density of the copper has changed. However, upon reflection he altered this stance when probed further, "actually no, come to think of [it is not more dense]. Because the sheet here, whilst being thinner width-wise, is also a lot wider". Whilst Steve offered probably the most convincing explanation of all learners in this inquiry it is still incomplete. For example, neither Steve nor any other learners seemed to be able to reconcile the strength of metallic bonding with the malleability of metallic copper (see p. 264). The remaining undergraduate learners offered simple explanations, like the secondary school learners, describing the rearrangement and movement of atomic species typically relating this to a perceived lack of strength of metallic bonding.

Interviewer. So you just see them as moving somehow do you?
Phill. They are not held there really tight they shift out.

Interviewer. So why do think they are able to move here? Why is that?

Phill. Um, 'cos...they just can [respondent laughs].

Interviewer. When you say flatten out. Can I just be quite clear on what you mean by that? Can you just tell me what that means?

Jane. It's able, they can go from being a cylinder type shape to like being flattened out, flattened out is—they are not, not the layers.

Interviewer. can you just tell me what you see that as being on the atomic scale if you like?

Jane. It's just rearranged. They have still got the same kind of bonding there. It's not bonding, the same kind of packing and it'd just change the shape of the whole thing. It's still, there's still on the atomic scale the same, the same pattern. Like you have only changed the real massive kind of shape.

Postgraduates also offered rather incomplete explanations for the event. Some like Rose had no idea at all, only describing the physical changes associated with the event.

Rose. I really haven't, I guess it must just be more spread out.

Interviewer. More spread out, OK.

Rose. I guess it's just the pressure of the rollers that's made them more spread out.

Interviewer. Why do imagine that say the thick block of copper is able to be spread out?

Rose. I haven't really thought about it [respondent laughs].

Terms like squishing and flattening were again common, although it seemed that postgraduates do not harbour the alternative conception that atom volume or spacing between atoms is reduced as exemplified by the views of Christine, Kevin and Brian.

Christine. When it's going through and coming out the other end it's much like you are squishing the different layers, and they are coming out so you have still got the copper interaction but they are more two dimensional.

Kevin. It's just that with the thick block you have got a lot more of a three dimensional lattice in which case you have got whole planes of atoms with the electron clouds associated with them, and this sort of goes on effectively almost infinitely. As you go through the rollers, the layers of atoms and their electron clouds remain pretty much as they are, but the number, I suppose it becomes more of a two dimensional

surface, as opposed to a three dimensional surface. I suppose the atoms would actually move around as they go through the rollers.

Brian. OK well in metals, as I mentioned before, the atoms are free to move next to each other. What happens is as the copper goes through the rollers the force that is exerted on the metal causes the entire, causes all of the, not all of the atoms, but some of the atoms to sort of move across each other so that to reduce the stress to, let me just think for a minute. Well because the atoms can move across each other, and they are not held by distinct bonds holding them in place, they, the whole structure can deform into a flat sheet.

James provided a reasonable, albeit rather brief explanation for the event.

James. I suppose you would somehow allow for all the positive centres being able to move around. I suppose if the electrons can move then the centres can move although.

Interviewer. So you believe the spheres are moving around?

James. Well that's how I would see it yeah. The spheres would have to sort of move past each other and come back to new arrangements.

Interestingly, Jason failed to use his mental model of sea of electrons to explain the malleability of copper, although his explanation was highly detailed.

Jason. I don't think I could really depict how [drawing array of circles close together; top part of Fig. 6.17], I don't have a good understanding of actually how the bonding between these atoms works.

Interviewer. OK, so you are just drawing those spheres together.

Jason. Yep I am drawing spheres together, but because the forces, because they are not particularly directional, each one has sort of twelve nearest neighbours, they can be pushed past one another with reasonable ease.

Interviewer. So what happens when they are pushed past each other?

Jason. Well I guess I basically see this [draws four more circles close together; middle part of Fig. 6.17] go through a process where they start in this kind of configuration here, which is hexagonal-close packed [writes *hcp* next to middle circles].

Interviewer. *hcp*, yep.

Jason. OK, and then it experiences a stress in one direction or another. It slips [draws arrow above middle circles] into this kind of configuration [drawing four spheres in cubic arrangement; lower LHS of Fig. 6.17, writes *bcc*] in which it has less nearest neighbours. I've just drawn it in two dimensions here to make it simple.

Interviewer. Yep, OK.

Jason. Like this one would have six nearest neighbours [indicating the *hcp* structure] and this one would just have four [indicating *bcc*]. So because the directionality isn't too strong, it can endure going from twelve, ah, six nearest neighbours, to four, and so that's *bcc*. Then as it experiences more stress, it sort of flops back over into the other one

here [draws four circles in diamond shape; lower RHS of Fig. 6.17, writes *ccp*].

Interviewer. So it's going from sitting in the gap to sitting on top and then back into the gap.

Jason. Exactly.

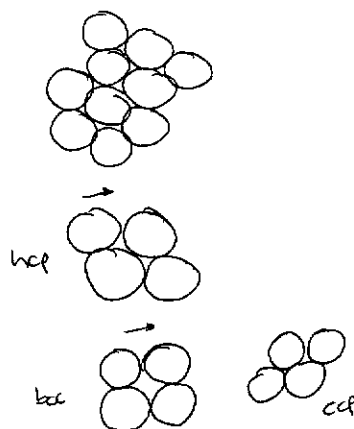


Figure 6.17 Jason's drawing illustrating of the malleability of copper metal

6.5 Summary

There was clear choice for the sea of electrons model across all academic levels of learner, particularly in the case of the secondary school learners. Learners seemed to see free or mobile electrons as a key feature of the bonding in metals, and undergraduates and postgraduates showed a greater appreciation of the continuous nature of metallic lattices than secondary school learners. In general undergraduate and postgraduates explanations were more detailed and complete, and were far more analytical and critical of models for metallic bonding; this was particularly so in relation to those depicted on the focus card MB01. Despite this latter observation, few learners at any level appeared to possess a complete and accurate mental model for metallic bonding that was in agreement with the scientific conceptualisation. Undergraduate's and postgraduate's appreciation of the continuous nature of the metallic lattice included the use of domain-specific terminology to describe lattice structure. This preference was reflected in choice of depicted models from MB01, with undergraduates and postgraduates choosing more open structures that depicted the three-dimensional lattice in more detail, whereas secondary school

learners preferred more realist space-filling depictions. All levels of learner deemed that the bonding in alloys was similar to that of pure metals and relatively few recognised that steel was an alloy. There was some correlation between model choice and model use for some physical properties such as conductivity; however, this was not carried over into the explanations of malleability. Learners used the sea of electrons model to explain the conductivity of copper, even if it was not their preferred mental model. Learners were unable to provide convincing explanations for the malleability of metallic copper, mostly resorting to descriptions of the macroscopic event rather than offering explanations on the microscopic level.

6.6 Learners' Mental Models for Ionic Bonding

Learners' mental models for ionic bonding, probed using part of the semi-structured interview protocol described in Chapter 4 (Table 4.1, p. 77), were deduced from two of the tasks contained within the interview protocol (Table 6.3).

Table 6.3 Interview protocol for the target system ionic bonding

-
1. Shown sample of sodium chloride—*please describe the bonding in this substance*
 2. Shown sample of lithium chloride—*please describe the bonding in this substance*
 3. Shown focus card IB02—*please explain this process*
 4. Shown focus card IB03A/B—*please explain this process*
 5. Shown focus card IB01—*which of these models appeals most/least to you?*
-

Learners were presented with a sample of solid sodium chloride and asked to describe the bonding in that substance, and were shown focus card IB01 (p. 80) which contained depictions of the bonding in caesium chloride. The remaining tasks of the interview protocol were used to provide learners with the opportunity to address the criterial attributes for ionic bonding (Section 6.7, pp. 183-197) and to

investigate learners' use of mental models to explain events that used ionic bonding in some way (Section 6.8, pp. 197-206).

6.6.1 Secondary School Learners

Secondary school learners possessed a number of mental models for ionic bonding with the preferred target model for the bonding in ionic compounds being the electrostatic model. Anne stated that "these have an electrostatic attraction between the two [ions]", Neil similarly viewed the bonding as involving charged species and he related the bonding to an attraction between charged species "because the sodium ions are positively charged and the chloride ions are negatively charged they are attracted to each other". David's mental model seemed more well defined. He related the bonding in sodium chloride to electron transfer and the resultant electrostatic attraction between oppositely charged species.

David. I know it's ionic bonding and that's where they donate electrons and receive electrons, the two things. So the way I would see that is the Na is the positive one and then Cl is the negative one. So because there's the attraction between the positive and negative charge, they are bonded together.

Interviewer. OK.

David. Like that [draws two vertical rows; (Cl⁻ Na⁺ Cl⁻) and (Na Cl Na) side by side, Figure 6.18].

Interviewer. So what's holding this together here?

David. The electrostatic attraction between the negative and positives I would imagine.

Interviewer. OK. What's electrostatic attraction meaning here? What do you mean by that here?

David. Um, the attraction between the positive and the negative, opposites attract.

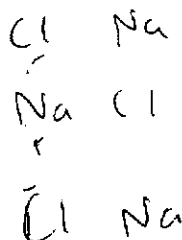


Figure 6.18 David's drawing illustrating the structure and bonding for sodium chloride (NaCl)

Learners related the electrostatic model directly to the octet rule of full-shell stability (Appendix A, pp. 321-322). Claire, for example, began by drawing a schematic of the Periodic Table (Figure 6.19), which she used to deduce the relative electronegativities for sodium and chlorine. She then used this to develop her model for the bonding in sodium chloride.

Sodium is over here somewhere [drawing Periodic Table outline; draws square on LHS], and the chlorine is up here somewhere [draws square on RHS]. The electronegativity goes that way [indicating from left to right on Periodic Table]. Chlorine, chloride, has a really strong attraction for electrons [drawing Cl⁻ with arrows pointing toward it] and, um, the sodium ion is holding that one electron in the outer shell really loosely [writes Na⁺] so it is easily attracted to the chloride [draws arrow towards Cl⁻]. The sodium loses and the chloride gains, spends most of its time with the chloride, so it is sort of ionic, yeah you can almost say it has been transferred.

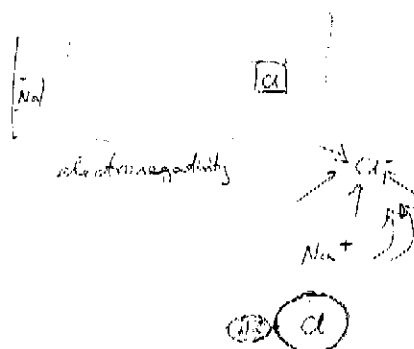


Figure 6.19 Claire's drawing illustrating the structure in sodium chloride (NaCl)

Anne also viewed the origin of the electrostatic attraction in the presence of charged species. The chloride ion, according to Anne, was formed by addition of an electron and the sodium ion from loss of an electron, which, like Claire, she related to the octet rule.

Anne. It gains an electron [i.e., sodium]. No it's got one electron in its outer shell, all by itself, and to make the outer layer full, the outer electron shell if you like, it loses an electron.

Interviewer. I see. The chlorine how do you see that?

Anne. That one's got seven electrons in its outer shell and so it's easier to gain one than lose all seven, so it gains an electron.

Some secondary school learners became confused when describing their mental models for ionic bonding, introducing inappropriate concepts. Keith, for example, seemed to believe there were van der Waals forces present in sodium chloride. After drawing a lattice structure for sodium chloride (Figure 6.20), he began with a description involving the octet rule (here he made the assumption that sodium gains seven electrons).

Keith. The sodium has got, the chlorides one, more, or it has got one electron in its outer shell, and the chlorine has got seven. So the chlorine requires one more electron to satisfy itself, and the sodium needs, the sodium needs I dunno...yeah...it's Na plus, so it gains seven.

Interviewer. And that's what it forms is it?

Keith. Yeah it just needs that to get its full outer shell.

He followed this description with the introduction of two notions; one that the attraction between the species is electrostatic in nature (Figure 6.20).

This one here with sodium, it's bonded directly to that [draws heavy line between Na and Cl, and encloses in ellipse; adds ellipses to other Na—Cl units]. Then there's sort of electrostatic forces bonding it to that as well [points to lines between ellipses in diagram].

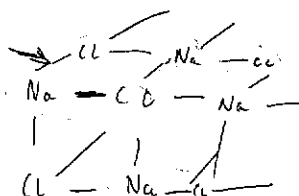


Figure 6.20 Keith's drawing illustrating the structure and bonding in sodium chloride (NaCl)

The second notion Keith introduced was the presence of van der Waals forces between NaCl "molecules", which he ostensibly believed to be covalently bonded.

Keith. So that sort of bond is the covalent bond, attracted to that electrostatically, van der Waals forces.

Interviewer. OK, can you just tell me a bit about those van der Waals forces?

Keith. Just weak electrostatic forces, not very strong, [they] can be broken fairly easily.

Frances seemed to hold a rather confused mental model for ionic bonding in sodium chloride; a model that consisted of concepts from ionic bonding and covalent bonding. Like other learners she stated that the bonding in sodium chloride consisted of a lattice of ions and was ionic in nature. However, she seemed to confuse ions with polar covalent species and subsequent comments indicated that, like Keith, she believed that the bonding in sodium chloride is covalent in nature.

Frances. Um OK...OK ionic solid with all atoms fixed in a lattice there's no free electrons. Ionisation energy is higher, there would be sort of, kind of like dipoles. So you have got your, they are not instantaneous, they are more like induced. That's what has formed, the sort of ionic bond. And you get the Na^+ attracting more of the electrons from the chloride, and they sort of stay on that side in chloride. That makes the chloride dipole negative, and the sodium dipole positive.

Frances. If there's a dimer, the chloride is electronegative which means it can give away an electron, and Na plus means it can accept the electron [drawing arrow from Cl^- to Na^+ , Figure 6.21]. So at one time that electron will be transferred to that, and that makes that dipole positive and that dipole negative. That sort forms a covalent bond, sort of sharing at any one time.

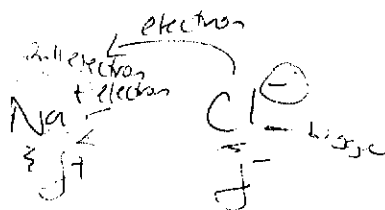


Figure 6.21 Frances's drawing illustrating of the bonding in sodium chloride (NaCl)

The fact that Frances has described the essentials of the electrostatic model and at the same time introduced the notion of covalency, may mean she has confused the concept of a covalent bond with the covalent character of an ionic bond (Appendix A, p. 329). Anita was the sole secondary school learner who seemed unsure about

the bonding in sodium chloride, although she did state that the bonding involved charged species where "there are pluses and minuses sort of all floating around".

Secondary school learners were given the opportunity to choose a depiction of the bonding in the ionic substance caesium chloride (IB01, p. 80). Their choices of depicted models were similar to their choices for metallic bonding in that four learners preferred a simple realist model, that is, depiction A. Aesthetic appeal may have been a factor, but several learners stated that they found depiction A familiar and simple. For example, Frances stated that "you can still very simply see how it would be" and Claire commented, "I like that kind of 3-D, it's like what I have seen before". In some instances, it seemed choice more reflected lack of appeal of other depictions. For example, Anita stated that the "lines on others are confusing". However, the view that choice represents underlying realist beliefs is supported by comments made by several learners, for example, Neil and Frances.

Frances. [depiction A] is like you would see on a microscopic scale.

Neil. Those balls represent the whole atom including the outermost parts not just the nucleus and they are actually really close, whereas the others they are not touching.

The three learners who chose depiction C reasoned that it was more informative, and that other depictions were confusing; Anne expressed her dislike of depiction D "this one has got caesium and it's got the chlorides around it, but then these ones don't have chlorides around them" and Keith likewise found other depictions confusing "I think B and D are too complicated and A is little simplistic, and I think C shows you pretty much exactly what's going on, and E sort of yeah, it's a little bit confusing as well". Richard was the sole learner who chose depiction B; his choice was based on the familiarity of the model to him, along with aesthetic appeal in that "its structure looks like, real easy on the eye. It just appeals. It's the way that things have been taught to me, that's why I picked it straight away".

It is interesting to note how learners may become confused by the more complex depictions of the bonding in ionic compounds such as those shown in

depiction C of IB01. Keith misinterpreted the diagram, mistaking the solid lines used to define the ionic arrangement for bonds.

Keith. The solid lines are the lines which are bonding each carbon directly, ah chloride I mean, to another chloride, and then the others carbon bonding to the chlorine.

Interviewer. So this is a bond between those chlorines?

Keith. The dark lines are the bonds between each chlorine, and then the dotted lines are the bonds between the chlorines and the caesium.

David's initial response seemed to indicate that like Keith he believed there were bonds between anions, however, his latter comments, made it clear that he understood the visual clues and was able to distinguish between the solid lines and dotted lines.

Interviewer. What appeals to you about C?

David. Well it's pretty clear, and it's kind of showing the lines.

Interviewer. Looking at C. You have got those lines. You have got solid lines on the outside circles or spheres, and then you have these dotted lines connecting those with the circle that's in the middle. Can you just tell me what those lines mean to you?

David. Those, they'd mean that there's a bond there, to me.

Interviewer. OK, that's both sets of lines is it? Is that what you are meaning ?

David. You mean the dotted lines as well?

Interviewer. Yes there are two sets of lines. I just want to be sure I know what you mean here.

David. Definitely the dotted lines would represent bonds to me.

Interviewer. Yeah.

David. I'd probably say those [indicating solid lines in depiction C of IB01] would just define the shape, maybe.

The most disliked depictions were D and E, D being too complex and confusing and E was seen as unclear, particularly the $\frac{1}{8}$ chloride at the corner of the unit cell as illustrated by Anne's response that it was "very strange". It seems that the single unit cell depiction intended to combine the elements of a space filling model with the symmetry elements of the unit cell has not proved meaningful for secondary school learners.

6.6.2 Undergraduate Learners

Undergraduate learners' preferred mental model for ionic bonding was the electrostatic model, but, as was the case for metallic bonding, they placed greater emphasis on lattice structure and the use of domain-specific terminology. Furthermore, undergraduates explanations of the bonding in sodium chloride tended to be more detailed than secondary school learners, as illustrated by Bob's and Alan's responses.

Bob. OK you have got obviously sodium, sodium cations, and chloride anions. Because of the negative and positive charges on either one, the anions tend to be bigger than the cations. The anions pack together in similar ways to the metal atoms in like cubic close-packed or hexagonal close-packed. I can't remember which one they told us it was. Cubic close-packed possibly. Yes quite possibly cubic close-packed, with sodium atoms located in the gaps [drawing 4 spheres in square pattern, Figure 6.22]. Like you've got, anions like that, and then another four on top. You are actually going to have a gap in here [draws a smaller sphere in middle], where a sodium can fit in there, and then the next one in there [draws another small sphere, top LHS].

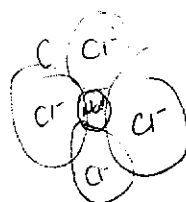


Figure 6.22 Bob's drawing illustrating the structure for sodium chloride (NaCl)

Alan....OK...well I would see the sodium chloride structure just like a close-packed layers. The way I envisage it is like a lattice with individual sodium and chloride atoms. So there's the sodium and chloride [draws three circles, two coloured, one plain, top of Figure 6.23].

Interviewer. So that sphere you have drawn there that coloured one what is that?

Alan. That's the sodium [writes Na with arrow pointing to coloured circle, and Cl with arrow to clear circle], and that's chloride.

Interviewer. So how would that look in three dimensions?

Alan. It'd be like [draws cube with some open circles at corners and filled in circles in faces].

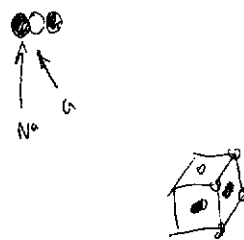


Figure 6.23 Alan's drawing illustrating the structure and bonding in sodium chloride (NaCl)

Interestingly, like Bob, Steve seemed to feel that he could be expected to remember the specific lattice structure for sodium chloride, perhaps as a result of recent instruction of ionic bonding.

Well once again you have got a regular repeating, a regular sort of repeating structure in an infinitely extended network of sodium plus [draws Na^+ , Figure 6.24] in cubic arrangement ions, ah, sodium plus cations and chloride minus anions [draws Cl^- in centre]. So you have, I can't quite remember what the exact structure is. I should remember that. But you have got a regular array of say Na^+ and then they have a Cl^- and they have repeating thing in three dimensional units. I can't quite remember, it's either face-centred cubic or body-centred cubic.

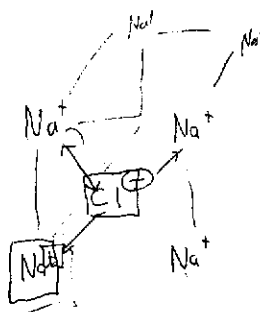


Figure 6.24 Steve's drawing illustrating the structure of sodium chloride (NaCl)

Undergraduates were clear that ionic compounds like sodium chloride consisted of ions. For example, they stated that the attraction was electrostatic in nature, and related this to the presence of ions typified by Renee's and Alan's responses.

Reneé. It's ionic. Yeah and, anions and cations in a lattice. You have like got surrounding each, um, that's in a three-dimensional structure. Surrounding each chloride ion you have got sodium and surrounding each sodium you have got the chloride ions.

Alan. Transfer of electrons from the sodium to the chlorine making it a positive charge, and a negative charge, making it ionic bonding.

Undergraduate learners also related the formation of ions to the octet rule. Reneé stated that ions form because "it's more stable in that state", and other undergraduates provided more detail in their explanations, as illustrated by the following responses.

Steve. Well basically it's the fact that the chlorine is heavily electronegative, whereas the sodium's electropositive. So the chlorine tends to take on an additional electron to form a complete octet, orbital, whereas the sodium is going to lose an electron. So that it has a filled valence shell. OK so in the solid, it's locked into that repeating structure and the electrostatic interactions are sort of holding it together.

Phill. Na positive one, 'cos it's lost an electron, and the chlorine is negative, so it's gained one.

Interviewer. That loss and gain of electrons, what in your mind is making it do that?

Phill. Just because it's sort of the stability. Like it likes to, say losing an electron, it can get back to, losing a losing a [respondent laughs]...

Interviewer. So it's lost an electron?

Phill. Yeah so it's more stable. Well it's quite stable before the electron loss, 'cos it's a full, a full shell, or half-filled or something [respondent laughs].

Interviewer. OK what about the chlorine? How would you see that?

Phill. It's just sort of in the same way gaining an electron so it just fills up that, fills up the shell.

Alan. Sodium's got one valence electron so it loses that electron so it's got a full outer shell, and the chlorine gains one.

Jane. It's got like the chlorides wants to gain one to form Cl minus, sodium it wants to give one away. It still the way I think of it. They both want to fill sets of orbitals.

Kim. Because it's more stable. 'Cos like chloride's only got seven, and then like to be stable to fill eight. You need an extra electron, and that's coming from the sodium [draws Cl with seven small circles around it, and curved arrow pointing to gap, Figure 6.25].

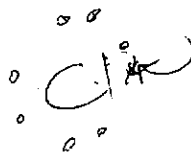


Figure 6.25 Kim's drawing of the chloride ion

Mary was the sole undergraduate that seemed confused about the nature of the attractive forces in sodium chloride. She identified sodium chloride as an ionic compound, mentioned cations and anions, and used the octet rule to deduce electronic configuration—"the chloride wants to gain one to form Cl^- . Sodium it wants to give one away, it's still the way I think of it, they both want full sets of orbitals". However, upon probing, she subsequently related the attractive forces in sodium chloride to "spare electrons".

Mary. Well I'd say it'd be ionic 'cos sodium plus Cl minus um...

Interviewer. Do you just want to tell me a bit more about that, what ionic means to you?

Mary. Um...ionic being, you have got one, you have got a compound which has one cation, one anion and they just bond together as opposed to say two cations together [respondent laughs] yeah.

Interviewer. OK what's holding them together?

Mary. Well I guess because the cations has got a spare electron. I don't know how many it could have. One, two, and the anion has got a spare electron, which can bond that cation to form a bond.

Interviewer. So what's actually holding them together then?

Mary. Um [respondent laughs] the spare electrons, spare electrons [respondent laughs] they are attracted to one another yeah.

In some instances, undergraduates confused terminology by borrowing terms from other models for bonding in their explanations for ionic bonding. For example, Alan used the term cloud in his description of the bonding in sodium chloride, but upon probing related this to the octet rule and equated "cloud" with "shell".

Interviewer. You used the term cloud [respondent laughs]. Do you want to tell me what that means to you?

Alan. Well I see the electron cloud as being the outer level of electrons. I know from high school the 2 8 8 rule.

Interviewer. So where does the cloud fit into the 2 8 8 bit?

Alan. Well for the chloride ion, the cloud would be the outer 8 electrons of the chloride ion.

Interviewer. You also used the term shell. Do you see that as the same or different?

Alan. Same sort of thing.

Learners' choices of depicted models from IB01 were similar to their choices for metallic bonding, with four learners preferring the simple realist depiction A. Again a similar pattern to learners' choice for metallic bonding depictions was observed; that is, undergraduates were more ambivalent about their choices, and more critical of the diagrams, weighing their choices before making a decision, typified by Bob's response.

Interviewer. OK you mentioned A, B and E. Is there any one of those that you prefer over the others?

Bob. A and B, probably over E.

Interviewer. A and B?

Bob. It's slightly easier to see what's going on. B especially you can see the ones behind.

The reason for choice typically was familiarity, Reneé stated that "it's familiar" and Mary that "you can see what's going on". Two learners chose depiction C; Phill identified familiarity again—"it looks like one we had in a lecture—it's just familiar", and Mary liked the clarity of depiction C "I guess 'cos you can, from this drawing you can kind of see that it's surrounded by eight chlorines". The remaining two learners chose depiction D. Alan stated that "it shows more how it's like how it carries on" and it seems he viewed the continuous nature of the ionic compound as important. Steve critically examined the lines on the diagrams and was able to discern the purpose of the two types of lines on depiction C; the dotted lines intending to indicate ionic forces, and the solid outer lines defining the symmetry of the unit cell. In his explanation he stated that the lattice structure for sodium chloride was body-centred-cubic rather than face-centred-cubic.

Steve. Well the diagram's showing through the dotted lines the ionic bonds between the chloride, the chlorine, and the caesium. It's also showing the regular repeating square unit which is body-centred, which

is shown here. But there is no sort of defined square unit, OK so that's shown there.

Steve. That's [the solid lines in depiction C of IB01] just to denote that they have got, between the cations, that is just to denote that they have got a sort of repeating cubic unit.

However, Kim, explaining her preference for depiction C, like some secondary school learners, seemed uncertain about the meaning of the lines in depictions B and C.

Kim. It's clear [i.e., depiction A]. There's no lines like telling you bonding.

Interviewer. Not telling you what sorry?

Kim. Telling you how the structure of it, like...doesn't that like, it's not bonding it's just the structure of it basically.

Interviewer. Oh yeah so those lines you are pointing to on B are not bonding did you say?

Kim. No they are just structures I suppose. But, um, yeah definitely that one [taps A].

Interviewer. So it's clear is it, did you say?

Kim. Yeah it's much clearer.

Interviewer. OK so the lines in the other ones, what do you find off-putting about them?

Kim. Well you can't, you're not too sure like sometimes whether it's like, they are like bonded in that way.

Depiction E was least popular for undergraduates, for similar reasons as stated by the secondary school learners, that is, undergraduates found the depiction confusing, Kim claimed "I don't understand it", Alan that "it's not clear to me" and others expressed similar sentiments.

Jane. I am not even sure what those are [pointing to corners of cube in E of IB01] what they are trying to show. It's they are like, they are the corner.

Interviewer. That's the corner you are pointing to.

Jane. Yeah. One eighth of a chlorine. It's like, nah, I mean I just can't see what's going on there.

Depiction D also was unpopular with some learners for similar reasons, as stated by Bob "it's very hard to follow, it looks like a jumbled, cluttered mess".

6.6.3 Postgraduate Learners

Postgraduate learners' preferred mental model for ionic bonding was the electrostatic model, their explanations being similar to those of the undergraduate and secondary school learners, typified by the responses of James and Grace.

James. It's mainly ionic, just having positive and negative sort of spheres packing together. Yeah it'd be almost purely ionic I'd say. There wouldn't be electron sharing like covalent bonds between centres.

Interviewer. Straight ionic?

James. Yeah.

Interviewer. Can you just clarify what you mean by ionic?

James. Oh I just mean when you have a positive charge and a negative charge, and it's the charges which sort of attract each other rather than sharing the electrons.

Interviewer. So you see the charges as being separated?

James. Yeah the charges are separated and it's like an electrostatic force which is bringing them together.

Grace. OK well it is ionic, a pure ionic species, so you have a sodium ion and then a chloride ion and by virtue of the fact that the chlorides got its electrons and the sodium got none. Because the sodiums are positively charged, then that is attracted to it. So you have got two separate things. I guess you have two separate things. The sodium and the chloride, but they are attracted to one another by virtue of the fact that there is a positive and a negative.

Although postgraduates exhibited a preference for a simple model of chemical bonding, their descriptions were typically more detailed compared with their counterpart groups. Interestingly, they invariably referred to a lattice structure, but were less inclined to draw lattice diagrams compared with the undergraduates and less inclined to use domain-specific terminology to describe the nature of the ionic lattice. Christine's response is rather limited, whereas Brian's is highly detailed.

Christine. I think of sodium chloride as basically like a lattice, you know, cube sort of extension.

Interviewer. So a lattice, can you just tell me what you mean by a lattice? What does that term mean to you?

Christine. Like sodium pluses, sort of like at the corner of a cube, but superimposed on that, the minuses, also surrounded by an equal number of pluses that's sodium plus, chloride minus.

Brian. Well the bonding in sodium chloride is what I know to call ionic bonding. Which involves like a matrix of chloride ions, that's Cl minus

in sort of sheets. Well not sheets but, sodium plus ions in a nicely ordered crystal matrix with basically one-to-one ratio of chlorine and sodium, but they are all arranged sort of [drawing rows of Cl^- and Na^+ , Figure 6.26].

Interviewer. OK so you have sodium's in the middle.

Brian. Sort of like that, but with sheets stacked on top.

Interviewer. On top.

Brian. Although they are not really in sheets they are just sort attached to, they are just one big mass. So yeah there is a positive charge with the sodiums attracted to the negative charge of the chlorines, and so on, so overall it doesn't have a charge.

Interviewer. So can you just think a little bit about the arrangement of those Cl minuses and Na pluses that you have drawn there. Can you just tell me a bit more about how you see them being arranged?

Brian. Well each sodium is effectively surrounded by chlorines. The chlorines are a very large molecule, and sodium is quite small. So it's really a whole lot of chlorines in a, well fairly close-packed sort of arrangement, and the sodium atoms sit in the holes between the chlorines. So every chlorine is surrounded by sodium and every sodium is surrounded by chlorines.

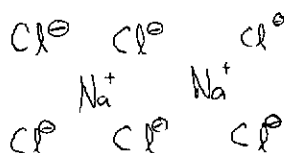


Figure 6.26 Brian's drawing illustrating the structure of sodium chloride (NaCl)

Kevin also provided a detailed response, similar in depth to his responses for the target system of metallic bonding.

Kevin. I see [the bonding in sodium chloride] a lot more as ionic bonding as compared to metallic. By ionic I mean, when I talked about metallic before you had the positive charges and you had the electrons were intrinsically associated with it and the electrons that were shared much more by the atoms. In this case each atom has a defined electron or electrons around it which aren't shared as such through the system. Each has got its own electrons associated with it. You also have positive, there is positive and negative charges associated with that. If they have got more protons than electrons, and more electrons than protons that sort of situation and the charge is associated with the atom.

Interviewer. OK so what's sort of holding the thing together if you like?

Kevin. Together? I see as the interaction between the positive sodium atom with all its associated electrons and the negative chloride,

chlorine, or chloride system. You have got the positive charge on the sodium, negative charge on the chloride, is holding the thing together, the ionic attraction.

Similar to undergraduates and secondary school learners, postgraduates related the formation of ions to the octet rule; for example, Christine stated "the sodium is losing an electron from its outer shell" and James and Brian likewise mentioned the noble gas configuration and full outer shells.

James. Its electron configuration, the sodium prefers to have a one plus and the chlorine prefers to have a one minus.

Interviewer. OK so how is that coming about?

James. It's just filled, having a sort of noble gas configuration of electrons. Yeah it likes to have all the electrons paired up so sodium loses one and chlorine picks one up.

Brian. Well with the sodium plus, well sodium metal itself has one electron in its outermost valency shell and losing that electron gives it a more stable electron configuration. So it prefers to be deficient in electrons you would say.

Interviewer. OK how about the chlorine?

Brian. Ah chlorine is well its outermost valency shell is almost completely full, and it doesn't have a charge. It just needs one more electron to make it completely full and to give it a stable structure as well. So gaining an electron to make chlorine minus is a favourable outcome for chlorine.

Only one postgraduate, Jason, showed any knowledge of the theoretical electrostatic model, and this was rather limited. His description of the bonding in sodium chloride was similar to the other learners, that is, the electrostatic model—albeit more detailed than most. However, he also introduced the notion of inter-anion repulsion, which has its origins in the theoretical electrostatic model (Appendix A, pp. 327-329), although he did not develop this idea further in subsequent discussion.

Jason. OK, sodium chloride is a sort of a classic cubic structure where you have each sodium and each chlorine surrounded by a six...[drawing Cl in a circle with Na in circles surrounding it, Figure 6.27]. So you get something that looks like this. So you get a chlorine which is surrounded by six sodiums and...

Interviewer. OK so you are just drawing a central chlorine and then there's six sodium, and you're drawing lines between them.

Jason. This is not really indicating the bonding in any way.

Interviewer. So what are those lines indicating to you what do you mean by those lines?

Jason. They're just showing the three dimensional nature of the diagram, I have drawn them more than to indicate bonding. In this case, I see the chlorine as being not a chlorine atom, but a chlorine ion. So a chlorine which has gained an electron from the sodium atom, so that the chlorine atom has a negative charge. The sodium has a positive charge. It's like this structure is essentially held together by electrostatic interactions.

Interviewer. OK I see what you mean.

Jason. Now there's also repulsions as well, because in this area here you also have another chlorine atom which is reasonably close to that chlorine atom so there's repulsions between the two.

Interviewer. Between those two chlorines.

Jason. Yep. Well it obviously this is extended into three dimensions.

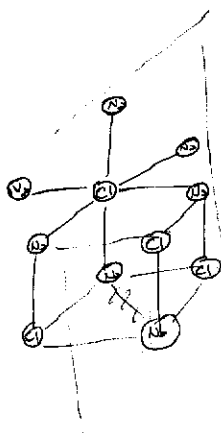


Figure 6.27 Jason's drawing illustrating the bonding in sodium chloride (NaCl)

Postgraduates choice of depicted models (IB01, p. 80) were different to the secondary school and undergraduate learners with six postgraduates preferring depiction C, one depiction B and one depiction D. Postgraduates liked the spatial aspects of depiction C and the fact that the diagram appeared to reinforce the continuous lattice structure of sodium chloride, as seen in Grace's response

You can repeat like, you can see that there's one in the middle, and they are all around it. You can pack you can see that you'd you just you can just spread that up—you could have like ten of those just all next to one another, you know you could stack them in all three directions.

As was seen for choice for depictions of metallic bonding postgraduates were more critical of the diagrams and in addition appeared to show greater

appreciation of visual clues. For example, Brian chose depiction C, and spontaneously offered an interpretation of the dotted lines.

Those dotted lines are a bit of a fallacy, because there are no actual direct bonds as such. There's just the attraction of charged species. So I guess A is good in that respect because it doesn't show direct bonds, it just shows a pattern of atoms. But I think C is good because it shows the size better.

The distinction made by Brian here is subtle; that is, it is evident that he views the attractive forces between ions as omni-directional rather than directional in nature. Christine chose depiction B for similar reasons to the others' choice of depiction C, namely, the implication of a continuous lattice structure for caesium chloride "because you can repeat like it you can see that there's one in the middle and they are all around it and you can see that you can pack in three dimensions". Kevin preferred depiction D because he felt it was less likely to lead to misunderstanding about stoichiometry in caesium chloride.

I like D because in all the other ones it seems to imply that you have got a large number of chlorides for the one caesium, which sure if just take a little system and do that sort of thing it makes it moderately clear, but it gives the incorrect impression that there is a lot more chloride than there is caesium. Whereas D seems to imply that you have got the caesium surrounded by eight chloride. But you have also got alongside it the chloride surrounded by eight caesiums.

Depiction E was least popular for similar reasons as other respondents; James describing it as "pretty funny", Grace stating "it doesn't really look like bonding", and Kevin that "it doesn't automatically spring to mind what it is referring to". The ability of postgraduates to discuss their views of bonding more critically is exemplified by Jason's response that he disliked B the most because "I think it contains potentially misleading information—especially the lines which are drawn here [indicating intersecting lines at the front of depiction B on focus card IB01] which I don't think mean anything". Postgraduate choice of depictions for the bonding in caesium chloride thus mimics their choices for the target system of

metallic bonding in that they were more critical of choices; however, by way of contrast, they did not show preference for realist models for ionic bonding in the same way that they did for metallic bonding.

6.7 Learners' Understanding of Mental Models for Ionic Bonding

Learners' understanding of their mental models for ionic bonding was probed by reference to criterial attributes for the sole target model identified, namely the electrostatic model. The criterial attributes for the electrostatic model described in Chapter 4 (Table 4.5, p. 87) are reproduced in Table 6.4.

Table 6.4 Criterial attributes for the *electrostatic model* for ionic bonding

	Level 1	Level 2	Level 3
1.	ion formation	ion formation	ion formation
2.	ion size	ion size	ion size
3.	ion shape	ion shape	ion shape
4.	ion type/charge	ion type/charge	ion type/charge
5.	lattice formation	lattice formation	lattice formation
6.	lattice structure	lattice structure	ionic-covalent
7.	ionic-covalent continuum	ionic-covalent continuum	continuum
8.	ion polarisation	ion polarisation	

Unlike the sea of electrons model, there are different criterial attributes for different levels of learner for the electrostatic model for ionic bonding. The researcher monitored learners' descriptions of their mental model as the interview progressed. In many incidences, learners made specific reference to criterial attributes spontaneously; if they did not, the researcher probed their views with prompt questions.

6.7.1 *Learners' Views of Ion Formation, Ion Type, Lattice Formation and Structure*

Criteria attributes 1, 4, 5 and 6 concerned learners' views for ion formation, ion type, lattice structure and lattice formation. Learners offered spontaneous responses for these attributes during their descriptions of their mental models for sodium chloride described above. To summarise these findings; learners across all three levels related ion formation to the octet rule of full-shell stability with metallic elements forming positive ions as a result of loss or transfer of electrons and non-metals forming negative ions as a result of the gain of electrons. Undergraduate and postgraduate learners appreciated that ionic compounds form continuous lattices whereas some secondary school learners viewed the structure as molecular in nature. Learners across all levels appreciated that lattice structures were definite and specific to the substance. These latter views were supported by the spontaneous drawing of lattice structures for sodium chloride and in discussions of the depicted models for caesium chloride (IB01, p. 80).

Responses for criteria attributes 7 and 8 were elicited by discussion of the bonding in lithium chloride; for the remaining criteria attributes learners' responses were probed with follow-up questions during their discussion of the bonding in sodium chloride.

6.7.2 *Learners' Views of Ion Size*

Learners' views of ion size were offered spontaneously during discussion of their mental models for the bonding in sodium chloride, or specifically elicited by prompt questions. Some learners also made spontaneous comments regarding ion size when describing their mental model for the bonding in lithium chloride.

Secondary school level learners seemed to hold a variety of views about ionic size; a number of learners asserted that the chloride ion is larger than the sodium ion; however, others believed that the sodium ion was the larger. David for example, stated "Na would be bigger, and the Cl would be smaller", and Richard, "I say the sodium is the larger one and the smaller ones would be the chloride". Others

seemed unsure of ionic size; Anne stated that "I can't remember which way around it is" and Frances "I think chloride's bigger than sodium, I am not sure, I think chloride is bigger". There is not necessarily a correlation between secondary school learners' diagrams and response to prompts about ion size. Anne seemed unsure about ion size, however, her drawing for sodium chloride (Figure 6.28) shows the ions to be of quite different size (note that she has drawn the sodium ion as larger than the chloride ion).

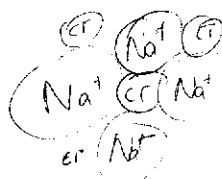


Figure 6.28 Anne's drawing illustrating the structure of the sodium chloride (NaCl) lattice

Although Neil also seemed uncertain about relative ion size of chloride and sodium ions, "yeah they would be different, one's bigger, one's smaller, I expect [respondent laughs]", but, unlike Anne, his response was inconsistent with his drawing of the structure for sodium chloride in which he drew similar sized spheres for both ions (Figure 6.29).

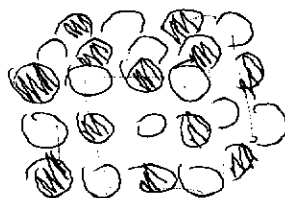


Figure 6.29 Neil's drawing illustrating the structure of the sodium chloride (NaCl) lattice

Secondary school learners failed to comment on the size of the lithium ion; the sole comment from Keith, who again seemed uncertain about relative ion size, stated

that "lithium would be bigger. It'd have more protons and electrons. It'd be bigger. I don't know if it would be bigger, smaller maybe, I don't know, I don't remember".

Undergraduates were more emphatic regarding ionic size for sodium and chloride ions. With a few exceptions, they stated that the sodium ion was smaller than the chloride ion and, moreover, provided explanations for their assertions. Bob, Alan and René, for example, related the size of the chloride ion to inter-electron repulsion.

Bob. Because you've got a greater negative charge floating around the outside of the small positive charge in the middle, there's a slightly higher amount of repulsion amongst the electrons pushing them apart, making it bigger.

Alan. The extra electrons means sort of repulsion of the electron cloud.

René. The chlorine well it's got an extra electron, so yeah repelling, like an extra electron.

Whilst undergraduates offered explanations for the larger size of the anion chloride, they did not offer particularly convincing explanations for the difference in sizes of the sodium and chloride ions. Alan, for example, stated that "I've always been told the sodium ion is smaller and the negatively charged ion is slightly larger", Phill explained that "they are not a lot different in size", and Jane said that "sodium has got a lower atomic number than chlorine". Others related the smaller size of the sodium ion to electrostatic model conceptions such as shell and loss of electrons, René stated that "the sodium ion has a reduced radius from the neutral atom because it's got less electrons" and Kim, "chlorine's like gained an extra shell and sodium's lost one". Only one learner, Steve, without the use of a Periodic Table, provided a comprehensive explanation, relating the size of the ions to the electronic sub-shells or orbitals in the respective atoms.

The Na^+ ion has simply the $1s^2$, the $2s^2$ and the $2p^6$, whereas the chlorine's filled the $1s^2$, the $2s^2$, the $2p^6$, the $3s^2$ and the $3p^6$ [Figure 6.30]. Because it's filled more orbitals, and as the orbital energy, um...I am just trying to think about this. As you get more and more orbitals,

they go out further and further and further away from the centre of the nucleus itself. So the radius, r , increases. So that as you go to a new energy level, so that's filled up to the end of the two. But that's filled up to the end of the three, and so that's going to be a larger radius by quite a bit.

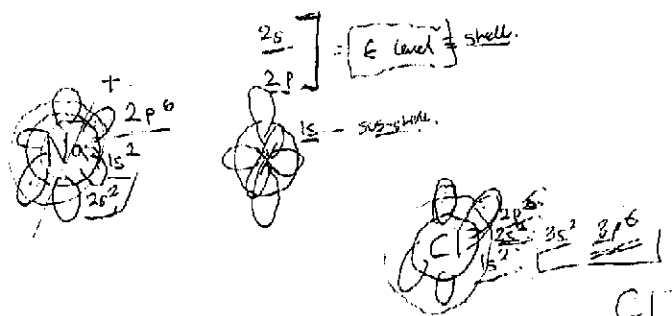


Figure 6.30 Steve's drawing illustrating the ionic radius for the sodium and chloride ions

Six undergraduates commented on the size of the lithium ion in relation to the sodium ion when discussing the bonding in lithium chloride. Four learners stated that the lithium ion was smaller, for example, Bob "it will be a lot smaller than sodium". Steve was the sole undergraduate to provide a detailed explanation.

It's different in the size [of the ion]. The lithium would be even smaller than the Na^+ . Because in lithium you have filled the $1s^2$. If it is going to be lithium plus, that would be it. So you have got hydrogen, helium, lithium, [writes H He Li], so only the $1s^2$ is filled. It's only got that first energy level filled whereas Na^+ has all of the second filled as well, so the lithium's radius is going to be less than the Na^+ .

The two learners who appeared to believe that lithium ion was larger than the sodium ion seemed rather uncertain; Alan stated "I would consider lithium to be slightly larger than the sodium", and Mary that "because it's exactly the same charge... maybe it could be a little bit bigger... maybe a little bit bigger than sodium, the lithium".

Postgraduate learners were surprisingly unsure about the relative sizes of the sodium and chloride ions. Five postgraduates stated that the sodium ion is smaller

than the chloride ion for similar reasons as provided by undergraduates, with Jason and James providing the most comprehensive explanations.

Jason. The sodium atom having lost an electron is a lot smaller, and because it has a positive charge now, it's attracting the electrons closer towards it. So it's holding what electrons it has left even tighter. Whereas the chlorine, because it has an extra electron, is much bigger, because the nucleus will now no longer hold all its valence electrons.

James. The sodium one gets smaller because it loses an electron and the charge on the nucleus pulls in all the other electrons even more. The chlorine one gets bigger because you have an extra electron on it. So they will sort of repel each other and then move out and the nucleus can't sort of pull all the electrons in as much as it was.

Interviewer. Could you perhaps compare the size of the sodium with the chlorine?

James. The chlorine would be heaps bigger I think.

However, Grace and Rose stated that the sodium ion is larger than the chloride; Grace stated that "the chlorine would be smaller 'cos it's got more electrons. It's got more electrons than protons so it's heaps smaller, it's got more attraction running around" and Rose believed that "the sodium is larger and the chloride is sort of packed around it". Christine seemed uncertain about the size of the two ions and related the size of the chloride ion to chlorine gas; she stated that "they are different, yeah. I think I think chlorine like a gas bigger [respondent laughs]". Jenny, like Christine, seemed uncertain about the relative size of the ions and stated that "well I know they are different but I visualise them as being the same". Interestingly, upon probing she was unable to explain why she believed the ions were similar in size "chloride might be larger, I know they are different, but when I visualise them they are the same". Postgraduates were more confident about the relative sizes of the lithium and sodium ions, with six learners stating that lithium was smaller than the sodium ion, but Jenny again was unsure on the relative sizes "I can't tell you which is bigger" consistent with her uncertainty about the sizes of the chloride and sodium ions.

6.7.3 Learners' Views of Ion Shape

Secondary school learners seemed rather unsure of the shape of sodium and chloride ions. Although most learners drew circles or spheres when constructing diagrams of sodium chloride, only one learner, Anita, explicitly stated that she saw the ions as circular or spherical in shape, "probably little balls again, it's like little circles". Secondary school learners, rather described ionic shape in terms of the underlying atomic structure as seen in Neil's response.

A sodium ion would probably be [draws solid circle with large circle around it, Figure 6.31] like that sort of thing and you would have it like that, a really long way out, and even further than that, that's not to scale [respondent laughs].

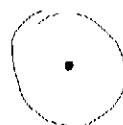


Figure 6.31 Neil's drawing of the sodium ion

Neil went on to describe the shape of individual ions as being "round, it's the sort of shape planets travel". Others were rather confused, for example, David stated that "it'd be like protons and neutrons in the nucleus" and "they would be white or something".

Undergraduates typically described sodium and chloride ions as spherical or circular in shape as illustrated by the following responses; Alan, " I suppose I have always envisaged them as spherical", Phill, "just circular I guess, sphere, spheres", and Renéé, "in the pictures it's depicted as spherical ". Some undergraduates used terms from other concepts of bonding, typically the molecular orbital theory. For example, Bob introduced the concept of orbitals in his explanation of the shape of sodium and chloride ions.

Bob. Well once again because all the orbitals, because all of the orbitals are now filled, once again there is a certain amount of symmetry there. It's got both. It's got the 3s as well as these 2p, so once again it's symmetrical in shape.

Interviewer. Symmetrical in shape. So is that spherical or not?

Bob. I have always thought of them as being spheres. Basically that's always been the image that we have been given, But just thinking about it now, because of the, the 2p have formed sort of fuzzy lobes, it's difficult to see that they can sort of merge together and form a sphere.

Like Bob, Kim and Mary related ion shape to other concepts such as clouds. Kim seemed to use the term "cloud" to define the shape, whereas Mary seemed to confuse electron clouds with shells.

Mary. I just think of circles surrounded by a cloud of electrons, the sodium would be a smaller circle than the chlorine.

Interviewer. You said cloud of electrons. Can you just tell me a bit more about that?

Mary. Just like surrounding the nucleus. I guess the thing like what I was drawing before. Like that would be [draws large dot, LHS of Figure 6.32].

Interviewer. That dot, yes.

Mary. That would be sodium and maybe that would be chlorine [draws second larger dot on RHS of first dot] and the sort of electron cloud surrounding it [draws concentric circles around each dot]

Interviewer. So that circle you have drawn there, that represents the electron cloud?

Mary. Electron shells I guess.

Interviewer. Shells? Do you see shells and clouds as the same?

Mary. Yeah, yeah, I do.



Figure 6.32 Mary's drawing illustrating the sodium and chloride ions

Postgraduates, like undergraduates, also viewed sodium and chloride ions as spherical in shape; for example, James claimed "it'd be more or less spherical", Christine said "I think of sodium plus as a round ball" and Kevin saw "a sodium ion as being spherical and I think of the chloride as being just larger and spherical". However, postgraduates extended the idea of spherical ions to include ideas relating to polarisation of the chloride ion described in detail in Section 6.7.4 (pp. 191-197). In addition, one postgraduate, Christine, employed an elaborate compound analogy

to describe the shape of the chloride ion (Chapter 7, pp. 260-261). The noteworthy point here is that it seems postgraduates are happy to use the concept of packing of spheres to model ionic bonding and structure, but have developed more sophisticated notions about details of the structure such as ion shape and were able to inter-link ideas from different models.

6.7.4 *Learners' Views of the Ionic-Covalent Continuum and Ion Polarisation*

Learners' views of the ionic-covalent continuum and ion polarisation were not elicited directly, but the use of lithium chloride as an additional prompt was intended to provide learners with an opportunity to discuss these concepts. Because the lithium cation is small and highly polarising, it induces significant covalency into the bond. Consequently, lithium chloride was chosen as the prompt. Since the two compounds contain a common anion (i.e., chloride) it was intended that learners would focus on the nature of the cation.

Secondary school learners almost universally believed there was little difference in the bonding in lithium chloride and sodium chloride. It seems that this view was related to the notion that they are both univalent ions. Anne, for example, stated that the bonding was "basically the same, 'cos lithium is one plus, the same as sodium" and Anita stated that there was no difference because "lithium is one plus and the chloride's just minus and so yeah it's the same". Probe questions about differences in the bonding in lithium and sodium chloride failed to produce further detail, although respondents appeared uneasy, perhaps sensing there were differences—but any answers offered were tentative. Keith, for example, viewed the lithium ion as smaller than the sodium ion, however, he seemed unsure as to what influence this might have on the bonding, thinking that "I don't know it might actually make it stronger or weaker, I don't know".

No secondary school learners responded to the use of lithium chloride as a prompt in the way intended; that is, they failed to realise the significance of the smaller more polarising lithium cation. However, during her description of the bonding in sodium chloride, Claire, showed some appreciation of the ionic-covalent continuum stating that "nothing is ever purely ionic". This she deduced from her

ideas about electronegativity, although confusion about electronegativity led to some ambiguity in her description. She stated that "the electronegativity increases going up" the Periodic Table and decided that lithium has a higher electronegativity (and is more reactive) than sodium. She then related the difference in electronegativity to the sharing of electrons.

Claire. It's still ionic because the lithium has a stronger attraction [drawing Li and Cl enclosed by circles, lower part of Figure 6.33].

Interviewer. Stronger attraction to what?

Claire. To the lithium. So the one electron they are sharing it will still spend most of the time around the chlorine or chloride. But it'll spend more time around here as well [draws small circle between Li and Cl and draws lines linking the "e" to Li circle].

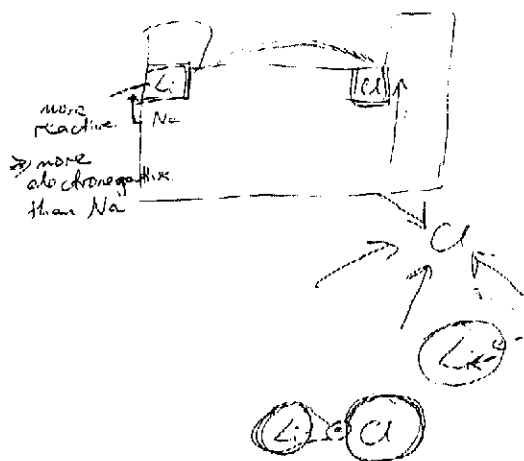


Figure 6.33 Claire's drawing illustrating the bonding in lithium chloride (LiCl)

Although Claire seemed to hold an alternative conception about electronegativity, that is, that it involved sharing of just one electron (see Chapter 7, p. 277), it appeared she possessed an appreciation of the ionic-covalent continuum.

Undergraduates descriptions of the bonding in lithium chloride centred on the relative sizes of the lithium and sodium ions (Section 6.7.2, p. 187). Like secondary school learners, undergraduates seemed unsure what the significance of the size difference would have for the bonding in lithium chloride again suggestions appearing rather tentative, as seen in Alan's response.

Alan. I basically see the bonding to be the same but I would consider lithium to be slightly larger than the sodium so could be slightly different ratio. So a different close-packing arrangement sort of thing. It might not be quite as compact.

Interviewer. So because of its size it is different?

Alan. Ratio of sizes of cation to anion would be different.

Interviewer. What would that effect?

Alan. The packing arrangement.

Interviewer. Do you see any other difference, say in the interaction between the lithium and sodium?

Alan. Um, no.

Similarly, Phill stated the difference in size "might affect the angles" and Steve and René believed that it would affect the number of chloride ions that could pack around a lithium ion compared with a sodium ion.

Steve. The chlorides have still got the same size. Well it's the same species and this [i.e., lithium] is smaller it's going to be difficult for more chlorines to get in quite as close to the lithium.

René. Because the lithium ion would be smaller than sodium which would probably mean you would have less of them around the co-ordinate sphere I think [respondent laughs].

Mary held a mixed model for the bonding in sodium chloride as described in Section 6.6.2 (p. 175). Upon further probing she seemed to become more confused by the concept of the sharing of electrons in the ionic compound.

Mary. Yeah they are sharing, like when they form a covalent type bond.

Interviewer. The line you have drawn...

Mary. You look at it as being like, I don't know you have got like [draws solid lines from Cl^- to Na^+ , Figure 6.34].

Interviewer. Those lines you just drew there now, what are you indicating by that?

Mary. Far out, um [respondent laughs], yeah 'cos I've always, I dunno, I've looked at it and thought of that kind of crystal thing and I know that they have the sharing of electrons between them. But then you think, well how do they actually...in that big crystal.

Interviewer. Can you tell me where you see the electrons? Say as you have drawn it there, where are the electrons?

Mary. Well yeah they are kind of like in between there [draws filled circle between Cl^- and Na^+].

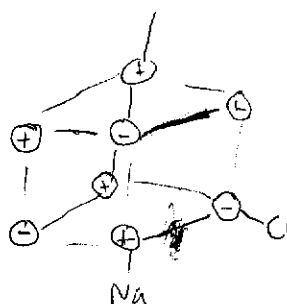


Figure 6.34 Mary's drawing illustrating the bonding in sodium chloride (NaCl)

Mary seemed clearer in her explanation for the bonding in lithium chloride, and she was more confident that lithium chloride contained covalent bonds; her drawing for the bonding (Figure 6.35) is more consistent with covalent bonding than ionic bonding.

Mary. I suppose it'd be the same. Just say once again you'd have like in the chloride [writes Cl^-], and you'd have it [writes Li^+] and you know they would come together, and they form like, um, a shared bond [writes $\text{Li}-\text{Cl}$ underneath].

Interviewer. So that's similar to what you drew before for the sodium. Do you see it as being different in anyway?

Mary. Um...probably the packing. That would be different, like the way it forms...the crystal and stuff, but I don't actually know.

Interviewer. So it'd be different, but you are not sure?

Mary. Yeah I am not, I'd still look at it as being a covalent bond.

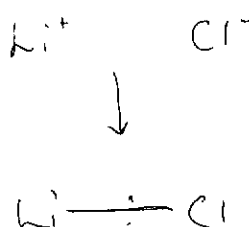


Figure 6.35 Mary's drawing illustrating the bonding in lithium chloride (LiCl)

It is not clear from these descriptions if Mary appreciates the concept of the ionic-covalent continuum for bonding in such compounds, or rather that she harbours an alternative conception about the bonding in sodium and lithium chloride. Her earlier description of the bonding in sodium chloride seems to indicate the latter. In

summary, none of the undergraduates made specific mention of the ionic-covalent continuum, although some suggested that ionic compounds like sodium and lithium chloride involved covalent bonding.

A similar situation existed with respect to polarisation. Interestingly, only one undergraduate, Bob, spontaneously introduced the concept of polarisation during his description of the shape of the chloride ion.

Bob. The chloride shape, big, floppy type of thing. Because you've got a greater negative charge floating around the outside of the small positive charge in the middle, the amount of repulsion amongst the electrons pushes them apart making it bigger.

Interviewer. When you say bigger. Bigger than what?

Bob. Than the sodium.

Interviewer. OK.

Bob. Um, and sort of big as far as anions go too. Not as big as iodine obviously, or iodide. Yeah, so big and floppy, the cloud shape can be influenced by the small positive charge of things like sodium.

Despite almost all undergraduates appreciating that the lithium ion was significantly smaller in radius than the sodium ion, only Bob related this to increased polarising power stating that "lithium one plus will be a lot smaller than sodium and quite possibly a lot more influencing on the electron cloud of the chloride".

Postgraduates responses to the lithium chloride prompt were similar to those of the undergraduates, with the commonly-held view being that the size of the lithium was the main difference. Postgraduates felt that this would offer little influence on the bonding with, for example, Grace stated "the lithium is positively charged, and the chloride negative, and I don't see any difference" and Brian claimed that "the lithium is in the same position as the sodium, where it prefers to lose an electron, so it should be exactly the same". Three postgraduates, Jason, James and Christine, made mention of the concept of polarisation, Jason and James offered comprehensive descriptions, with Jason in particular going into considerable detail in his description of the shape of the sodium and chloride ions.

Jason. I see them [the chloride ion and sodium ion], because neither of them are particularly polarisable, they are fairly spherical.

Interviewer. OK, you mentioned polarisable. What do you mean by that term?

Jason. I kind of regard polarisability as sort of the floppiness of the anion [respondent laughs]. It's sort of big and easily deformed. I guess I sort of associate it with the softness of the anions as well. Now I have to describe what floppiness and softness is?

Interviewer. OK that's alright, you can keep going. So you are saying floppy or soft...

Jason. Yeah, and if you have a polarising anion, ah, cation, the cation would be small and highly charged and so it would have a tendency to distort the electrons that are near by, of the nearby anion. So, for example, if you had your sodium and your iodide or something, you'd have a very strongly polarising cation and a very polarisable anion. So you're probably not going to have strict ionic bonding like you have here quite a different thing altogether.

Interviewer. So what would be different? What would be the different type of bonding other than ionic?

Jason. That's when you would get more into covalent with the sharing of the electron.

Despite his detailed spontaneous description offered for sodium chloride, Jason made no mention of polarisation when describing the bonding in lithium chloride. Rather he saw any differences in terms of packing and bond strength stating that "I sort of see the lithium atom perhaps as instead of filling that cavity like the sodium did, sort of floating in the middle which perhaps weakens the bond". James was more specific about polarisation relating the size of the ions to the electrostatic potential, although he asserted sodium chloride would be more covalent in nature.

James. Lithium is higher up [i.e., the Periodic Table], so the charge would be a lot smaller, so there'd be a much higher, it's called electrostatic potential, so the bonding might be a bit stronger.

Interviewer. Stronger?

James. A stronger bond, and if there was going to be any covalency in it at all, there'd be more in the sodium chloride than in the lithium chloride.

Interviewer. Can you just tell me what you mean by electrostatic potential?

James. It's like when you've got the charge-to-the-density on the surface, sort of how concentrated that charge is.

Christine also mentioned charge density but was unable to use the idea to explain the bonding in lithium chloride.

Christine. Lithium is smaller than sodium, it'd have a higher charge density. So it's trying to fit the same amount of charge into a smaller space.

Interviewer. How do you imagine that in terms of the bonding?

Christine... I don't really think it would, because they are so close on the Periodic Table. Like I know there is a difference in size, and that will have an effect on bonding, and I know that lithium will have a higher charge density. But...because they are reasonably close...they'd be slightly different. Sodium chloride, I can't actually think in what way it'd be different.

The rather mixed responses found here suggest that using lithium chloride as a prompt for the concepts of polarisation and the ionic-covalent continuum may have been too subtle. However, it is not particularly obvious how learners' views of such esoteric concepts can be easily accessed without the use of leading questions which may introduce bias. The data here do provide some insights and perhaps the most notable feature of this is that concepts like the ionic-covalent continuum, unlike, for example, lattice structure and ion size, do not form a major part of the learners' mental models for ionic bonding.

6.8 Learners' Use of Mental Models for Ionic Bonding

Learners' use of mental models for ionic bonding to explain properties of ionic compounds was probed in a similar manner to that for metallic bonding; namely, by the use of focus cards depicting events involving model use. Focus card IB02 (p. 80) depicted an event in which the conductivity of solid and molten sodium chloride were compared, with conductivity indicated schematically by the presence of a glowing light bulb.

6.8.1 Learners' Explanations for the Conductivity of Molten Sodium Chloride

Secondary school learners offered essentially the same explanation for the conductivity of molten sodium chloride that they did for the conductivity of copper wire (pp. 153-154), namely, the movement of free electrons; Frances claimed that "the molten frees the electrons...giving them more energy from the heat allows the electrons to be released into the circuit" and Richard stated that

"once the sodium chloride has been heated up all the electrons are free to move". Conversely, the lack of conductivity for solid sodium chloride was associated with lack of electron freedom or movement as illustrated by Keith, Neil and Richard's responses.

Keith. A solid block the bonds are...are rigid, and aren't allowing the sodium chloride to sort of ionise...holds the electrons from flowing on through the sodium 'cos the molecules are held like tightly together by the bonds in the sodium chloride so they can't move around, so the electrons can't flow. But in that one [points to RHS circuit in IB02, p. 80].

Interviewer. The molten one?

Keith. The molten sodium chloride, 'cos its molten, the electrons are more free.

Neil. The molten sodium chloride, 'cos it's molten, the electrons are more free.

Richard. The electrons aren't free to move, they are locked in position.

Some learners' explanations suggested that they believed ions and electrons were interchangeable. Neil, for example, began by talking about the conductivity being due to electrons, and then ions stated that "the sodium chloride in that fixed structure has got all electrons committed, they are not free, but with the molten [sodium chloride], all the bonds have been broken and these ions are free to move". Anne, however, related conductivity directly to the presence of free ions, rather than electrons.

Anne. Well the sodium chloride requires energy to break the bonds so and that's supplied by the heat and they are broken into sodium ions and chloride ions so they allow the current to flow through them and light the bulb.

Interviewer. OK in what way is that different to the solid block of sodium chloride?

Anne. Well they are fixed in their structure [respondent laughs] and so there's no electrons can flow through there's, no ions too.

Claire related the conductivity to the movement of ions although she stated that the ions were in solution rather than in the liquid phase.

Well they are all stuck in there and they are all attracted to each other because of the electromagnetic force. So no ions or electrons can move to carry the current through the circuit. Whereas in this one, when you heat it and make it molten, you've broken the intermolecular forces which are between the particles. So you've got ions in solution so they can move around and carry the current through the circuit.

Upon further probing she stated that "it's all ions, there's no water or anything in it because it's molten" and that the two situations were similar since "a solution would still carry current because the ions are still free to move".

Undergraduates more typically believed that conductivity of molten sodium chloride was related to the movement of ions as opposed to free electrons, for example, Phill stated "the ions can move about", Reneé claimed that "the molten state will have sodium ions and chloride ions moving about so it can conduct the current", and Kim stated that "there's no free electrons there's no free ions, whereas that one [pointing to molten sodium chloride in IB02] has got free ions". Steve offered the most comprehensive explanation.

In the solid there are no actual free ions present at all so it's not possible to get any current flowing through the crystal. In the case of the molten sodium chloride that structure is now broken and we have got free Na^+ and Cl^- ions, so consequently you end up with free ions that are capable of moving and that's equivalent to current.

However, like secondary school learners, a number of undergraduates believed conductivity was due to either ions or electrons, for example, Bob stated that "in the crystal the ions are quite so free to move...whereas in the liquid the charges don't have to be used to hold the shape and the electrons are free". Similarly, Alan attributed conductivity to "loose electrons" in molten sodium chloride. Again like their secondary school counterparts some undergraduates, like Jane, related their ideas for the molten state with the solution state, saying that "in the molten sodium chloride, I imagine them all being kind of free—it's almost like as you would imagine it as in kind of aqueous solution".

Postgraduates associated lack of conductivity of solid sodium chloride with the idea that the electrons are fixed in the solid structure, but like undergraduates

viewed conductivity of molten sodium chloride as due to movement of ions rather than electrons.

Jason. There's no mechanism for which the electrons can move through, and so I guess that's why you don't get a current in the crystal. The molten sodium chloride, you have got in this case, I would sort of see it more as I guess discrete cations and anions moving about the system rather than rather than electrons.

James. In the crystal, it's highly ionic and the electron is held very tightly, and there's no sort of sharing of electrons or delocalisation. So there's nothing to carry the charge. In the molten sodium chloride, the ions are free to move around so the ions will be able to carry the charge from one electrode to the other.

Grace. I see it that in the left-hand side when it's a crystal, because it's a solid, and is so rigid, you don't really associate it with much interaction going on because everything is stuck where it is. But then on the right-hand side where it is molten, things are moving around more. So the sodium chloride has dissociated, so as things warm up there's more interaction with things whizzing around. So in the right-hand one sodium chloride is all moving around more, and because of that you are able to get transition of the charge I guess, flowing through because the ions can move more freely whereas in the solid they are stuck where they are.

Brian. In the crystal matrix the atoms are stationary they can't move at all, or the ions rather are stationary. So while there are charged species there, they can't move from one electrode to another. Whereas in the molten sodium chloride, you have got sodium plus and chlorine minus still attracted to each other, with the electrical charge they have got. But the because they are a liquid, they are able to they are not held in place as they would be in a solid. So they are able to move to the electrodes and pass the current.

However, again some responses related conductivity of molten sodium chloride to electron movement rather than ion movement, for example, Jenny stated "the electrons aren't sort of free to move", and Rose in a more ambiguous explanation claimed "in the molten one they would be a bit more free to move, and the electrons would be able to go and light up the bulb". Christine seemed surprised that molten sodium chloride conducted electricity at all—"that's funny I would have thought the light would have been going on there [indicating the LHS of IB03, p. 80]". She considered that solid sodium chloride would conduct electricity since "there's some room for flexibility, like there's room for electrons to shuffle around". Upon

reflection, she concluded that molten sodium chloride could conduct electricity as a result of the liquid behaving "like a liquid metal, as in the free electrons".

6.8.2 *Learners' Explanations for the Friability of Sodium Chloride*

Learners' use of mental models for ionic bonding was also probed by discussion of their understanding of the friability of sodium chloride. In focus card IB03A (p. 80), shown to secondary school learners, the friability of sodium chloride was compared with that of diamond, and in focus card IB03B, shown to undergraduates and postgraduates, it was compared with silica. Secondary school learners mostly attributed the friability of sodium chloride to weak bonding in the ionic compound, for example, Anne stated "the bonding in chloride is weak" and Keith similarly "the bonds in sodium chloride I don't think are as strong". However, several learners commented that the bonding in sodium chloride is strong, and friability is due to displacement of the lattice resulting in repulsion between like-charged species; Claire in particular offered a quite detailed explanation.

The sodium chloride, they are held in place by really strong electromagnetic forces between them, between the atoms because of the big electronegativity difference [drawing cube with Na and Cl inside circles, Figure 6.36]. So when the force pushes them closer together these two strongly negative ions will repel each other, same with the positive ions [draws double-headed arrows between ions]. Because they are very strongly charged so that causes the crystal to break up into smaller bits.

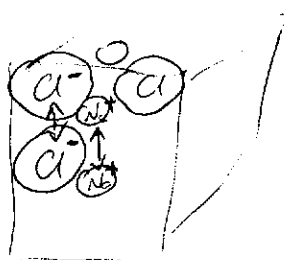


Figure 6.36 Claire's drawing illustrating the friability of sodium chloride (NaCl)

Although Keith seemed to believe that the bonding in sodium chloride was weak, he also pointed out the force will result in a situation in which "those positive ends go together and sort of repel", and David likewise stated "the negative and positive

charges would align and then they would break into smaller ones". The lack of friability for diamond was attributed to the presence of stronger bonds, for example, David stated "in the diamond, covalent bonding is a lot stronger" and "it takes a lot more force to break them up". But learners also showed an appreciation of the significance of the giant-covalent network structure. Anne, for example, stated that in the diamond "you have got bonds between layers" and Anita that "the diamond is all stuck together and they can sort of support each other". Others offered more detailed explanations—Claire drew a covalent network structure and pointed out that unlike sodium chloride, there are not charged species present in the lattice.

The diamond is not ionic bonding. It's something else, probably covalent. No, yes that's right, it's carbon, covalent carbon. One two three four bonds [drawing series of Cs joined together, Figure 6.37] yeah so it's still held in a covalent lattice but [adds extra lines] but there's no charges involved, so they don't repel each other when you try and squish them.

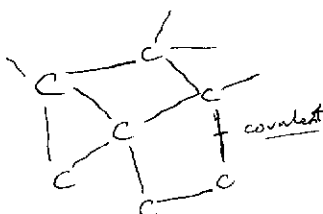


Figure 6.37 Claire's drawing illustrating the structure of diamond

Likewise Frances stated that she saw diamond as containing "giant covalent bonding" in which the carbons were held together by a "tetrahedral arrangement" of carbon atoms.

Diamond's the hardest known sort of material in the world. Because they have got these strong [drawing small circles in a tetrahedral arrangement, Figure 6.38], I am trying to draw a tetrahedral, or something like that shape.

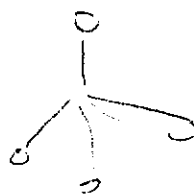


Figure 6.38 Frances's drawing illustrating the structure of diamond

Undergraduates mostly attributed the difference in friability between sodium chloride and silica to strong bonding in silica and weak bonding in sodium chloride for example Kim, "the sodium chloride's got weaker bonds than silicon dioxide, it'd be easier to break I suppose", and Jane, "I think 'cos you think of them as being heaps stronger". However, undergraduates also showed an appreciation of the importance of the network structure of silica—Steve offered a detailed explanation.

Steve. OK I think back to my high school years [respondent laughs] about this. With the sodium chloride of course you have got ionic bonding [writes ionic bonding, Figure 6.39], and the silica has covalent [writes covalent]. So that's the key difference between the two. In the case of the sodium, in general if I remember the order the covalent bonding tends to be stronger than the ionic bonding [writes covalent > Ionic bonding].

Interviewer. OK.

Steve. Yep, and as a consequence, if one is to apply a certain force to the NaCl, it's possible to say, if you have got an infinitely extended network as you had before [draws Na's in diamond pattern linked by lines], of these repeating units, you could say break one unit, it would break a whole unit cell from another block and split the crystal.

Interviewer. Why is that able to happen in that case?

Steve. Well because the ionic bonding that is holding this crystal together here is weaker than is the case of the covalent, so it's forming once again a network. But it's a covalent silica network [draws two Si's linked by O in triangular shape], and the covalent bonds being stronger they are more difficult to break and therefore it's more difficult to break apart than the network.

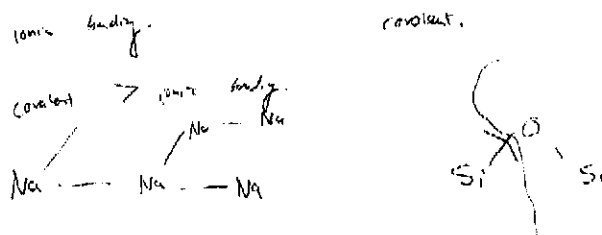


Figure 6.39 Steve's drawing illustrating the friability of sodium chloride (NaCl) and rigidity of silica (SiO₂)

One undergraduate, Bob, remarked on the presence of charged species in sodium chloride. However, he related the brittle nature of sodium chloride to the inverse square law of electrostatic forces rather than to the repulsion of like-charges.

It's maybe related to the positive and negative charges on that. If enough force is applied to get them far enough apart so that, that one over r squared term, they um, the electrostatic force between them can, if it knocks them far enough apart, so it's not valid anymore, then they are going to let go.

Postgraduates were more ambivalent in their explanations for the event although their explanations were more detailed. Strength of bonding and covalent network structure were common ideas, for example, Jenny stated that "I see them [the bonds in silica] as being strong so they would be harder to break", but postgraduates also introduced other ideas such as the "stretching" or "flexing" of bonds.

James. Probably because there is no stretching in it [i.e., sodium chloride] because if you just move them apart a little bit, and it may take a bit of force, then the interaction drops off and there's nothing holding them together anymore and so it's broken. Silica, it's a covalently bonded with silicon and oxygen so you can sort of stretch the bonds a bit, and that that way you could apply a force and they wouldn't break.

Christine. The fact that they didn't break up means that the bonds are stronger than the sodium chloride. At least they're more, they are not actually stronger...they would have to be quite rigid to not...I think of them as rigid as a like a rigid bond. Like snap really easily.

Interviewer. OK.

Christine. So it's not that it's held or it would have to be so strong and it's like a like a brick I guess. It's holding it very rigidly so even if you are applying a force it's not going to break it. It's a strong bond but it's going to have to be extensive like a real network of bonds because that's the only way to hold the whole...

Interviewer. This is the silica you mean?

Christine. Yeah the silica. With the sodium chloride I guess you have got I'm thinking it's easier to just break up into discrete little packets like, it's still the same type of bonding, but maybe it's got places where it will break more easily even though it's the same everywhere.

Grace ostensibly believed ionic compounds are "not actually bonded" and suggested that they are instead "physically attracted" in contrast to silica in which "everything is covalently bound". According to Grace the difference between a bond and an attraction is that the latter involved "sharing of electrons" whereas the former was simply an "electrostatic attraction", and it appears she sees these as substantially different in strength. Kevin attributed the brittle nature of sodium chloride to defects in the crystal.

Kevin. In terms of the sodium chloride again you are looking at a lattice configuration in three dimensions. As you apply the force you apply a stress which is able to fragment the lattice and it fragments along lines, such that each of the smaller crystals is effectively the same in all three dimensions as the large crystals were, but on a smaller scale. So it's been compacted in the three dimensions I suppose, but effectively the same lattice arrangement exists.

Interviewer. OK. So why is it fragmenting? Can you sort of focus on that?

Kevin. Why is it fragmenting? Ah the reason as I see it, probably the reason for that would be the large crystal of the sodium chloride, as you get larger and larger, there are defects in the crystal, lines where edges and cracks sort of thing where as you apply the force you have got a tendency to fragment them along those sort of defects.

Jason claimed the brittle nature of sodium chloride arose as a result of repulsion of like charges.

Jason. The sodium and sodium chloride [drawing rows of Na^+ and Cl^- , top LHS of Figure 6.40], you start with a situation where opposing charges are lining up and that's providing the attractive force. OK so you have this sort of system, and then when you apply a force, so say a shear force which pushes [drawing an arrow at top of one row of ions].

Interviewer. Along one line yep OK.

Jason. There's sodium, chlorine, sodium and then that force has all of a sudden pushed the chlorine next to the chlorine [drawing second row of Na^+ and Cl^- alongside each other]. So there is now no sort of bonding forces in this direction now [draws diagonal lines linking Na^+ and Cl^- , top RHS of Figure 6.40].

Interviewer. So those are the ones on the angle, and they are the bonding forces?

Jason. Yep, and now you have a repulsive force which is right next to each other [drawing double-headed arrows between ions] pushing each other apart, and so therefore you get a shear down there [draws a line between rows of ions].

Interviewer. Right down the middle OK.

Jason. So it's broken apart. Silica on the other hand is a lot stronger. So that's why we don't end up with grains of sand on our beaches. Silica has got covalent bonding where each silicon is surrounded tetrahedrally by a by four oxygen atoms [drawing SiO_4 unit in tetrahedral configuration] and these are covalent bonds which are extremely strong, and they don't break particularly easily at all.

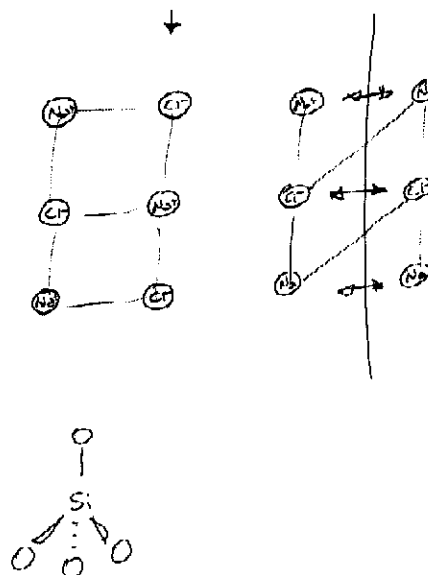


Figure 6.40 Jason's drawing illustrating the friability of sodium chloride (NaCl) and rigidity of silica (SiO_2)

6.9 Summary

Learners' preferred mental model for the target system of ionic bonding is the simple electrostatic model, although like the target system metallic bonding, a few learners held mixed models and used concepts from other target models. Secondary school learners identified the bonding as an attraction between charged species which they related to the octet rule. Undergraduates and postgraduates provided similar but more detailed descriptions of their mental models, used domain specific terminology and showed a greater appreciation of the continuous nature of ionic lattices. Secondary school and undergraduate learners preferred simple realist depictions of ionic bonding from those illustrated on focus card IB01. Postgraduates in contrast preferred a more complex depiction that illustrated the continuous nature of the ionic lattice more clearly. Learners' understanding of the electrostatic model for ionic bonding varied depending on level of learner. Secondary

school learners appeared to hold a number of alternative conceptions about ionic size and ionic shape and had little appreciation of the concept of the ionic-covalent continuum or polarisation of ions; although the latter concept was not probed directly. Undergraduates and postgraduates descriptions for ionic size and ion shape were more in accord with the scientific conceptualisation, although a number held alternative conceptions about ionic size. Likewise, few undergraduates and postgraduates offered explanations for polarisation and the ionic-covalent continuum that were in agreement with the scientific conceptualisation. Learners across all academic levels used the octet rule based model to explain the conductivity of molten sodium chloride and non-conductivity of solid sodium chloride. Secondary school learners, however, stated that conductivity of molten sodium chloride was due to the presence of free electrons rather than ions. In contrast, undergraduate and postgraduate learners typically asserted that the conductivity was due to the movement of ions, in accord with the scientific view. Learners across all academic levels inappropriately attributed the friability of sodium chloride to the presence of weak bonds in the ionic compound, although they related the hardness of diamond and silica to the strength of bonding and giant covalent network structure.

6.10 Learners' Mental Models for Covalent Bonding

Learners' mental models for covalent bonding were probed using the third phase of the interview protocol detailed in Chapter 4 (Table 4.1, p. 77). The portion of the protocol that pertains to the target system of covalent bonding is reproduced in Table 6.5 (p. 208). Like the other target systems, learners were shown two samples, two IAE focus cards, and one focus card that contained depictions of the bonding in a covalent compound. Learners' mental models for covalent bonding centred on two prompts; in this case Prompt 1 and Prompt 5 (Table 6.5). The second sample used was chloroform (i.e., Prompt 2, Table 6.5), and learners generally provided shorter descriptions of the bonding in chloroform than they did for molecular iodine. Initially, like the other target systems of metallic and

ionic bonding, learners stated that the bonding in the second physical prompt was similar to that in the first but drew diagrams to illustrate the bonding in chloroform and described the bonding in detail.

Table 6.5 Interview protocol for the target system covalent bonding

1.	Shown sample of molecular iodine— <i>please describe the bonding in this substance</i>
2.	Shown sample of chloroform— <i>please describe the bonding in this substance</i>
3.	Shown focus card CB02— <i>please explain this process</i>
4.	Shown focus card CB03A/B— <i>please explain this process</i>
5.	Shown focus card CB01— <i>which of these models appeals most/least to you?</i>

Hence, in describing learners' mental models for covalent bonding, results for Prompt 1, Prompt 2 and Prompt 5 are summarised. The remaining prompts were used to address specific criterial attributes the results of which are described in Sections 6.11 and 6.12.

6.10.1 Secondary School Learners

Secondary school learners did not appear to hold any clear preferred mental model for the bonding in molecular iodine (I_2); the single consistent idea being that it involved covalent bonding and that covalent bonding involved sharing, although views on what was actually shared varied. Most learners specified that the bonding in I_2 was covalent in nature, but many were unable to clearly articulate what the term meant to them. Anne, for example, stated that the bonding in molecular iodine is "pure covalent" which she subsequently related to the concept of electronegativity. However, she was unable to provide a definition of covalent bonding, and it is interesting to note that her drawing of the bonding in I_2 (Figure 6.41) does not contain any links between the two I symbols.

Anne. It's pure covalent, they are, um, iodine atoms [drawing two I]. They are identical, they are electronegative charges, is that what it is? Yeah.

Interviewer. Can you just tell me, you used that term covalent bonding. Can you tell me what that term means to you?

Anne. Um...[respondent laughs] yeah...um.

Interviewer. OK you have drawn two Is there. What would hold those together?

*Anne....*The electrons I suppose.

Interviewer. The electrons OK.

Anne. Yeah [respondent laughs].



Figure 6.41 Anne's drawing illustrating the bonding in molecular iodine (I_2)

Anita simply described the bonding in molecular iodine as "strong I think" and stated that it would possess some order "but I don't know what kind of order it would be". Upon probing she described the bond as consisting of the overlap of "bits of iodines".

Interviewer. What does covalent mean to you then?

Anita. It's another picture I have got in my mind. Two things sharing it, and sort of overlapping in the middle, like one little ball and another little ball, and they are joined together and cross over and then they share that cross-over bit.

Interviewer. OK spheres crossing over? Do you mind just drawing it?

Anita. OK [drawing two overlapping circles with Is inside them, Figure 6.42].

Interviewer. OK, OK I have got you.

Anita. Yeah and they share that bit [colours in the overlapping portion].

Interviewer. OK so that stuff in there, that's the bond is it? Is that what you mean?

Anita. Yeah joined there [draws second figure comprising two circles joined by line].

Interviewer. OK so the little bit you have filled in there, the dark bit. What actually is that?

Anita. That's where the two bits of iodines actually cross over, and the bond actually happens.

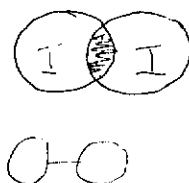


Figure 6.42 Anita's drawing illustrating the bonding in molecular iodine (I_2)

Such a description is reminiscent of the valence bond approach (Appendix A, pp. 338-343). However, given that this model is not part of the secondary school curriculum, it seems more likely that Anita has recalled mental images of space-filling diagrams or models of covalently bonded substances which are similar in appearance to the diagram she drew. Richard appeared to possess no mental model for covalent bonding and was unable to offer any response at all; Frances stated that the bonding in molecular iodine comprised "van der Waals forces" which she described as "like covalent, not as strong". Only three learners related the sharing specifically to electrons and to the octet rule of full-shell stability as seen in Claire's response.

Claire. That one is covalent, because they are identical [drawing two Is inside overlapping circles, Figure 6.43] and there's no electronegativity difference and...

Interviewer. Between what?

Claire. Between the two atoms that are bonded together. So it's not polar the electrons spend an equal amount of time between each atom. The shared ones that is. They share two electrons because each of them needs to gain one [draws two crosses between Is].

Interviewer. Each I is it?

Claire. Yeah, that's it yeah.

Interviewer. Why is gaining that one, why does it need to gain that one?

Claire. Um, to get a full shell [draws two Is surrounded by circles with 7 dots on one circle, and seven crosses on second circle].

Interviewer. OK, I see OK.

Claire. And you join those two [circles one cross and one dot] that one can count that one.

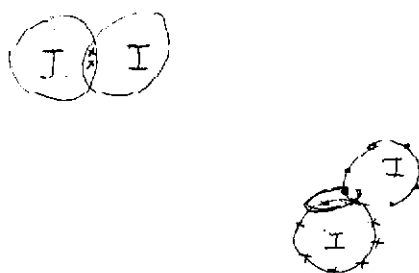


Figure 6.43 Claire's drawing illustrating the bonding in molecular iodine (I_2)

Secondary school learners' preferred mental model for the bonding in chloroform was the octet rule. Learners initially simply stated that the bonding in chloroform was similar to that of iodine. For example, Anita stated that “they are similar because they are both covalent” and Claire that the carbon and chlorines “are sharing two electrons”. However, they were quick to draw structural diagrams of the molecule and, unlike their explanations of the bonding in molecular iodine, these explanations were based on the octet rule of full-shell stability. Neil's view is typical.

Neil. Yeah it's the same kind of thing, but it's more complicated because there's more. Do you want me to draw it?

Interviewer. Yes.

Neil. So you'd have the same kind of thing. You'd have your carbon [draws C, Figure 6.44], and it's got room for like another, it's got four electrons in its outer thing. So it's got room for four more, and it can get one from, like share one with Cl [draws 3 Cl and H next to central C], who only wants one more.

Interviewer. Alright.

Neil. So they can share these [draws small circles in between C and Cl].

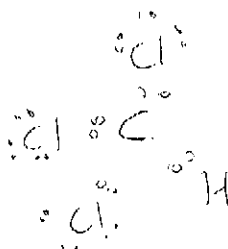


Figure 6.44 Neil's drawing illustrating the bonding in chloroform ($CHCl_3$).

Secondary school learners' preference for depicted models of benzene (C_6H_6) (CB01, p. 81) evidenced high commonality of views. Six learners chose depiction C as their preferred model, one depiction B, and one depiction A. Learners offered two reasons, one being familiarity, for example, David, "yeah I have seen it before" and the other that depiction C was more informative. For example, Anne stated "it's got all the information" and "it's showing where the double bonds are" and Keith said that "you can tell clearly the bonds between each carbon and then the bonds between carbon and the hydrogens". Keith's response and the responses of other learners, indicated that secondary school learners believe benzene possess double bonds. For example, Keith declared a preference for depiction C, but also indicated that depiction B held some appeal. However, he stated that "they are the same" and it seems that the concept of resonance indicated by the ring in depiction B has eluded him. Anita, who preferred depiction B, stated that this was because "I have seen it before" and Frances who preferred depiction A found that it was a "simpler" depiction than the others. Not surprisingly, the least appealing depiction was E and lack of clarity and familiarity was the overriding reason; for example, Keith stated "it looks a bit weird", Anne said "I don't even know what it is", and Anita claimed "I have never seen anything like that before".

6.10.2 Undergraduate Learners

Like their secondary school counterparts, undergraduates appeared to hold a variety of views for the bonding in I_2 . However, there was more commonality of views, with five learners expressing a preference for the octet rule. Undergraduates see the bonding in I_2 as covalent in nature, which they described as the sharing of electrons.

Phill. Yeah that's covalently bound with each other they are, the valence electrons they'd probably have an electron out on its own looking to share with another one. So another iodine will come along and they just share electrons, quite happily share with each other.

Interviewer. OK so it's the sharing of that one outer valence electron?

Phill. Yeah and that makes the bond to be formed.

Renéé similarly viewed the bonding in I_2 as sharing of electrons, and utilised a Lewis dot diagram to illustrate her mental model.

Renéé. OK in this case they are sharing electrons equally, like neither of them has a higher affinity if you like, and they are forming an electron pair which makes it into a molecule.

Interviewer. OK can you just tell me what that sharing looks like to you. How does that come about if you like?

Renéé. Lewis dot diagrams [respondent laughs].

Interviewer. OK that's fine. Whatever way you see it. That's what I am interested in.

Renéé. OK [draws two Is, one with small crosses, and the other with dots around it, Figure 6.45].

Interviewer. OK you have drawn a couple of Is there, and you have drawn some crosses around one [respondent laughs]. OK that's fine. So the crosses and dots, what are they indicating?

Renéé. They are the electrons for each respective atoms, and, um, just to complete the octet the, the single electron, one from each iodine, forms a covalent bond.

Interviewer. Right OK. So the cross and dots they are...

Renéé. Oh they are just sort of representative of the electrons, like seven electrons for one, and seven electrons for the other.

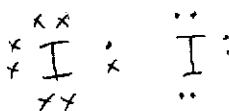


Figure 6.45 Renéé's drawing illustrating the bonding in molecular iodine (I_2)

Kim's response was similar to that of Renéé. However, she seemed less certain of the number of electrons shared, although she related the formation of the covalent bond to the octet rule.

Kim. I_2 , OK [draws two Is each with eight small circles around them, Figure 6.46]. I, I, and they would be sharing [draws ellipse enclosing circles between Is] I am not sure how many.

Interviewer. OK, that's OK. So they are sharing electrons. So why are they doing that do you think?

Kim. Just to fill up the eight I suppose. Eight, I don't know how many electrons they share, but up it's to fill up the eight so that they are more stable.

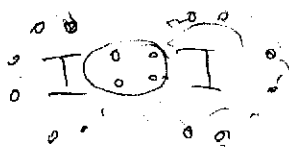


Figure 6.46 Kim's drawing illustrating the bonding in molecular iodine (I₂)

Although Kim has stated that each iodine atom requires eight electrons to complete its octet, in her diagram (Figure 6.40) she has indicated that the formation of a bond involves four rather than two electrons. Alan began his explanation of the bonding in molecular iodine by stating that it was like that in metals. He stated that iodine is "semi-metallic" and "slightly ionic", and initially considered that the bonding would be like the "sea of electrons". However, upon probing he produced an explanation similar to that of Kim and Reneé, that is, based on the octet rule, "just a covalent bond between the two, share the bonding electrons. you have a pair of bonding electrons shared between the two". The remaining two undergraduates, Steve and Bob proposed a molecular orbital theory-based model. Bob's model was rather confused in that he combined ideas from several models. The first part of his description is consistent with the localisation of electrons, or electron density, that is, consistent with the octet rule or valence bond approach, however, he extended this and went on to discuss the molecular orbital theory.

Bob. I see covalent bonding as being an overlap of two orbitals to complement each other to make up an octet if you like for each other. They both have seven electrons in their octet, in their valence shell, and want to get another one, and so they sort of one lift off each other and, each orbital has got one electron in it in this sense [drawing two Is separated, with overlapping ellipses joining them, Figure 6.47]. So you get this sort of thing with the two electrons being sort of throughout them.

Interviewer. Throughout them OK. So those sort of ellipses you have drawn between the two Is you have got there, what are they actually indicating?

Bob. The electron cloud I was talking about I suppose. But in specific orbitals now, rather than just as a generalised area.

Interviewer. OK before you mentioned two types of orbitals, atomic and molecular. Which of those orbitals do you see those ones you have drawn there as being?

Bob. I'd actually thought what I have been taught and how, I have understood it that atomic orbitals tend to be almost a myth. I might have picked it up wrong, but...

Interviewer. I am just interested in your views.

Bob. Yeah, I don't see many bonds as being atomic orbitals anymore, I see them as being molecular orbitals where it's over the whole molecule.



Figure 6.47 Bob's drawing illustrating the bonding in molecular iodine (I_2)

Steve began his highly detailed explanation with a description that was based on the octet rule (Figure 6.48).

Steve. Well iodine has molecular bonding which is a sub-set of covalent bonding, more or less covalent bonding. So the iodine as I see it, you have got an iodine atom there, and an iodine atom there [draws two large Is with line between them, top LHS of Figure 6.48, p. 218], and it's the formation of a covalent bond between them, where an electron from the iodine, an electron from each iodine, is sort of shared between the two.

Interviewer. Between the two?

Steve. And that forms, that forms a communal bond if like.

Interviewer. Communal, OK.

Steve. So the electrons are shared and they are free. They are free to orbit around both so it will go around both atoms to make, making up the I_2 [draws dumbbell shaped perimeter around I—I diagram].

However Steve spontaneously introduced the molecular orbital theory, and went on to produce a description that was enormously rich and detailed; all the more remarkable given the spontaneous nature of his response. He began by considering the atomic orbitals involved in the formation of a bond.

Steve. Of course I suppose you could look at that in terms of a molecular orbital diagram and draw the molecular orbital which covers both [draws larger perimeter encircling I—I group, Figure 6.48] which covers both atoms as well.

Interviewer. OK how do you see that?

Steve. Well if you were to take the iodine, if I remember it, you are going to have your $1s^2$, and your $2s^2$, $2p^6$, your $3s^2$, and then it's going to be $3p^6$ as well isn't it, $4s^2$? Oh hang on a sec, $4s^2$, $3d^{10}$, $4p$ that would

be 5 I guess, if I can remember it right [draws $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^{10}$ and $4p^5$ in a column, RHS top of Figure 6.48]. It's a bit of a struggle sometimes. So you would have atomic orbitals there [draws two sets of three closely spaced lines, writes AO next to them], there, and there, and then they come together and form the same number of molecular orbitals. I could draw a diagram I suppose. You don't need to worry about these ones because they are completely filled [draws line through $1s^2$, $2s^2$, $2p^6$, $3s^2$ and $3p^6$], so it's just the overlap of the, of these...

Interviewer. OK the outer ones.

He then constructed an energy level diagram from the atomic orbitals that he described previously.

Forming the bonding and antibonding combinations [draws series of lines between two previous sets of three lines and links up]. OK yeah [writes bonding and antibonding at top and bottom of lines respectively] and of course you would have to have the same number of molecular orbitals as atomic orbitals.

This was followed by a detailed description of the role of bonding and antibonding molecular orbitals.

Interviewer. OK. The bonding and antibonding you talked about there. Can you just tell me little bit more about those?

Steve. OK well if you take the case of iodine [writes I_2] you have got in this case two atomic orbitals, one for each iodine—two atomic orbitals. Now when the covalent bond is formed the atomic orbitals overlap and they form the same number of molecular orbitals.

Interviewer. Right.

Steve. That's the conservation of orbital rule.

Interviewer. Right.

Steve. Four and six is actually going to give you three isn't it?

Interviewer. Three, OK.

Steve. So you have got three different p orbitals.

Interviewer. p , yep, OK.

Steve. So you form these two overall combinations depending on the phase of the lobes when they overlap [draws two sets of dumbbells linked by line at centre].

Steve then related the boundary surface depictions to molecular orbital energy levels which he used to relate to bond formation.

Interviewer. That's those sort of dumbbells you have drawn is it?

Steve. Yeah dumbbell drawings, and so you get the two molecular orbital states; bonding, which is lower in energy than the individual atomic orbitals that you started with, and the antibonding, which is higher in energy than the two atomic orbitals that we started with.

Interviewer. Could you just sort of relate those lobes you drew to the bonding and antibonding, just so I am clear on that?

Steve. I need to be sure of my signs in this case, I believe, I am just trying to think about it now...

Interviewer. What is it that those signs are indicating, that you have drawn there?

Steve. OK I am trying to think of how to describe that. Well it's basically the sign of the wavefunction [writes Ψ under each lobe and + and - beside them]. So you have got the wavefunction describing each individual atomic orbital, and each one has overall a positive sign or a negative sign and so when the two are, I think when the two are positive maybe the bonding combination, the positive and negative the antibonding I can't actually quite remember.

Finally he used the energy level diagram to deduce bond order for molecular iodine.

Interviewer. OK that's fine. OK so in this case how would you see the bonding form in relation to say that energy level diagram you have drawn there.

Steve. Well take each one of these orbitals here, they would be occupied by, in this case there is five, so you would have, one, two three, four five [draws half arrows in atomic orbital levels].

Interviewer. Right, that's in your atomic orbitals, yep.

Steve. Yep and I am just trying to think how the degeneracies and what have you work out, but I think some of these would be degenerate [indicates closely spaced lines].

Interviewer. That's your molecular orbitals you have drawn there right.

Steve. Yeah and I think there maybe a non-bonding level, I can't quite remember [draws two lines in centre of molecular orbital diagram]. But they would fill from the lowest energy to the highest energy, so you get X number in the bonding, and maybe something similar in the non-bonding, and some in the anti-bonding, and the number in the antibonding cancels out some in the bonding.

Interviewer. Cancels out, right.

Steve. That determines the overall strength of the bond. So it's essentially the net number of electrons that is in the bonding orbital [draws rectangle around lower levels in molecular orbital diagram].

Interviewer. OK so it'd be that rectangle you have drawn. So the net number in there?

Steve. Yeah, after you have taken into account the number in the antibonding it's an indicator of the bond strength.

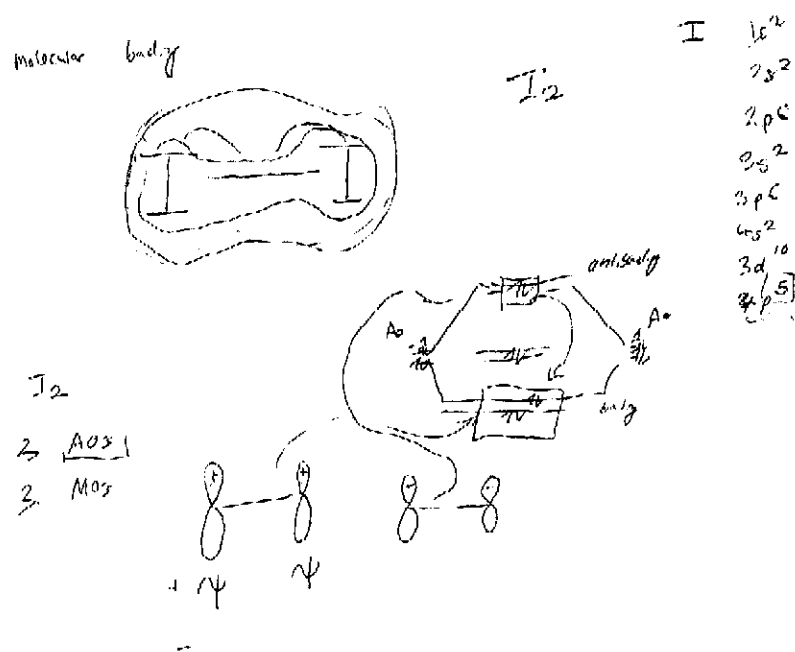


Figure 6.48 Steve's drawing illustrating the bonding in molecular iodine (I_2)

Undergraduates' views of the bonding in chloroform were the same as those that they held for molecular iodine. Bob, for example, again used a combination of ideas from the octet rule with those from molecular orbital theory.

Similar to iodine, the fact that it's covalent, made up of atomic orbitals again. In that case from what we established in the last one then between the carbon and [drawing CH_2Cl_2 structure in planar arrangement, Figure 6.49]. No that's Cl [writes Cl over top H, top part of Figure 6.49]. Those anions are going to want to be as far away, and the hydrogen obviously, they are not, I shouldn't call them anions. These groups on the carbon are going to want to be as far away from each other as possible. Because, because chloride, because of their electron clouds around them repelling each other. Therefore adopts a tetrahedron obviously.

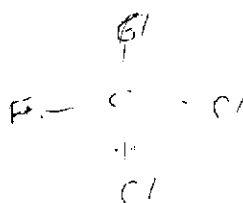


Figure 6.49 Bob's drawing illustrating the bonding in chloroform ($CHCl_3$)

In contrast to Bob, Steve held two clear mental models for the bonding in I_2 , one based on the octet rule and the other based on molecular orbital theory; however, like Bob, he combined ideas from molecular orbital theory and the octet rule to describe the bonding in chloroform. Steve introduced aspects of the molecular orbital theory describing the structure in terms of σ -bonding and delocalised orbitals across the chloroform molecule.

Steve. Well with the carbon to hydrogen bond, that's a σ -bond. Which is essentially just one electron contributed from each, to form the bond, and it's spread as I said before over the carbon and hydrogen.

Steve. OK to look at it from a quantum mechanical distribution, which would give a sort of a relationship I suppose, something like that [draws perimeter over C—H, Figure 6.50] which I see as rather ill-defined, with a carbon and hydrogen. I think because the polarity of the bond is so low, the density around both would be relatively the same. Whereas in the carbon chlorine case, the electrons are attracted much more towards the chlorine [draws new C—Cl with distorted dumbbell shape perimeter]. So that would mean that you would get a sort of swelling around the chlorine.

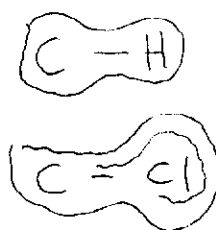


Figure 6.50 Steve's drawing illustrating the bonding in chloroform ($CHCl_3$)

The production of a molecular orbital theory energy level diagram for a compound like chloroform is more challenging than for a homonuclear diatomic like I_2 (see, e.g., Appendix A, pp. 351-353), and it is possible that this is one reason Steve chose to describe the bonding without employing a molecular orbital energy level diagram. Other undergraduates produced explanations that mimicked those they provided for the bonding in iodine, as seen in Phill's response (Figure 6.51).

Phill. Each chlorine would donate an electron, because they have one spare, and they would have lone pairs around here [draws dots around LHS Cl].

Interviewer. Right OK, so that's those dots you have drawn.

Phill. Yeah. The carbon has four, and so that would donate one to each of these bonds, and hydrogen as well.

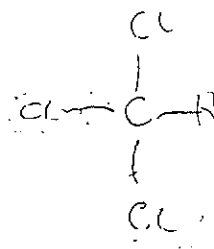


Figure 6.51 Phill's drawing illustrating the bonding in chloroform (CHCl_3)

Undergraduates' choice of depicted models (CB01, p. 80) varied with four choosing depiction B, two A, one D and one E. The undergraduates who preferred depiction B stated that it was because it was a more accurate representation of the bonding. Steve, for example, stated "it's clear, it's simple, it shows the ring and it shows the σ -bonding", and Alan "it's showing that the actual π -bonds are in no set position, they are resonating around the ring". Reneé stated that she liked both A and B, with a slight preference for A and also stated "we used them pretty interchangeably". However, she went on to state that "A can be misinterpreted in such a way that people think the double bond to carbon is actually fixed rather than delocalised", but Reneé was able to use the two representations without generating this alternative conception. Jane also indicated that depiction A held some appeal and stated that it was simply because she found it easy to draw, but she, like Reneé, was clear on the meaning of the visual clues provided in the diagrams.

Jane. Well when I think of benzene I think all the bond lengths should be the same. When I look at that, A, it doesn't tell me that. But in my mind it's actually telling me that. That A means that length there, that length there, that length there.

Interviewer. That's those double bonds?

Jane. Yeah, the doubles, are the same, are shorter and stronger whereas B is clear that they are not. Whereas [indicating depiction B on CB01] here that's indicating that they are all the same, all the same length and that's how I think of benzene.

However, upon probing, Jane preferred depiction E because it showed "what's actually going on with the delocalisation of electrons" and Bob liked depiction D because it possessed "more detail". Dislikes were also mixed with three undergraduates disliking depiction C typically because it was seen to be misleading, as seen in Steve's response, "it's trying to show discrete carbon-carbon double bonds and it's more cluttered with the hydrogens there". Jane disliked depiction A because, like Steve's concern with depiction C, she considered that it was potentially misleading as "it's not explaining that it's not a conjugated alkene". Two undergraduates disliked depiction D, Jane because she didn't understand part of the diagram very well "I understand this one [taps RHS of depiction D in CB01], I understand the right part of D but the left is kind of...", whereas Kim found the molecular orbital theory-based boundary surface representations in depiction D confusing.

Kim. They use positive and negative signs [i.e., on the boundary surface depictions] and like you relate that to ionic bonding with the electrons or whatever.

Interviewer. So in the way it's used here as far as those dumbbells if you like, what does the positive and negative mean to you here?

Kim. Like positive's overlaps and you get like instead of positive an negative overlapping like you would for ionic compounds, you get positive and positive overlap, and negative and negative overlap instead.

Other comments were similar to those of the secondary school learners and Bob, for example, disliked depiction B and described it as "very simplistic".

6.10.3 Postgraduate Learners

Postgraduates' preferred mental model for the target system covalent bonding was the octet rule, with all learners describing covalent bonding as consisting of the sharing of electrons and relating this to full-shell stability. An interesting difference was that postgraduates were more emphatic about the molecularity of I_2 and spontaneously introduced the concept of van der Waals forces between molecules. It should be noted that the interviewer did not use the

term *molecular iodine* when prompting learners; rather they were shown a sample of solid iodine and asked what the bonding would be like in *iodine*. James provides a typical response.

James. Just covalently bonded dimers, and sort of van der Waals as weak forces holding all those dimers together in a big crystal.

Interviewer. That's dimers was it?

James. Yeah, yeah.

Interviewer. So what's holding it together within the dimers?

James. Oh that's sort of covalent bonds between the two iodines. Sort of like the electrons are shared in the middle.

Interviewer. OK could you just tell me what you mean by van der Waals forces?

James. Um...it's where you have...sort of like a momentary polarisation or something of the dimers and the other dimer beside is polarised the same as that, so they polarise at the same time and they sort of attract.

Brian similarly described the bonding in molecular iodine in terms of the octet rule of full-shell stability.

OK well it's a molecule where there are two iodine atoms which are linked by a single covalent bond [drawing two Is linked by single line, Figure 6.52]. Essentially it's just the sharing of two electrons between the two iodine atoms that, well both iodine atoms are one short of attaining their complete valency in their outermost shell. So by sharing an electron between each one they both get the stability of the full shell. So the sharing of those two electrons is the covalent bond between them. So they exist as discrete I_2 molecules.



Figure 6.52 Brian's drawing illustrating the bonding in molecular iodine (I_2)

Like undergraduates, some postgraduates introduced concepts from other target models such as molecular orbital theory. Christine, for example, stated that molecular iodine consisted of "discrete little iodine molecules" and produced a diagram (Figure 6.53) consistent with this concept to illustrate her mental model.

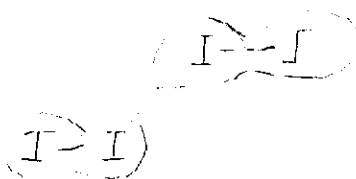


Figure 6.53 Christine's drawing illustrating the bonding in molecular iodine (I_2)

Christine stated that she saw the bond as arising from the "sharing of electrons", but upon further probing she then introduced the notion of an electron cloud, although she seems unclear in her own mind what a cloud actually is.

Interviewer. The line you have drawn between those two Is there, what are you trying to indicate by that?

Christine. They are attached.

Interviewer. OK it's just showing that they are attached.

Christine. Yeah I'm not actually thinking distinct electrons. I am just thinking, I guess of a cloud of whatever that is holding them together. I am not thinking electrons.

Interviewer. OK so you are thinking of a cloud?

Christine. Yes.

Interviewer. As opposed to?

Christine. Yeah I am not thinking about...

Interviewer. Individual electrons is that it?

Christine. Not a...it's not like a plus minus where you have got a like an interaction. I mean because one is positive it has something that is minus around it. It's more that they're just I guess a cloud around them like a [drawing outer circles enclosing Is, Figure 6.53].

Interviewer. Can you just tell me what you mean by that?

Christine. [respondent laughs] I am not quite sure that I can [respondent laughs]. I guess I think of...what do I think? Well they are obviously held together by something. I guess I don't think of electrons. I think of stuff, if I can use that word, with everything moving around the whole time.

Interviewer. OK.

Christine. I am not thinking in discrete I. Do you know what I mean? Not just Is, I think of then just as a two thing floating around.

Grace stated that the bonding in I_2 comprised "sharing of electrons", but later stated that the iodine atoms would "both have filled orbitals" and Rose described the bonding in molecular iodine in a similar manner to the other postgraduates, namely, that is a molecular compound that contained a covalent bond arising as the result of

the sharing of electrons. However, she also seemed to hold the alternative conception that the I_2 molecule contained charged species (see Chapter 7, p. 276).

It is interesting to note that despite their rather detailed explanations for the bonding in molecular iodine described above, both Jason and Christine seemed distracted by the shiny appearance of the solid substance. This led them to state that they considered that the substance possessed some metallic characteristics. This concept is described in detail in Chapter 7 (pp. 278-279) but their descriptions provided here are more consistent with a octet-rule based model for the bonding in molecular iodine.

Postgraduates generated descriptions for the bonding in chloroform ($CHCl_3$) that were identical in nature to those they provided for molecular iodine, as seen in Jason's response.

Jason. Chloroform is a tetrahedral molecule in which a central carbon atom is covalently bonded to three chlorine atoms and a proton, or a hydrogen atom [drawing spheres with C, 3xCl and H inside linked by lines, top part of Figure 6.54]. It's sharing electrons with each of these, so carbon has, shall I draw a Lewis diagram?

Interviewer. Whatever you like, yep.

Jason. OK [drawing Lewis dot diagram of $CHCl_3$, lower part of Figure 6.54] so you have a carbon which has four electrons [drawing crosses], a proton has one, and each of these, each of the chlorines, about it has eight, oh seven sorry. Ah, they want eight OK, so this configuration satisfies the valence requirements of each of the elements. Because hydrogen can only have a 1s orbital. It only needs two to fill its valence shell, but carbon and the chlorines, all need eight, and they can form eight by sharing an electron each. This sharing is very strong so these four bonds are all very strong. But the bonds between each chloroform is quite weak [draws two $CHCl_3$ in column and draws dotted line between them, top RHS of Figure 6.54].

Interviewer. Quite weak OK.

Jason. The van der Waals forces.

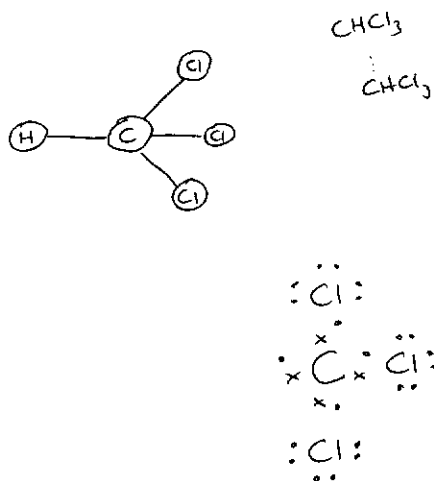


Figure 6.54 Jason's drawing illustrating the bonding in chloroform (CHCl₃)

Whilst Jason provided a highly detailed explanation here, there is some evidence of misuse of terms. For example, he stated that "a proton has one [electron]" and though this may be an exercise in semantics, the issue is discussed in more detail in Chapter 7 (pp. 272-274). Similarly to Jason, James stated economically that chloroform would contain "covalent bonds between the carbon and hydrogen and the chlorines", and Grace saw "covalent bonds from the carbon to a hydrogen and three chlorines". Like their models of bonding in I₂, a clear appreciation of molecularity for CHCl₃ was evident, and for example, Christine stated that "the bonding in chloroform I think of as distinct little species".

Postgraduates' choice of depicted models were fairly uniform with five learners choosing depiction B as their preference. As was seen for the target systems of metallic bonding and ionic bonding, postgraduates were more discerning as exemplified by Jason's response.

A is sort of a sequence of double and single bonds which is the structure Kekulé proposed for benzene in the first place, and he came up with the most correct answer to begin with and it's a good way of depicting benzene in that it is sort of roughly hexagonal but it didn't explain some of the other aspects about benzene. For example, the structure of benzene shows that all the bond lengths are the same and the strength of the bonds is all about one and a half. When you hydrogenate benzene you get less energy back that you would expect from cyclohexatriene.

It's almost like there is extra bonding there that you would expect compared with a sequence of double bonds. B shows this effect, which is called aromaticity, where you have a sequence of double and single bonds. Neither of these structures show the individual hydrogens or carbons, you are assumed to know that they are there. C shows each of these carbons and hydrogens, and again it's essentially structure A drawn out showing each hydrogen each carbon. Structure D shows the collection of orbitals which shows the 1s orbitals of the hydrogens as well as the sp^2 orbitals of the carbon. The remaining diagram shows the other p orbital or the other pure p orbital if you like of each of the carbons.

Jason eventually decided he preferred depiction B, because "B is the most simple and useful, certainly for everyday use". Other postgraduates provided similar, albeit less detailed responses in that they discussed and evaluated the depictions before settling on their choice. As well as simplicity, the main appeal of depiction B was that it indicated clearly and simply that the electrons were delocalised over the hexagonal ring system as illustrated in Grace's response "because it emphasises that the electrons are shared over all the carbon atoms".

A dominant feature of the discussion for all postgraduates was the delocalisation of the bonding in benzene, and like the other target systems of metallic and ionic bonding, choice in some cases was more a reflection of dislike of alternative depictions. Most disliked depictions were A and C (seven learners) because they were seen to imply the presence of localised double bonds in the structure for benzene, as seen in Grace's response.

Mainly because it emphasises that the electrons are shared over all the carbon atoms. I guess with A and C you get the misconception that there's a double bond between two particular carbon atoms. Whereas that's not the way it is. Those electrons are actually shared around. So A and B are an easier way to draw it, but you could get a misconception.

Some interesting responses were produced during the discussions of the delocalisation of electrons or bonds around the benzene ring. Depiction D was seen by some learners as "more accurate" but less convenient to use. In considering postgraduates' views of the relation between depiction D and the resonance concept, the notion of one-and-a-half bonds between adjacent carbon atoms in the

benzene ring seems counter-intuitive. However, despite their predisposition towards the concept of delocalisation of bonds or electrons, it seems some learners find the one-and-a-half-bond concept less conceptually challenging than the notion of delocalisation. Kevin's response is interesting.

D, I see automatically when I look at it I see benzene as in the way I have been taught. I also see it as being more accurate because it hasn't specifically shown which are double bonds and which are single bonds. That's shown by the circle the fact they are all a mixture of both. When it comes down to benzene, I see more a mixture of carbon-carbon one and a half bonds than I do see π -electron clouds circling above and below.

Brian similarly found the notion of delocalisation of electrons counter-intuitive—"I find it difficult to believe that there are just two little donut-shaped clouds hanging around there".

Postgraduates response to visual clues in the depictions provided in CB01 were not necessarily obvious. As indicated above, most respondents saw depiction C and A in a similar light. However, Jenny, ostensibly saw A as correct, but C as wrong.

Interviewer. So why do you think you see C as being wrong, and yet not A?

Jenny. Because A is quite often depicted like that. I mean I am doing lignin chemistry so I see lots of that. We do lots of ring aromatisations. So it's easier to draw three distinct double bonds.

Interviewer. I see.

Jenny. I know when I look at that O [i.e., the circle inside the hexagonal ring in depiction B for CB01] I know it's delocalised.

Interviewer. OK it's one you have used yourself quite a lot is it?

Jenny. Yeah. Whereas that one there [indicating depiction C] when I look at it as being a representation of three distinct double bonds, but I look at that and see that as being benzene. Almost like they are not related, although I know they are. It's like they are two separate things.

Jenny's response seems to indicate that her difference in perception of the depictions A and C are related to her greater experience in the use of structures that resemble depiction A over C.

6.11 Learners' Understanding of Mental Models for Covalent Bonding

Learners' understanding of their mental models for covalent bonding were probed by reference to the criterial attributes as detailed in Chapter 4 and those for the octet rule are reproduced in Table 6.6 (p. 229). Steve was the only participant who used a different mental model to describe the target system of covalent bonding; his choice being the molecular orbital theory. Consequently, learners' understanding of the octet rule is discussed first, followed by Steve's understanding of the molecular orbital theory.

6.11.1 Learners' Understanding of the Octet Rule

Learners across all levels discussed the octet rule spontaneously, and in some depth, during their description of the bonding in I_2 and $CHCl_3$. Hence most learners addressed the criterial attributes for the octet rule during this discussion with little or no prompting. Criterial attributes 1, 2, and 3 were addressed and the results are summarised here. Learners across all academic levels evidenced a good understanding of full-shell stability and pairing of electrons (see e.g., Figure 6.43 p. 211, Figure 6.44, p. 211, & Figure 6.45, p. 213). Although it should be noted that a few secondary school learners namely, Anita and Anne, and one undergraduate, Kim, appeared to be confused about some aspects of electron pairing (see Figure 6.46, p. 214) and undergraduate and postgraduate learners showed a greater appreciation of the concept of molecule formation than their secondary school counterparts. Criterial attributes 7, and 8 were evaluated by reference to focus card CB01 which showed depictions of the bonding in benzene (C_6H_6). The criterial attributes for the octet rule in Table 6.6 are different with Level 3 learners (i.e., secondary school learners), not expected to show understanding of these concepts. This was borne out in the inquiry with secondary school learners showing little appreciation of the concept of multiple structures or the resonance concept; apparently they believed that there were double bonds in benzene (see, p. 212).

Table 6.6 Criterial attributes for the *octet rule* model for covalent bonding

	Level 1	Level 2	Level 3
1.	full-shell stability	full-shell stability	full-shell stability
2.	electron pair formation	electron pair formation	electron pair formation
3.	molecule formation	molecule formation	molecule formation
4.	bond directionality	bond directionality	bond directionality
5.	unequal sharing	unequal sharing	unequal sharing
6.	non-bonded pairs	non-bonded pairs	non-bonded pairs
7.	multiple structures	multiple structures	
8.	resonance	resonance	

Key. Level 1=postgraduate learners, Level 2=undergraduate learners, Level 3=secondary school learners

In contrast, undergraduates and postgraduates readily discussed the concept of multiple structures, and it is clear from these data that these learners appreciate that for compounds such as benzene no single Lewis structure can adequately represent the bonding. Understanding of the resonance concept was less fully addressed during discussion, and whilst undergraduates and postgraduates introduced the term resonance, few expanded on the meaning of this concept.

6.11.2 Learners' Understanding of Bond Directionality and Unequal Sharing

Learners' understanding of the concepts of bond directionality and unequal sharing of electron pairs were probed by discussion of the bonding in CHCl_3 . Learners were asked to describe their mental model for the bonding in CHCl_3 and asked if they saw the C—H and C—Cl bond as different in any way. In addition, they were probed as to their views of the shape of the CHCl_3 molecule in order to probe their understanding of the directional component of the bonding in the compound.

Secondary school learners showed little appreciation of the concept of unequal sharing of electron pairs. Learners described the bonding in CHCl_3 in the same way that they did for molecular iodine, namely in terms of the sharing of electrons and full-shell stability. Anne stated that there would "not really" be any difference in bonding and others offered other vague explanations, Neil stated that they "could be different strengths" and Richard that the chlorine atoms were "loosely bonded" compared with the hydrogen. Only two learners stated that they saw any difference between the C—H and C—Cl bond, as a consequence of differences in electronegativity between H and Cl atoms. Claire and Keith related the difference in bonding to the electronegativities of the hydrogen and chlorine atoms. Keith, however, seemed to have little appreciation of the influence this might have.

Interviewer. The bond you have got there between the carbon and the chlorine, and the carbon and the hydrogen, do you see those as being different at all?

Keith. Yep, the electronegativities are different, like the hydrogen and chlorine would have different values. So the bond depending on which is the biggest, won't be as strong between the smaller difference.

Interviewer. OK, so what's electronegativity meaning here?

Keith. How much an atom wants to bond with another atom. A high value means it's really eager to get in there and bond with another atom.

Claire's explanation was more detailed. She spontaneously introduced the term electronegativity and went on to relate this to the concept of polar covalent bonding.

Claire. They are all kind of covalent bonds. The carbon-chloride bond is polar. It will be polar because of that electronegativity difference, the same as the sodium. It's not enough of a difference to become an ionic bond. So it's just polar covalent with the chloride.

Interviewer. Can you tell me what you mean by polar covalent so I am clear on that?

Claire. The electrons that they are sharing, they are sharing two electrons. Because the chloride, the chlorine, wants to gain one, so it just borrows one of the carbon ones. But these two shared electrons aren't, they are not equally shared. Because the chloride's got a strong, a more strong attraction. So that's going to go [draws arrow from C to Cl, Figure 6.55] and the hydrogen is still a polar bond because it can't be exactly non-polar because the atoms aren't identical like the iodine ones. But it's not much of a difference so it's a little bit polar.

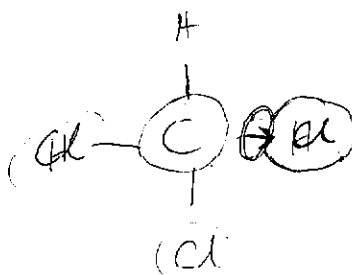


Figure 6.55 Claire's drawing illustrating the bonding in chloroform (CHCl_3)

In contrast, all secondary school learners showed a clear appreciation of the directional component to the bonding in the molecular covalent compound CHCl_3 . Claire attributed the shape of the molecule to the arrangement of the electron pairs and the fact that, "being of like charge, they would repel". Anne provided a detailed

response. Originally she discussed the bonding in terms of the octet rule and drew a Lewis diagram. However, upon prompting, she drew a stereographic projection for the CHCl_3 molecule, and she explained the visual clues she used in her diagram.

Interviewer. In terms of the structure you have drawn there can you just tell me how in terms of the shape how you interpret that structure as you have drawn it there?

Anne. Um, I ah [drawing stereo diagram, Figure 6.56] like a pyramid there.

Interviewer. Sorry did you say pyramid?

Anne. Yeah. That one [indicating the solid wedge in lower figure] is like sticking out towards you. That one is behind [indicating broken line in lower figure]. So that's a pyramid sort of shape.

Interviewer. OK. What's made it adopt that shape?

Anne. The, the electron pairs push them, like to the corners.

Interviewer. OK. Why are they doing that?

Anne. [respondent laughs] there's no lone pairs.

Interviewer. No lone pairs OK. So you said the electron pairs and you said that was pushing them to the corners. I am just interested to know in your view why that pushes them to the corners.

Anne. Well they are like charges so they repel.

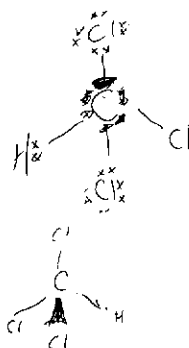


Figure 6.56 Anne's drawing illustrating the bonding in chloroform (CHCl_3)

Other secondary school learners drew similar diagrams and provided similar responses. Anita, who struggled to describe her mental models of the bonding for other target systems, showed an appreciation of the directional component of the bonding in CHCl_3 . Her initial drawing simply showed the connectivity.

Anita. OK I think it's like that [draws planar CHCl_3 molecule, Figure 6.57]. That's a normal single bond.

Interviewer. A normal single bond OK, and how do you see those bonds? What does single bond mean to you?

Anita.....um...covalent, like those other ones. But yeah, covalent bonds.
Interviewer. So are they similar or different to the iodine ones we talked about before?
Anita. Similar because they are both covalent.

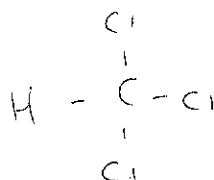


Figure 6.57 Anita's drawing illustrating the bonding in chloroform (CHCl_3)

However, upon probing Anita went on to describe the bonding as "3-D" in nature.

Interviewer. How do you see the shape of the molecule?

Anita. Ah, 3-D.

Interviewer. 3-D? Can you just sort of expand on that a bit for me.

Anita. [respondent laughs] Yeah it'd have, oh I can't draw 3-D.

Interviewer. OK but even if you just describe it that's fine, or you can try drawing it.

Anita. [draws tetrahedral CHCl_3 molecule, Figure 6.58] one's at the top there and that's at the back [draws broken line to bottom, middle Cl] there's the Cl.

Interviewer. Oh, OK.

Anita. Yeah, it's a sort of 3-D.

Interviewer. The two you have drawn straight out, where are they in relation to the...

Anita. It's like a big 3-D triangle.

Interviewer. A big 3-D triangle, OK.

Anita. Yeah with a C sort of in the middle, and with each of the others at the corners.

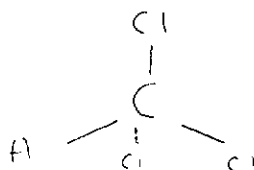


Figure 6.58 Anita's drawing illustrating the structure of chloroform (CHCl_3)

Undergraduates showed a greater understanding of the concept of unequal sharing of electrons than their secondary school counterparts. Five out of eight

undergraduates introduced the concept of electronegativity when asked if they saw any difference between the C—H bond and C—Cl bond. Interestingly, Steve, who described the bonding in CHCl_3 in terms of his molecular orbital theory mental model (p. 219), also indicated that "there is significant electronegativity so that's [indicating Cl] much more electronegative than the carbon and so you get significant polarity in the bond". Electronegativity was seen by undergraduates as providing a "pulling" or "drawing" of an electron, or electrons, towards the more electronegative halogen atom.

Bob. The more electronegative the groups are, the more the electrons in each bond are sort of drawn to that group.

Reneé. The chlorine would be more electronegative because it has a higher affinity for the electrons. It could effect the bond strength as well as the size of the chlorine.

Undergraduates extended the concept of electronegativity to the concept of polar covalent bonding as seen in Kim's response.

Kim. Chloride is like delta minus [writes δ^- next to one Cl, Figure 6.59], which makes the hydrogen delta plus I suppose [writes δ^+ next to H on adjacent structure and draws wavy line linking Cl and H], so...

Interviewer. So and you have drawn a line between those two.

Kim. There would be like interaction there.

Interviewer. OK. So the delta minus and delta plus. Can you just tell me a bit about that? What are you indicating by that?

Kim. Well that's like electron rich [indicates δ^-], and that's electron deficient [indicates δ^+], because chloride has a high electronegativity. It has a strong pull for the electrons, and hydrogen doesn't.

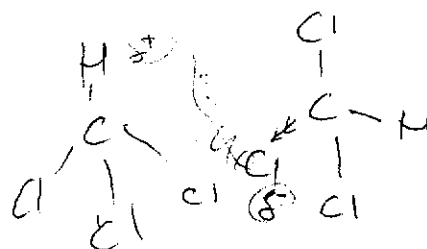


Figure 6.59 Kim's drawing illustrating the bonding in chloroform (CHCl_3)

However, three undergraduates seemed to have little idea of the concept of unequal sharing in covalent bonding. Alan stated that "I haven't considered that" when asked if he saw differences in the C—H and C—Cl bond, Phill stated "there should be", and Mary seemed confused about the bonding in chloroform in general.

Like their secondary school counterparts, undergraduates showed a good appreciation of the directional component of the bonding in chloroform; all either drew stereographic projections or specifically stated that the atom arrangement in the chloroform molecule was tetrahedral in nature. However, their reasons proposed for this shape varied considerably. Steve, for example, stated that "the tetrahedral angle of 109.5° minimises steric interaction", whereas Alan simply stated that "the carbon is sp^3 hybridised". Interestingly, a number of undergraduates, like Alan, introduced the concept of hybridisation, but were unable to describe the meaning of the concept. Kim, for example, stated that "I just have the idea that carbon attaches tetrahedrally automatically", and René stated that "it's just the way we learnt it". Hence it seems that undergraduates are clear that covalent bonding is directional in nature, but are unclear as to the underlying reasons for this.

Postgraduates showed a clear appreciation of the concept of unequal sharing of electrons in polar-covalent bonds. Learners related unequal sharing to electronegativity of the chlorine atom which resulted in pulling of electrons towards the Cl.

Grace. The chlorine wants another electron to have its orbitals full. So I guess it's going to take the carbon electrons and sort and bond with them, pulling them towards itself 'cos it's wants to have a full p orbital. So you have got the covalent bond between the carbon and the chlorine, but the chlorine is more electronegatively charged because it's stronger.

Rose. I guess the electrons would be pulled more to the Cl because it's more electronegative than in the carbon to hydrogen.

Perhaps the most well articulated description was provided by Kevin.

I have the view that when I have drawn the covalent bond, you have got, as I have drawn there, two crosses for the electrons. At the moment I have drawn them in the middle of the bond. I wouldn't really consider them purely in the middle of the bond [indicates crosses in Figure 6.60]. They are more shifted towards the chlorine atom than they are the carbon [draws crosses closer to RHS Cl]. The reason yeah, then you get into electronegativity. The chloride atom is more electronegative than the carbon atoms is, which means it will attract the electron density to a greater degree.

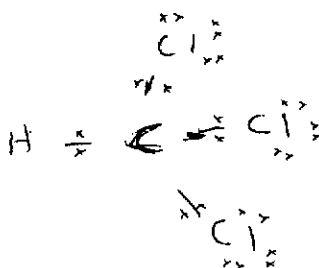


Figure 6.60 Kevin's drawing illustrating the bonding in chloroform (CHCl_3)

Some postgraduates related the concept of electronegativity to polarisation as seen in James's response.

They'd be different. The carbon-chlorine bond would be polarised to the chlorine and make it sort of slightly negative and the carbon-hydrogen would slightly polarise to the carbon making the hydrogen slightly positive.

Christine, however, despite introducing the notion of polarisation, seemed rather confused about the concept, particularly in relation to the C—H bond.

Christine. I probably wouldn't see it as being polarised. I mean hydrogen's not, I wouldn't see that as partly negative. So I guess having said that I am probably...yeah I don't actually see it as positive.

Interviewer. OK.

Christine. I wouldn't see it as positive, but I guess maybe it would have to be to balance up the negative charge but I don't see it as positive.

Postgraduates were emphatic about the directional component of the bonding in chloroform. With the exception of Rose, all postgraduates stated that the arrangement of the atoms in chloroform was tetrahedral in nature, and drew projection-like diagrams (see, e.g., Figure 6.54, p. 225). Nonetheless, Rose also

produced a diagram (Figure 6.61) that showed the tetrahedral co-ordination of the chloroform molecule and that resembled those produced by the other learners.

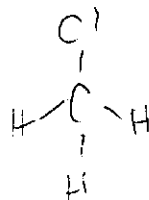


Figure 6.61 Rose's drawing illustrating the structure of chloroform (CHCl_3)

Like their undergraduate counterparts, postgraduates were unable to offer clear reasons for the atom arrangement. Rose, for example, stated that "that's the arrangement it adopts", Jenny stated "I know carbon is tetrahedral" and "because carbon is always tetrahedral", and Grace bluntly stated "I dunno". Three postgraduates offered some explanation; Brian described the arrangement as arising from repulsion of substituents, recalling concepts from his high school instruction.

I'd see that as tetrahedral. I suppose back when I was in high school anyway I would see it in terms of a like planar square almost. That's the way we always drew it. But as you move on, I see it as a tetrahedral, in which case, um, it, um. Why is it tetrahedral? It wants to arrange the substituents as far as part as they can be from one another, and the maximum for that is 109.5 degrees apart from one another, which is the tetrahedral geometry.

James was more specific in his explanation, and pointed out that the structure and arrangement would be slightly distorted from a pure tetrahedral arrangement because "it'd be like tetrahedral with the chlorines sort of pushing themselves up. The chlorine-carbon-chlorine angle's a lot bigger than say the chlorine-carbon-hydrogen". The most detailed explanation and drawing (Figure 6.62) was produced by Jason who specifically referred to the directional component of the bonds, which he attributed to hybridisation.

In this case the directional component is very strong because you have a specific bunch of hybrid orbitals. The hybrid orbitals in this case are on the carbon are the sp^3 hybrid, in which an s orbital and three p

orbitals have come and sort of recombined together and formed these four identical orbitals which have a tetrahedral shape.

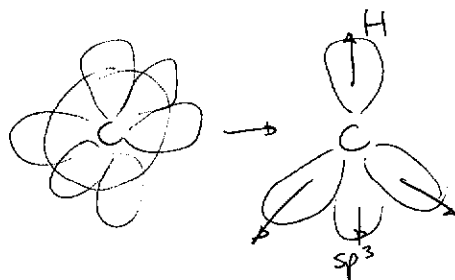


Figure 6.62 Jason's drawing illustrating the concept of hybridisation

Jason did not specify why hybridisation occurs, or why it was necessary. Furthermore, he stated that the hybridisation produces sp^3 orbitals that are tetrahedral in *shape* rather than arrangement.

6.11.3 Steve's Understanding of the Molecular Orbital Theory

Steve was the sole participant to identify the molecular orbital theory as his preferred mental model for the bonding in molecular iodine (I_2). The details of Steve's mental model are described above (see, pp. 215-218), here his understanding of molecular orbital theory is described. The criterial attributes for a Level 2 Learner (i.e., an undergraduate) were detailed Chapter 4 (Table 4.9, p. 91) and are reproduced in Table 6.7.

Steve had a good understanding of the molecular orbital theory as evaluated against the criterial attributes, spontaneously introducing a number of subtle and relevant conceptions, for example, the concept of atomic orbitals stating that "they come together and form the same number of molecular orbitals".

Table 6.7 Criterial attributes for the *molecular orbital theory*: Level 2 learner

-
- | | |
|----|--|
| 1. | Linear Combination of Atomic Orbitals (LCAO) |
| 2. | electron delocalisation |
| 3. | boundary surface |
| 4. | orbital geometry |
| 5. | orbital size/shape |
| 6. | Aufbau principle |
| 7. | bond order |
| 8. | relative energy level |
-

He went on to describe how they combine to form molecular orbitals "if you take the case of iodine you have got in this case two atomic orbitals. One for each iodine, two atomic orbitals. Now when the covalent bond is formed the atomic orbitals overlap, and they form the same number of molecular orbitals". These statements indicate that he has a good appreciation of the LCAO concept (criterial attribute 1). He also stated "that's the conservation of orbital rule" and went on to say that the formation of molecular orbitals resulted in two sets—bonding and antibonding. However, he seemed unsure about the sign of the phases involved in the combination of orbitals, "I think when the two are positive, maybe the bonding combination, the positive and negative the antibonding". His statement that "the molecular orbital covers both [i.e., both Is]" shows appreciation of the concept that molecular orbitals are delocalised (criterial attribute 2). Furthermore, his diagram of the molecular orbitals for I_2 (Figure 6.63, LHS part of drawing) substantiates his view of delocalisation. Steve's drawing contains depictions of boundary surfaces for the molecular orbitals involved.

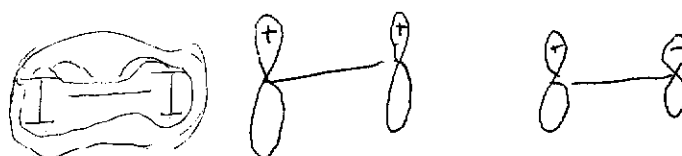


Figure 6.63 Detail from Steve's illustration of the bonding in molecular iodine (I_2): Depictions of the boundary surface concept

Steve stated that "the orbitals overlap" and that "the combinations depend on the phase of the lobes" (criterial attribute 3). Steve's description of the bonding for chloroform where he described the molecule as tetrahedral and stated that this occurred because "the tetrahedral angle of 109.5° minimises the steric interaction" is indicative of an appreciation of the importance of geometry. However, he did not relate this to the LCAO or to orbital symmetry (criterial attribute 4). Likewise, he made little mention of orbital size and shape other than that depicted in his drawings in Figure 6.63 (criterial attribute 5). He did show an appreciation of orbital occupancy rules of the Aufbau Principle (criterial attribute 6) which he related to the relative energy level (criterial attribute 8) in his drawing of the molecular orbital energy level diagram depicted in Figure 6.64.

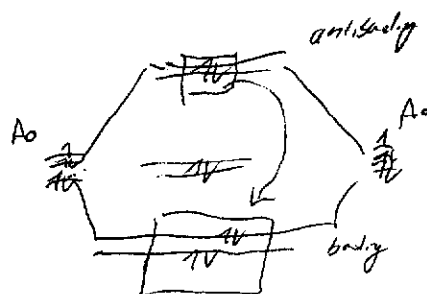


Figure 6.64 Detail from Steve's illustration of the bonding in molecular iodine (I_2): Energy level diagram

Steve's drawing possesses some limitations compared with the scientists' conceptualisation (see, e.g., Figure A26, p. 349). However, his model and statements indicate that he appreciates that the antibonding orbitals are higher in energy than bonding orbitals although his molecular orbital diagram does not contain the correct number of bonding and antibonding orbitals perhaps as a result of his confusion about the role of non-bonding orbitals when he stated that there "may be something similar in the non-bonding". He clearly possessed an understanding of the use of molecular orbital energy level diagrams to explain bond order (criterial attribute 7), and he began by stating that there were degenerate energy levels in the energy level diagram and stated "they fill from the lowest energy to the highest".

His diagram reveals his understanding, with the lower energy bonding orbitals filled, and the higher energy level antibonding orbitals indicated as incomplete. Steve stated "the net number of electrons that is in the bonding orbital" is what effects the bonding order since "the number in the antibonding cancels out some of the bonding". Hence whilst Steve was confused about the exact number of electrons involved in the I_2 molecule (allocating 8 electrons instead of 10 into the molecular orbitals), he has evidenced a sound understanding of the molecular orbital theory as it applies to I_2 . In addition, he was able to use the salient points to describe the bonding in chloroform ($CHCl_3$) and this suggests his understanding of molecular orbital theory is not confined to simple molecules such as homonuclear diatomics.

6.12 Learners' Use of Mental Models for Covalent Bonding

Learners' use of mental models for the target system covalent bonding were probed by reference to three IAE focus cards. Secondary school learners were first shown focus card CB02 (p. 81) which depicted the reaction between an aqueous solution of copper(II) sulfate and 0.880 ammonia solution. The card was accompanied by a demonstration of the reaction. Second, they were shown focus card CB03A (p. 81) which depicted variations in flow of liquid streams as they passed a positively charged rod. Undergraduates and postgraduates were likewise shown focus card CB02 along with the demonstration. Subsequently, they were shown focus card CB03B (p. 82) which comprised a line drawing illustrating the relationship between boiling point and periodic group number for a series of analogous hydrides.

6.12.1 *Learners' Explanations for the Reaction of Copper(II) Sulfate with Ammonia Solution*

Secondary school learners were unable to offer an explanation of the event depicted on focus card CB02 in terms of bonding changes. Due to time constraints the focus card was omitted from the interview protocol for three learners, Frances and Keith and David. Anne offered no response and the others offered simple

explanations that were not strongly related to chemical bonding. For example, Anita stated that "the ammonia attracted the copper and that gave deep royal blue". Neil stated that "the structure of it has changed and I don't know why that changes the colour" and offered the explanation that "it reflects light in a different way". The most detailed explanation was offered by Claire who explained the bonding in the aqua complex which she related to the negative nature of the oxygen atom on the water molecule.

Well the first picture is the hydrated copper ion. That's why it is bonded. The Os are written because they are slightly negative in the water molecule and then you add the ammonia and the ammonia molecules displace the water molecules because they're more δ^- , so they're more strongly attracted to the copper.

However upon probing, she was unable to explain why the tetra(ammine) complex (a term introduced by Claire in earlier discussion) was a different colour; it seems she considered copper ions to be inherently blue in colour stating that "the copper ion is blue and nothing else with ammonia is blue. So unless the waters around it make the blue lighter, and the loss of those will make it darker again, but I don't really know"

Many undergraduates also struggled to explain the event depicted in CB02 (p. 81); Kim stated "I have no idea really", Jane said "I don't have any idea" and Mary's response was that "nothing is actually jumping to mind". The remaining undergraduates related the colour change to electronic transitions between orbitals or the spectrochemical series.

Alan. Yeah stronger bonds, sort of lowering the energy levels of the orbitals and the transitions between them will be different and therefore a brighter colour. So there'd be electrons, which gives a different colour.

Reneé. That's a co-ordination complex what you have got in the diagram is different ligands bonded to the copper atom. Let's see, ammonia is higher on the spectrochemical series than water, and it would increase the crystal field splitting in the crystal field diagrams the octahedral splitting, Δ_o , would be greater for ammonia.

Bob was the sole undergraduate to offer a comprehensive explanation.

Bob. This is co-ordination chemistry obviously. This copper can't form six bonds to anything else with the electrons that it has. Water, well why water is not as good a ligand as ammonia I have no idea. But I know that it is not as strong as separating the *d* orbitals. In an octahedral complex the *d* orbitals split up, and the stronger that a ligand is at splitting those *d* orbitals, what colour it will emit will depend on that, because of the transition between the electrons from the lower energy to the higher energy orbitals. When they come back down, they emit light and it's going to give off different frequencies of light with the different gap between the two.

Interviewer. Right.

Bob. So if water doesn't split it as much as ammonia does, so the gap between, or Δ_o as it is called, isn't as much in the water co-ordinated complex as in the ammonia co-ordinated complex.

Interviewer. OK.

Bob. So the energy given out is gonna be higher, and it's gonna give you higher wavelength whatever that turns out to be, blue, and then purple being higher wavelengths obviously. It makes sense, towards the ultraviolet end.

Steve's explanation was different to his mental model of the bonding in I_2 and $CHCl_3$, for which he used the molecular orbital theory. He attributed the colour change depicted in CB02 (p. 81) to dative bonding, a model based on the octet rule (Appendix A, p. 335).

Well in this case here you have got your copper centre and you have got your oxygen, your waters co-ordinating by the oxygen of water [draws Cu with bent H_2O molecule linked to it by an arrow, Figure 6.64]. So that forms a co-ordinate bond, or a dative bond, I suppose you could say. Which goes to the copper like that and it's the same with all the other ones in the octahedral arrangement. Whereas with the ammonia case, you have got a similar sort of thing but now your ammonia NH_3 is co-ordinated by a dative bond through the nitrogen.

However, when he went on to clarify dative bonding, he reverted to a molecular orbital theory-based model.

Interviewer. OK could you just clarify one thing. You used the term dative. Can you just tell me what you mean by that?

Steve. Rather than having a covalent bond say between carbon and hydrogen, where each one contributes one electron to the bond, you have got a molecular orbital formed [draws C—H with dumbbell

perimeter, Figure 6.65]. In a dative bond, you have got both electrons in this case coming from the oxygen. You have got a free electron pair from the water [draws two dots on O], both being contributed to the copper, hence the one sided arrow.

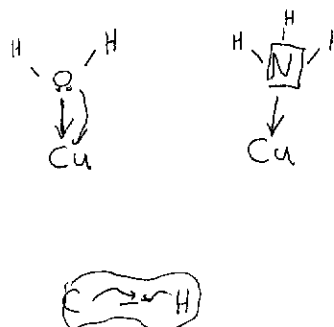


Figure 6.65 Steve's drawing illustrating the concept of dative bonding

Postgraduates also struggled to offer explanations for the event depicted on CB02 (p. 81) in terms of the bonding in the two complexes. Grace stated, "it's got the choice, so it obviously prefers the ammonia, I am not actually sure why" and Rose said "I don't know really". The idea that ammonia is bound, or bound more strongly, to the copper than water was stated by a number of postgraduates. Jenny, for example, appeared to believe that the water molecule is not bound to the copper in the aqua complex, "I don't really sort of visualise the water as being bound so much, I guess I see it more as solvated", a view shared by Kevin—"when they are in solution they are surrounded by as solvent sphere" and Brian "I guess the nitrogen bonding to the copper must be stronger than water because it seems to displace the water". James related the changes to differences in interaction with molecular orbitals on the copper atom.

They interact differently with the orbitals on the copper. So they sort of move further up or further down or whatever. So the transitions from the highest occupied molecular orbital, to the lowest occupied are going to be different in energy, so you see different colours.

Christine held a similar view to that of James, although she was less specific about the orbitals involved.

I am thinking like in copper there's been a change in energy levels. There's been a change to where they have got access to [drawing energy levels and joining up with straight arrows, Figure 6.66]. Which has caused the change in colour. So they are going somewhere different to give a different colour.



Figure 6.66 Christine's drawing illustrating the colour change in the copper coordination complex

Jason offered an explanation in terms of charge-transfer rather than inter-configurational *d-d* or molecular orbital transitions—"I dare say the intense blue colour is probably due to with a charge transfer band, where you get some of the charge transferred from the copper to the ligands". However, he was unable to relate this to the bonding and stated "I am sort of scraping the memory banks".

6.12.2 Learners' Explanations for the Relationship Between Physical Properties and Intermolecular Forces

Secondary school learners indicated that they had performed an experiment such as that depicted on focus card CB03A (p. 81) before the interviews. Due to time constraints the focus card was omitted in David's interview, however, the other secondary school learners were able to explain the events depicted in the focus card. Learners stated that the difference in behaviour of the three liquid streams arose from a difference in charge, or polarity, and shape of the molecules. Anne offered a typical response.

Anne. Water is bonded like that to give it that shape [drawing bent H₂O molecule, RHS of Figure 6.67]. There's like a slightly negative charge end in this one here like this [drawing δ⁻ on oxygen end] and so that this charge here [drawing circle with + inside it] is attracted to that.

Interviewer. OK perhaps looking at the CHCl₃. How do you see that?

Anne. Well that is very slightly positive [drawing CHCl₃ molecule in tetrahedral shape, writes + near RHS H] [respondent laughs].

Interviewer. OK that's alright. So the hydrogen's very slightly positive.

Anne. Whereas the...[writes - near Cl] is slightly negative and there's a bit of attraction there.

Interviewer. So there's a bit of an attraction there. OK how about the CCl_4 ?

Anne. It's just the structure [drawing CCl_4 in tetrahedral arrangement] [respondent laughs].

Interviewer. OK, so what is the difference there why is there no effect there?

Anne. It's like, it's all the same all the way around.

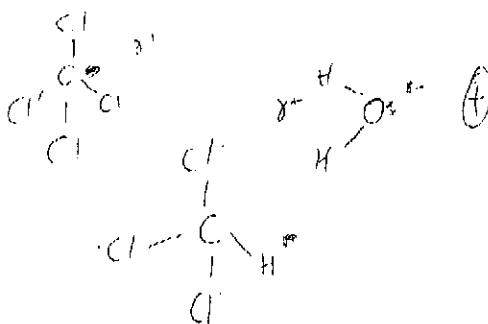


Figure 6.67 Anne's drawing illustrating her explanation of the event depicted in IAE focus card CB03A

Although Anne has not specifically related the polarity of the C—Cl or H—O bond to a difference in electronegativity, it seems that she appreciates there is a difference in bond polarity and furthermore understands the importance of molecular shape. Other learners made similar statements—Claire's response was the most detailed.

They sort of all equally pull on this carbon, and they all cancel each other out. So the molecule is non-polar. So there's no effect, whether you put a positive or negative rod, because the molecule itself is not charged. Chloroform on the other hand [draws planar CHCl_3 molecule, top middle part of Figure 6.68] has got those three, which are highly polar bonds [draws arrows from C to the Cls]. That one is not as polar, so you have got those and just a little one [draws small arrow from C to H]. I don't know which way it goes, but those two cancel each other out [indicating Cls opposite each other]. So you are left with the effect of those two [indicating the H and remaining Cl] which makes that one δ^- and that δ^+ [writes δ^+ near H and δ^- near Cl] so they line up. The δ^- end is attracted towards the positively charged rod. Water is quite highly charged because that's [indicating oxygen] the second most electronegative atom [drawing bent H_2O molecule] apart from chloride and fluoride. So you have got two polar bonds here, which can be represented by those two vectors [draws arrows under H_2O molecule] which add to give that [draws heavy arrow between arrows].

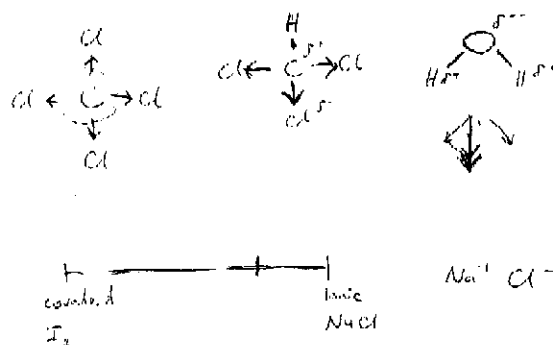


Figure 6.68 Claire's drawing illustrating her explanation of the event depicted in IAE focus card CB03A

Claire went on to explain the origin of the polar covalent bond which she related to the concept of the ionic-covalent continuum and to samples she had encountered previously during her interview, that is, NaCl and I₂.

Interviewer. Can you just tell me a little bit about those δ^- and δ^+ signs. What are they indicating to you?

Claire. Because it's a polar bond. There's the continuum between the covalent like iodine [draws line, writes covalent and I₂ at one end, and ionic and NaCl at other, lower part of Figure 6.68], and the ionic which is usually taken to be sodium chloride and like all the other bonds fall into the sort of continuum. I don't know where the carbon chlorine would be, but it'd be, it's quite polar.

Only one secondary school learner, Richard, was unable to offer an explanation for the event. Nonetheless, Richard related the events to the nature of the bonding in the compounds, "I think it would be something to do with the bonds, polar, non-polar...", and made the connection to the electronegativity of the elements involved "I think it's electro, electronegativity".

Undergraduates explanation for the event depicted in CB03B (p. 82) suggested that they believed that boiling points of liquids were related to molecular size. Learners stated that the boiling point for group-14 hydrides was related to the strength of inter-molecular forces. For example, Steve stated that "the boiling point is going to be a measure of the degree of attraction between these particles in the liquid", and went on to relate this to the concept that "you are getting to a larger

and larger species down the series. There is a larger and larger surface area around the around the molecule, and that is facilitating a greater area for van der Waals attractions between the molecules". Similarly, Alan stated "the gradual increase in boiling point I would probably attribute to the increase in mass", Phill's supposition was that "they would increase because they are getting bigger", and René believed that "those are showing an increase in molecular weight and so the boiling point would be increased". Reasons for the anomalously high boiling points of the first member of group-15 and group-17 series (i.e., HF, NH₃) varied. Three learners, Steve, Kim, and Mary, stated that hydrogen halides were ionic in nature. However, the concept that the bonding in hydrogen halides is ionic seemed to result in Steve becoming confused about the intermolecular forces in these compounds.

Well in that case in the liquid you don't have that [writes HF, Figure 6.69] you have H plus F minus [draws H⁺ and F⁻]. So looking at H⁺ and Cl⁻ [writes HCl, and draws H⁺ and Cl⁻], and so in this case going from the fluorine to the chlorine, you have got a significant decrease in electronegativity. So consequently that tends to suggest that because this is an electrostatic interaction and it is dependent upon how strongly the fluorine is going to tack on the electron to form the fluoride. Then if you have a decrease in electronegativity, then the chlorine [draws box around Cl⁻], will have much less of a tendency to take on an electron and form the chloride [writes dec electroneg]. Hence the electrostatic interactions will be weaker.

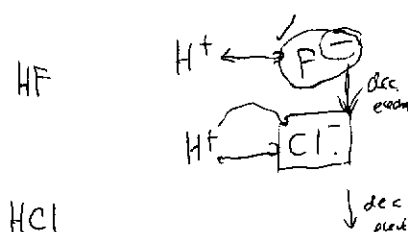


Figure 6.69 Steve's drawing illustrating the intermolecular forces in hydrogen halides

Kim, in contrast, was able to explain the high boiling point of HF more convincingly.

Interviewer. I am just interested in the shape of the lines if you like. One feature of that is the fact that say HF as you have started with that group there, is higher than, significantly higher, than its next member HCl.

Kim. OK I suppose it's more electronegative, so the bonding's stronger.

Interviewer. OK. So what's more electronegative here?

Kim. Um, fluoride.

Interviewer. Fluoride...OK. So how does that make the bonding, stronger did you say?

Kim. Yeah, so like you need more energy to break the bonds, to boil the thing.

Interviewer. When you say the bonds. Which bonds are you referring to there?

Kim. The HF.

Interviewer. HF?

Kim. The HF bonds. These bonds [writes HF under original HF and draws dotted lines linking them, Figure 6.70].

Interviewer. Oh OK, I see.

Kim. The intermolecular bonds.

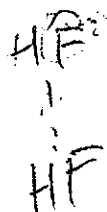


Figure 6.70 Kim's drawing illustrating the intermolecular forces in HF

Learners were less clear on why there were increased intermolecular forces in NH_3 . Bob stated "I would only be speculating", Alan "I suppose the lone pairs on the nitrogen", Phill "I can't say" and neither Mary nor Renée were able to offer any explanation at all. Jane simply stated "it could be the electronegativity", but Steve was able to provide explanations, Steve's being the more detailed.

Steve. Well you have got a lone pair of electrons on the nitrogen. I suppose it means that part of the molecule is slightly electronegative, and the other part is slightly electropositive. So naturally there is going to be some sort of attraction between the two, which is van der Waals. In this case here [indicated PH_3] you have got the same thing.

Interviewer. That's the PH_3 is it? [see, CB03B, p. 82].

Steve. Yes. But in this case now with the PH_3 , the electronegativity of the phosphorus with respect to the nitrogen is once again significantly reduced. So that's not so electronegative so therefore the interaction is not as strong.

Postgraduates were quick to relate the boiling point of the hydrides to intermolecular forces, for example, Christine stated that "a higher boiling point means that the intermolecular interaction must be stronger". Postgraduates went on to state that the gradual increase in boiling point was due to the increase in size of the central atom down the group. Grace stated that "I just see it as a size thing. The bigger it is the less volatile it is", Jason "as the hydride gets heavier the boiling point increases", and James "I'd say 'cos they are getting heavier". Learners also related increased size to increased polarisation. Grace's view was that it is like "the more polar. If the compounds end up being polar they are attracted to one another more, so the boiling point is higher". Rose, Jenny, and Kevin were unable to offer an explanation for the trends in boiling points although Rose stated that the increase in boiling points was related to an increase in the strength of bonds, but it seems she thinks this is due to intramolecular bonds as she referred to bonding between "hydrogen and nitrogen". The high boiling points of NH_3 and HF were attributed to increased intermolecular interaction and specifically to polarisation or hydrogen bonding. As seen in the following responses, postgraduate's explanations tended to be more detailed than their undergraduate or secondary school counterparts.

James. I just sort of think HF and NH_3 would be quite, the bonds would be quite polarised. So there'd be these dipole-dipole type interactions, which makes it harder to boil. As you move down, it's like phosphorus and chlorine and so on, they become more covalent. So you have less of the sort of dipole-dipole bonds, so it's easier to boil.

Christine. The interaction between the discrete molecules is weaker than the HF one is. Because of that it's easier to boil methane.

Interviewer. Than HF alright.

Christine. So therefore the to strip them apart is easier. So therefore there must be a weaker interaction which I guess comes back to the fact it's more polarised.

Grace. Fluoride's like really electronegative, it's really electronegative, and so it's pulling the electrons towards itself. Between that hydrogen and along the hydrogen fluoride bond. The fluoride, the fluorine, is holding the charge more, so it's an induced polarity, there's polarity over that bond. Because the hydrogen fluoride is a polar species, then there's going to be an intermolecular interaction. So you've got intermolecular interactions going between a whole lot of hydrogen fluoride, hydrogen fluoride, molecules. So because they are attracting

they are staying together in the liquid more, and wanting to split up into, or vaporise less. They are not wanting to go into the gas phase so much. So you still have got the size thing going on, but in the case of fluorine, I think that's because it's really electronegative and it's induced polarity attracting other molecules.

Brian. Well the boiling point I would guess would be directly related to the interactions between molecules, rather than within molecules themselves. So it means the stronger the interaction between the molecules, the more closely they attract each other, the higher the boiling point, because you have to break those intermolecular bonds to boil. For NH_3 and HF you would have hydrogen bonding going on in the liquids, which you wouldn't have for... Well the reason for which you wouldn't have in any of the other ones, fluorine and nitrogen are both highly electronegative, which causes the H end to polarise dramatically.

As was characteristic, Jason offered a highly detailed explanation, and went on to describe his understanding of hydrogen bonding.

Looking at the general trend in this line in this diagram you can see that as you increase the molecular weight of whatever hydride you are dealing with. For example, the carbon, silicon, germanium, tin series is a good one. As the hydride gets heavier the boiling point increases. However, that trend is broken by both the group three and the group five and the seven one by ammonia and HF. In this case the reason the boiling points are different is because of something called hydrogen bonding. This is where you have a bond between ammonia, for example, where you have [drawing ammonia molecule, Figure 6.71]...and hydrogen bonding is the bonding between the hydrogen of an adjoining ammonia [drawing second ammonia]. In this case say this hydrogen, and a lone pair on another nitrogen [draws dotted line from H to lone pair]. I think the reason for this bonding is because the within each nitrogen—hydrogen bond you have a covalent bond which is sharing of the electrons, but because nitrogen is quite electronegative, that means it likes to hold the electrons as close to it as possible. It holds the shared electrons very close to it, rather than the hydrogen. So the hydrogen is effectively electron deficient, and so you can get a bond with the lone pair on the nitrogen, because a lone pair of course contains spare electrons if you like. And they're attracted to the electron deficient hydrogens. Now you only get that in cases where you have a very electronegative main atom. So that's why you see it mainly for HF and ammonia.

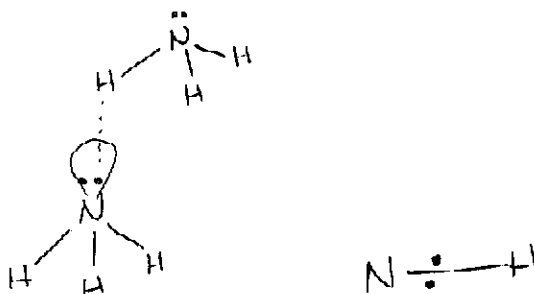


Figure 6.71 Jason's drawing illustrating the intermolecular forces in ammonia (NH_3)

Although the diagram produced by Jason here clearly indicates the molecular nature of the substances, neither Jason nor any of the other learners articulated explicitly the difference between intermolecular and intramolecular bonding.

6.13 Summary

Learners' preferred mental model for the target system of covalent bonding was the octet rule. Learners viewed covalent bonding as arising from the sharing of electrons and the driving force behind this process was the formation of a stable octet. Postgraduates evidenced a fuller appreciation of the molecular nature of the covalent molecular substances used in the inquiry than their secondary school or undergraduate counterparts. Secondary school learners preferred a more detailed depiction for the bonding of those illustrated in CB01 and, unlike undergraduates and postgraduates, appeared to hold the alternative conception that benzene contains double bonds. Undergraduates and postgraduates preferred simple depictions, but showed an appreciation of the delocalisation of bonds in conjugated alkenes and the resonance concept. Learners across all academic levels evidenced a clear appreciation of the directionality of covalent bonding although they were unable to explain the underlying cause. All but one secondary school learner failed to understand the concept of unequal sharing of electron pairs, whereas undergraduates and postgraduates related this to electronegativity difference in atoms. Few learners were able to explain changes in colour of metal complexes upon

changes to the co-ordination. However, most were able to relate physical properties such as boiling point and polarity to the bonding and structure of covalent molecular compounds, with undergraduates and postgraduates specifically relating physical properties to intermolecular forces and hydrogen bonding.

Chapter 5 comprises a description of the data analysis as it pertains to the second and third research goals; learners' use of analogy and alternative conceptions for chemical bonding.

CHAPTER SEVEN

LEARNERS' USE OF ANALOGY AND ALTERNATIVE CONCEPTIONS FOR CHEMICAL BONDING

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CHAPTER SEVEN
LEARNERS' USE OF ANALOGY AND ALTERNATIVE CONCEPTIONS
FOR CHEMICAL BONDING

Overview of the Chapter

This chapter comprises the data analysis of the clinical interviews with respect to the two subordinate research goals, beginning with learners' use of analogy, followed by learners' alternative concepts for chemical bonding. The chapter concludes with a summary of the results.

7.1 Learners' Use of Analogy for Chemical Bonding

The second research goal for this inquiry as reported in Chapter 1 is to

Establish the prevalence of the use of analogies for the understanding of the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

Learners' use of analogy was determined by examination of interview transcripts and were classified according to Dagher's (1995a) typology, that is, compound, narrative, procedural, peripheral or simple. Compound analogies are those which draw on more than one domain source to explain related ideas in the target domain. Narrative analogies are those which take the characteristics of a story—with one source domain used to explain several concepts in the target domain. Procedural analogies are those that pertain to the procedures with which science is conducted. Peripheral analogies are analogies that are used to support a central analogy, and simple analogies are analogies that involve a single link between target and source. Simple in this sense does not mean that the connections between target and source are trivial or obvious; rather, simple analogies are characterised by the brevity of analogical reference (Dagher, 1995a).

Some target models, notably the sea of electrons model, are clearly analogical in nature and for the purposes of classification have been deemed an analogy. The sea of electrons model entails the analogical mapping of two concepts; the mobility of electrons—likened to the fluidity of a gas—and the packing of spheres. If both these elements were present in a description, the analogy was classified as a compound analogy. If only one element was present, the analogy was classified as a simple analogy, since the model entailed mapping from two domains. Similarly, the use of physical models involving the packing of spheres during chemistry instruction is ubiquitous. As described previously (see, e.g., Section 6.3.1, pp. 145-149), use of terminology pertaining to specific packing models also is common, for example, cubic close-packing, hexagonal close-packing and so forth. In effect, this terminology represents the use of analogy. However, it is not always clear from the interview data if learners *perceive* such a description as use of analogy, or if rather, they in fact believe that atoms and ions are spherical. One reason this occurs is that criterial attributes for ionic bonding include reference to shape of ions, hence, learners' views of the shape of ions were probed during interviews (Chapter 6, p. 189). Hence, such references in interview transcripts were not classified as analogy use, unless the learner has explicitly stated that an atom or ion is *like* a sphere. Other analogies identified in learners' descriptions were classified by reference to Dagher's (1995a) typology.

Secondary school learners made extensive use of analogies to describe aspects of their mental models for chemical bonding, with a total of 29 analogies identified (Table 7.1). Of these, 25 were classified as simple analogies, the remainder being compound analogies. The use of simple analogies involved a single statement or link, with mapping clearly superficial in nature. Keith, for example, used a simple comparison of concrete to illustrate his views regarding the strength of bonding in metals.

Because the bonds aren't so strong they are electronic, I don't know, like in concrete or something harder, steel.

Table 7.1 Classification of learners' analogies according to Dagher's (1995a) typology

	Secondary School	Undergraduates	Postgraduates	Total
Compound	4	3	6	13
Narrative	0	0	0	0
Procedural	0	0	0	0
Peripheral	0	0	3	3
Simple	25	13	18	56
Total	29	16	27	72

Richard discussed his preference for depictions E and D of covalent bonding in benzene (C_6H_6) (focus card CB01, p. 81) and generated a simple analogy of bowling pins "D looks like a bunch of ten pin bowling things" to describe the appearance of boundary surface representations of molecular orbitals (Appendix A pp. 346-347). Similarly, Neil used two simple analogies, one in which he related the shape of ionic species to the trajectory of planets, and a second in which he related the spatial arrangement of ions in sodium chloride to a die.

Neil. Shape of Na^+ ions, so yeah they are round. They are round; it's the sort of shape planets travel, like that I suppose [respondent laughs].

Interviewer. In rows is it? OK, how would you see one row in relation to another row?

Neil. Sort of just like...you would have like one in the middle, and you'd have six around it like dice [sic] sort of shape.

Interviewer. A dice, OK.

Neil. That's not how, that's not the shape of it.

Interviewer. All right.

Neil. But if you look, that's actually like stacked up like, like where the dots are.

Anita made extensive use of analogies describing a total of nine analogies, nearly a third of the total for secondary school learners. As she described her mental models she related them to simple real-world experiences; cartoon pictures, balls, and spyograms (i.e., an interactive computer game).

Interviewer. What do actually see as holding them together if you like? Do you have a picture of what that might be like?

Anita. Just what you see in textbooks little lines [respondent laughs]. Yeah and they are pretty much like little cartoons showing ways of joining them.

Interviewer. What does covalent mean to you then?

Anita. It's another picture I have got in my mind. Two things sharing it, and sort of overlapping in the middle. Like one little ball, and another little ball and they are joined together and cross over and then they share that cross-over bit.

Interviewer. Is there any one of those that particularly doesn't appeal to you?

Anita. E [i.e., choice E from CB01, p. 81]. Because I have never seen anything like that before.

Interviewer. OK, so it's unfamiliar to you. How about D? Have you ever seen that before?

Anita. Yeah that's a bit weird. It's like one of those spyograms.

One learner, David, introduced a compound analogy when he described his mental model for the organisation of aluminium atoms on an atomic scale. He likened the arrangement of aluminium atoms or ions to that of a die and a grid "I'd see them...in a grid sort of, you know. Straight up and down, like a dice [sic]". The remaining compound analogies identified for secondary school learners comprised the sea of electrons model.

Overall undergraduate learners made less use of analogies than their secondary school counterparts (using 16 compared with 29 analogies) and demonstrated a preference for simple analogies; the most common example of compound analogy was the sea of electrons model. For undergraduate learners, analogy use also was dominated by one individual, Bob, who like Anita frequently struggled to express his views of bonding, and resorted to the use of analogies to explain his ideas. However, unlike Anita, as well as making extensive use of simple analogy, Bob generated a compound analogy—comprising a ball-and-stick model, and a glove when he described his preferred model for the bonding in aluminium foil. In addition, he introduced the simple analogy of a rubber band to aid his description of the friability of the sodium chloride (IAE focus card IB02, p. 80).

Interviewer. You said molecular orbitals. I am interested to know what you envisage as being a molecular orbital. What does that term mean to you?

Bob. To me, like an electron density around atoms. You know how you have atomic orbitals, they have been told to us as being like a stick between two balls or whatever like that. I see the molecular orbitals more of as an electron density that sort of surrounds the whole thing, and binds them together, like, I don't know, a glove over them or something like that.

Interviewer. So just say focus on the sodium chloride. Why do you think that's breaking down? I understand what you are saying about that silica, it's that structure you were talking about and the strength. But it's not quite obvious to me why you believe the sodium chloride is breaking down.

Bob. Um...it's more brittle, why I am not sure. It's maybe related to the positive and negative charges on that. If enough force is applied to get them far enough apart so that, that one over r squared term.

Interviewer. Oh, yeah.

Bob. The electrostatic force between them can, if it knocks them far enough apart so it's not valid anymore, then they are going to let go then.

Interviewer. So the force would change that distance.

Bob. Well shearing, you know if the force is enough to shear those bonds and move them apart from each other enough to let go.

Interviewer. OK.

Bob. It's like a rubber band I suppose in that way.

However, more typically undergraduate learners employed simple analogies, involving the use of a single term, and made little attempt to develop links between source and target domains. Terms such as floppy electron clouds and bonds represented by sticks were used to describe the bonding in covalently bonded substances.

Bob. The chloride shape, big, floppy type thing. Because you've got a greater negative charge floating around the outside of the small positive charge in the middle it's got a slightly higher amount of repulsion amongst the electrons, pushing them apart, making it bigger.

Jane. So I look at the, um, you know how they have those stick like kind of things.

Interviewer. Yes. Feel free to draw it.

Jane. [draws SiO₄ unit in tetrahedral arrangement, see Figure 7.1], um...

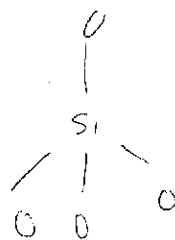


Figure 7.1 Jane's drawing of the structure for silica (SiO_2)

Kim's description of the structure of sodium chloride, upon probing about the shape of sodium ions, appeared to use spheres as an analogy to explain their shape.

Interviewer. Do you have a picture of what the shape would be?

Kim. Ah in the pictures it's depicted as spherical [respondent laughs].

Interviewer. Is that the way you see it?

Kim. I suppose they would be. Like they are not physical, like tangible entities which stay in the same shape all the time like. Um, you have got electrons that are moving around. The nucleus. So they are roughly spherical [respondent laughs].

Kim did not seem to think that sodium ions are "tangible entities" that happen to be spherical in shape and she appeared to be mapping between the source and analog domain, viewing the packing of like-sized spheres as an analogical model for the structure of the ionic substance sodium chloride.

Although Steve described the structure of the ionic compound sodium chloride in terms of orbitals, his description shows how the use of analogy may result in conflict with certain target models. In this case, Steve used the analogy of the packing of spheres to describe the nature of the ionic lattice in sodium chloride, but it appears that this resulted in conflict with his concept of the overlapping of p -orbitals to form π -bonds, a valence bond concept (Appendix A, pp. 338-340).

Well when we talked about the ionic bonding with the repeating units, I have always thought of them as being, as, as being spheres. Basically that's always been the image that we have been given. But just thinking about it now because the $2p$ have formed sort of fuzzy lobes. It's difficult to see that they can sort of merge together and form a sphere.

Thus, it appears that Steve has confused the boundary surface depiction of an atomic or molecular orbital with the analogy of the packing of spheres.

The incidence of analogy use by postgraduates was similar to secondary school learners, that is, greater than undergraduate learners (Table 7.1, p. 256). However, in contrast, postgraduates made greater use of compound analogies and their analogies, like their mental models, tended to be more detailed. Christine, for example, mapped a number of concepts from different domains as she explained the bonding in sodium chloride. She began by relating the shape of the chloride ion to a saucer, a banana, a cupped hand, and a flower petal. With little prompting she drew a diagram of a saucer (Figure 7.2) and used this and other analogies to describe the shape of the chloride ion in sodium chloride.

Christine. It's sort of like a like a saucer if it was in two dimensions. I think of it like that, even though I think of chlorine like a banana almost.

Interviewer. Banana, OK.

Christine. Kind of curved. But probably in three dimensions, almost like a cupped hand or something.

Interviewer. Sorry what did you say? Cupped hand?

Christine. Yeah. Like a flower petal or something. Not just a banana, not in two dimensions like that.

Interviewer. Could you perhaps just draw it so I know what you mean by that?

Christine. You'd have got your [drawing Na⁺ inside sphere, RHS of Figure 7.2].

Interviewer. That's your sodium is it?

Christine. Yeah.

Interviewer. OK that's alright. I just want to be clear on what shape you are describing so I understand what you mean.

Christine. Like it's a saucer. You know how, how it [draws a saucer shape and labels it saucer] I can't draw a saucer.

Interviewer. That's OK I understand what you are saying.

Christine. Like it's, um...

Interviewer. So that there is the large circle, with the smaller one inside it. That is this other curve here?

Christine. If you are looking at it flat on.

Interviewer. From the side OK

Christine. Yeah. So it's three dimensional like a saucer. Like a cupped hand.

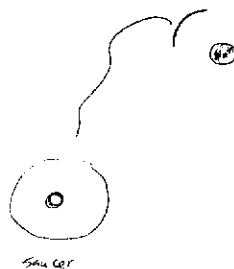


Figure 7.2 Christine's drawing illustrating her compound analogy for the shape of the chloride ion

Similarly, Jenny introduced a compound analogy to describe the bonding in aluminium foil. She began with the analogy of the packing of spheres (see Figure 7.3); however, as she struggled to recall specific terminology, she introduced a second analogy, a star, to aid her description of their geometrical arrangement.

I guess I sort of see it as spheres, a whole heap of aluminium atoms like this. Sort of really close packed together. Not, not sort all most like I guess a star sort of description, sort of a star.

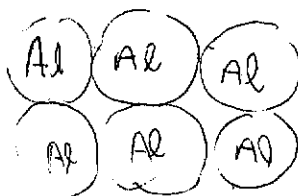


Figure 7.3 Jenny's drawing illustrating the structure of the aluminium lattice

Jason's use of analogy, like Christine's, was extensive and detailed. He generated a compound analogy, the sea of electrons model for metallic bonding in aluminium foil and subsequently introduced a peripheral analogy, that of proton transfer. The statements made by Jason clearly indicated that he appreciated that he was using analogy during his description.

The picture I have is whole lot of metal atoms, basically all stacked as closely as possible together. There's a bunch of different metal structures, like cubic and hexagonal close-packing and then the body-centred cubic. So basically all the metal atoms are as close together as they can possibly be and the valence electrons, the outer electrons, are basically, can transfer from one, from one metal to another very easily. So that the electrons can

flow backwards and forwards through the metal. I sort of analogise it with the way kind of the way the protons go through water. The conductivity of protons is much more than any of the ionic species, because it can sort of latch on to one side of the water molecule, and another other one falls off the other end. Then goes onto the other and I guess that's how I see it, the same sort of thing.

Jason and James were the only learners to make use of peripheral analogy during this inquiry. Jason described his compound analogy for the bonding in sodium chloride and aided his description with the use of a peripheral analogy. He introduced of the concepts of floppiness and softness to describe the polarisability of electron clouds.

Jason. I kind of regard polarisability as sort of it's almost the floppiness of the...

Interviewer. Floppiness?

Jason. [respondent laughs] of the anion, it's sort of big and easily deformed. I guess I sort of associate it with the softness of the anions as well.

James similarly introduced the concept of softness to aid his explanation of his compound analogy the sea of electrons model which he employed to explain the bonding in aluminium foil.

I'd sort of see like transition metals, especially like the hard transition metals like say titanium, as having like highly charged positive spheres with electrons flowing all around it. But I'd sort of see say main-group metals as maybe softer metals. Sort of having a bit more covalent bonding so the spheres aren't as highly charged.

Classifying James's use of the term soft here as analogy may be somewhat tenuous, since the terms soft and hard are frequently used during instruction to describe the polarisability of anions and cations. However, unlike spheres, soft, floppy and hard are terms less likely to be associated with atoms and ions in a realist sense.

Learners' use of analogy was classified according to the target system, namely, metallic, ionic and covalent bonding (Table 7.2).

Table 7.2 Learners' use of analogy classified according to the target system

	Bonding		
	Metallic	Ionic	Covalent
Secondary School	11	11	7
Undergraduates	7	6	3
Postgraduates	14	8	5
Total	32	25	15

It is evident from Table 7.2 that most use of analogy was made for the target systems of metallic and ionic bonding. This is mostly due to the analogical nature of the target models used for these two target systems; that is, the sea of electrons model for metallic bonding and packing of spheres model that forms part of the electrostatic model for ionic bonding.

7.2 Learners' Alternative Conceptions for Chemical Bonding

The third research goal for this inquiry as reported in Chapter 1 is to

Establish the prevalence of alternative conceptions for the concept of chemical bonding for secondary, undergraduate, and postgraduate chemistry learners.

Learners' alternative conceptions for chemical bonding were identified by examination of interview transcripts. In this chapter, a conception has been classified as an alternative conception if it meets the following two criteria—the view was in disagreement with the scientific view and the conception was related to some aspect of chemical bonding, including specific details of a particular model for chemical bonding. For example, to describe the bonding in ionic compounds, learners typically described the size and shape of ions as well as the packing. Hence views at odds with the scientific view about ion size, shape or nature of packing have been classified as alternative conceptions. However, during discussions

centred on IAE focus card MB02 (p. 79) which compared the electrical conductivity of metallic copper with that of glass, there was evidence that some learners held alternative conceptions about electrical conductivity. However, because such alternative conceptions did not pertain to chemical bonding, they have not been included in this thesis.

Alternative conceptions were compiled into *Concept Profile Inventories* (CPIs) and expert-validated by the instructors involved in this inquiry (Appendix B, p. 363). It is important to note that this research question is subordinate to the main aim of the inquiry, namely, to establish learners' preferred mental models for chemical bonding. Consequently the results reported herein should not be deemed as an exhaustive catalogue of learners' alternative conceptions for chemical bonding. Rather, these data represent a compilation of alternative conceptions revealed when learners discussed their mental models for chemical bonding.

Learners' alternative conceptions identified in this inquiry are provided in Table 7.3. Many of these 20 alternative conceptions were not widely held, several alternative conceptions being held by a sole individual. Because the inquiry does not comprise a systematic attempt to uncover learners' alternative conceptions, a given alternative conception may have been identified for only one learner, but this does not necessarily mean only one learner holds this alternative conception.

The alternative conception that chemical bonding is weak was prevalent across all levels of learners (AC 1-3, Table 7.3) who seemed unaware that this view conflicted with direct physical evidence such as the hardness of metallic copper. Keith, for example, attributed the malleability of copper to weak metallic bonding (AC 1) (IAE focus card MB03, p. 79).

I think as it goes through rollers the copper atoms just spread out. Like, the bonding, the bonding between them isn't so strong.

Table 7.3 Learners' alternative conceptions identified in the inquiry

Alternative Conception 1 <i>Metallic bond is weak bonding</i>	Alternative Conception 11 <i>Metallic lattices contain neutral atoms</i>
Alternative Conception 2 <i>Intramolecular covalent bonding is weak bonding</i>	Alternative Conception 12 <i>Electronegativity comprises attraction for a single electron</i>
Alternative Conception 3 <i>Ionic bonding is weak bonding</i>	Alternative Conception 13 <i>Molecular iodine is metallic in nature</i>
Alternative Conception 4 <i>Continuous metallic or ionic lattices are molecular in nature</i>	Alternative Conception 14 <i>Ionic bonding comprises sharing of electrons</i>
Alternative Conception 5 <i>The bonding in metals and ionic compounds involves intermolecular bonding</i>	Alternative Conception 15 <i>Ionic and metallic bonding contain an element of directionality</i>
Alternative Conception 6 <i>The ionic radius of the sodium ion is greater than the chloride ion</i>	Alternative Conception 16 <i>Ions in close-packed metal lattices possess other than eight nearest neighbours</i>
Alternative Conception 7 <i>The ionic radius of the lithium ion is greater than the sodium ion</i>	Alternative Conception 17 <i>Metal to non-metal bonding in alloys is electrostatic in nature</i>
Alternative Conception 8 <i>Polar covalent compounds contain charged species</i>	Alternative Conception 18 <i>Ionic shape and packing is influenced by pressure</i>
Alternative Conception 9 <i>Molecular iodine contains I minus ions</i>	Alternative Conception 19 <i>Intermolecular forces are influenced by gravity</i>
Alternative Conception 10 <i>The charged species in metallic lattices are nuclei rather than ions</i>	Alternative Conception 20 <i>Glass is an ionic crystalline substance</i>

David suggested that the intramolecular bonding in chloroform (CHCl_3) is weak. In his view, so weak that it resulted in the release of gaseous hydrogen and chlorides.

David. I'd see the bonding as pretty loose, not strong bonding 'cos this is the stuff that puts you to sleep.

Interviewer. Yes it has been used for that.

David. So it must be letting off some hydrogens and stuff, so I don't think it would be that strong.

Interviewer. OK, so when you say loose, can you just expand on that a bit.

David. Not strong bonds.

Interviewer. So that CHCl_3 , can you just tell which part of that you would see as being loose.

David. Was it CHCl_3 [writes CHCl_3]...the chlorides probably.

Interviewer. You would see the chlorides as being loose in your view?

David. Yep.

Interviewer. So can you just clarify for me. Do you see that as actually breaking away from the CHCl_3 ?

David. ...Yeah I do.

It is possible that such confusion arises from inappropriate use of nomenclature, it being common to refer to molecular hydrogen, that is, dihydrogen gas (H_2), simply as hydrogen when describing organic compounds. Hence, when learners are told that chloroform or other hydrocarbons contain hydrogen, it is possible that they confuse this with molecular hydrogen. This situation is likely exacerbated when the substance, like chloroform, is rather volatile in nature—the volatility perhaps suggesting to learners that a gas has been given off.

David also appeared to believe that "chlorides" are released from the chloroform. In an attempt to clarify this suggestion, the interviewer may have inadvertently led David to the view that it is the intact chloroform molecule that is volatilised.

Interviewer. So what has become a gas here, is it the chloroform itself or the chlorides?

David. Yeah, yeah it's the chloroform.

Interviewer. The chloroform sample?

David. Yeah it's becoming a gas

David's rather eager response may mean that he has picked up on a suggested alternative rather than indicating he has changed his view. His response seems to contrast with his earlier responses, where with more neutral prompts, he indicated that he believes the bonding in chloroform is "loose" and that something had broken away from the chloroform molecule.

The view that the electrostatic forces holding ionic compounds together are weak was prevalent (AC 3, Table 7.3). This view was the most common explanation offered for the friability of ionic salts such as sodium chloride (IAE cards IB03A and IB03B, p. 80) and was identified across all levels of learner from secondary school to postgraduate.

Anne...Um, sodium chloride is weak.

Neil. In the sodium chloride the force can just break it, the bonds are not very strong.

Steve. The ionic bonding that is holding this crystal together here is weaker than is the case of the covalent.

Kim. Would it be like the sodium chloride's got weaker bonds than silicon oxide?

Jane. I don't know, I mean it's really that it's stronger.

Brian. It's much harder to break bonds, actual direct covalent bonds like this than it is to break weak ionic bonds.

Other learners, whilst not explicitly stating that such forces were weak, made statements that seem to imply this. For example, Jason asked "can you actually melt sodium chloride with a Bunsen?" and Bob also expressed some surprise at the fact that a Bunsen was able to melt the salt and commented that "pretty hot Bunsen". It seems that Bob thinks to break down sodium chloride would require considerable energy input—more energy than a Bunsen can provide. Furthermore, his explanation of the friability of sodium chloride (IAE focus card IB03A, p. 80) indicated that he views electrostatic forces in sodium chloride as weak.

The sodium chloride is only relying on an electrostatic force to hold together, whereas the other one's got a lot of covalent bonds locking it rigidly together making it strong.

Hence, whilst Bob identified the importance of the network nature for the bonding of giant covalent structures, the fact that he dismissed the bonding in the ionic substance as merely "electrostatic force" indicates that he views such forces are somehow inferior. Christine's view appeared similar to Bob's, but it is more evident that she believed ionic electrostatic forces in sodium chloride are weak.

I see that bonding in sodium chloride can't be as strong [as in SiO_2] although I see it, I guess I see it as the sodium chloride as different type of bonding. But if it's going to crack it must have like...little sections or something. Like that's the only way I can explain it away, like if it's the same type of bonding the silica one must be stronger otherwise the same thing would happen to it.

It was revealed in Chapter 6 that undergraduate and postgraduate learners seemed to possess a greater appreciation of the continuous nature of ionic and metallic lattices than secondary school learners (see, e.g., Section 6.3.1, pp. 145-149). Interestingly, learners across all levels possessed alternative conceptions about the nature of metallic and ionic lattices, seeming to believe that such lattices were molecular in nature (AC 4, Table 7.3). For example, learners used the term *molecules* to describe particles in metals and ionic substances; Frances, Keith and Richard described the motion of particles in molten sodium chloride as they explained the conductivity of molten sodium chloride (IAE focus card IB02, p. 80).

Frances. When you are heating it up, it's making the solid molecules move around more giving them more energy from the heat. That allows the electrons to, some of them to be released into the circuit to make the bulb glow, where this in this [indicating the solid crystal on LHS of IB02A, p. 80) all the molecules can only move a little bit side to side so they can't move and make the bulb glow.

Keith. The sort of bonds are rigid and aren't allowing the sodium chloride to sort of ionise and holds the electrons from flowing on through the sodium 'cos the molecules are held tightly together by the bonds in the sodium chloride, so they can't move around.

Similarly, Keith introduced the concept of molecules in metallic copper and Bob in the metal lithium.

Keith. The copper molecule, it's flowing. Like it's going from positive to negative so the electrons can flow along.

Interviewer. Can you tell me what appeals to you most about depiction D [in MB01, p. 79]?

Bob. The packing together of the molecules in a regular fashion.

It is possible that in some instances this merely represents inappropriate or careless use of nomenclature, such as in Brian's statement that "each sodium is effectively surrounded by chlorines. The chlorines are a very large molecule and sodium is quite small", and Bob's earlier remarks (see, pp. 154, 160). However, some learners identified specific molecular species in metals and ionic substances, suggesting that their use of the term molecule is purposeful, as for example, in Alan's description of the structure of sodium chloride and caesium chloride and in Grace's description of the bonding in sodium chloride.

Alan. I assume it's a regular lattice, so all the ions would be paired, so it'd have a neutral charge on it.

Alan. It shows how the caesium atom makes contact with all these chlorides in the middle. That sort of interaction between the caesium and chloride, like how you are taught NaCl, the NaCl molecule.

Interviewer. The attraction in this case you are referring to as what?

Grace. As within the actual molecule.

A related alternative conception, that metals and ionic compounds possess intermolecular bonds, was held by three learners (AC 5, Table 7.3). David, Keith and Kim described the electrostatic attraction holding aluminium foil together as consisting of van der Waals forces, although David also made mention of electrostatic forces.

Kim. With van de Waals in between.

Interviewer. OK. That's in between what?

Kim. Between the atoms.

David. I suppose there is always the van der Waals things with just the attraction of the electrostatics and stuff, maybe, I am not sure about the actual metal.

Keith. And then bonding between another [draws second similar Li—Cl unit] and another, and another [draws wavy lines between units and off bottom of second unit, writes van der Waals next to wavy line, Figure 7.4].

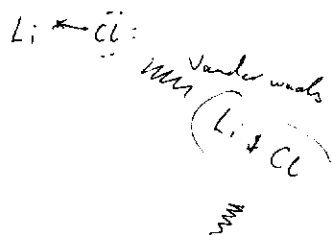


Figure 7.4 Keith's drawing illustrating the bonding in lithium chloride (LiCl)

There were two remarkably prevalent alternative conceptions related to the size of ions identified; one in which the sodium ion was viewed as being larger in size than the chloride (AC 6, Table 7.3), the other that the lithium ion was larger than the sodium ion (AC 7, Table 7.3). Again these views were held across all three levels of learner; Anita, Neil, David, Richard, and Rose all stated that sodium was the larger ion of the two in sodium chloride.

Anita. The sodium would be bigger than chlorine.

Neil. OK lithium's smaller than sodium and, and chloride is smaller than sodium.

David. I would say the Na would be bigger, and the Cl would be smaller.

Richard. Well I would say the sodium is the large one and then the smaller ones would be the chloride.

Rose. Yeah the sodium's larger, and the chloride is sort of packed around it.

Likewise, Neil, Alan, and Mary stated that they believed the lithium ion was larger than the sodium ion, despite being in possession of a Periodic Table at the time.

Neil. Because lithium would be bigger it'd have more protons and electrons it'd be bigger.

Alan. I basically see the bonding to be the same but I would consider lithium to slightly larger than the sodium.

Mary. To me I see it just the same, because it's exactly the same charge. Maybe it could be a little bit bigger maybe.

Interviewer. Sorry what would be bigger?

Mary. I am just trying to work it out here, maybe a little bit bigger than sodium, the lithium.

The data above reveal the tentative nature of the learners' views when the size difference is described as being "slightly larger" and "maybe a little bit bigger". Similarly, Jenny seemed uncertain, her immediate mental picture is inconsistent with the scientific view; that is, the chloride ion being the larger of the two, but in her drawing of sodium chloride (Figure 7.5) the ions were depicted as similar in size.

Jenny. Well I know that they are different, but when I visualise them I see them being the same.

Interviewer. Being the same?

Jenny. I know that chloride is smaller, or is it larger, chloride might be larger. I don't really know [respondent laughs]. I know they are different but when I visualise them they are the same.

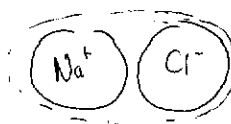


Figure 7.5 Jenny's drawing illustrating the bonding in sodium chloride (NaCl)

It is interesting to consider why this alternative conception should be so prevalent. It is common to illustrate the structure of ionic substances such as sodium chloride using space-filling and ball-and-stick models; informal interviews of all of the instructors in this inquiry indicated that this formed part of their teaching strategy. The ball-and-stick models often have the ion size depicted as similar; whereas there is a significant difference in ion size in space-filling models. Furthermore, it is common to point out that the structure comprises two

interpenetrating lattices of sodium ions and chloride ions, and that in effect the lattice positions are interchangeable. It is possible that this latter view, taken literally, may have resulted in confusion. However, views expressed by some of the secondary school learners offered clues to the origin of the alternative conception that the chloride ion is smaller than the sodium ion. It seems that learners at this level at least, may have confused *ionic* size with the Periodic trend in *atomic* size.

David. I would say the Na would be bigger and the Cl would be smaller, I imagine they would be.

Interviewer. Why do you see it that way?

David. The explanation I have had of that is that as you move across the Periodic...well there's more electrons in the same shell with an increasing number of protons as well.

Interviewer. Oh, OK.

David. And that like attracts them closer which just means it is smaller.

Potential origins for the ion size confusion between lithium and sodium ions are less obvious. The high charge density of the Li^+ ion results in the formation of a strongly held co-ordination sphere containing two layers of polar solvent molecules resulting in an increased effective ionic size in comparison with other ions such as sodium which typically contain a single solvation sphere. This effect is used to explain the low mobility of the lithium, a common explanation in undergraduate chemistry classes and a possible source of confusion for undergraduates and postgraduates; but it seems unlikely to be of relevance for secondary school learners.

The inappropriate use of nomenclature may result in some alternative conceptions. Jason, one of the most academically able and more erudite of the participants in this inquiry, exemplifies the situation. His academic ability coupled with his extensive tutoring of undergraduate chemistry suggest that he is likely to be aware of the importance of nomenclature. Upon describing the formation of the chloride ion from neutral chlorine, he clearly showed that he understands the difference between an ion and a neutral atom, that is, chlorine and chloride. However, he made inappropriate use of nomenclature in subsequent explanations.

Jason. I see the chlorine as being not a chlorine atom but a chlorine ion, so a chlorine which has gained an electron from the sodium atom so that the chlorine atom has a negative charge. The, the sodium has a positive charge.

Interviewer. Yep.

Jason. It's like this structure is essentially held together by electrostatic interactions.

Interviewer. OK I see what you mean.

Jason. Now there's also repulsions as well because in this area here you also have another chlorine atom which is reasonably close to that chlorine atom so there's repulsions between the two.

In a similar way, he used inappropriate terminology when describing the structure of chloroform, although he corrected himself upon realising his error.

Chloroform is a tetrahedral molecule in which a central carbon atom is covalently bonded to three chlorine atoms and a proton, or a hydrogen atom.

Because of his expertise and experience, it seems that Jason is clear in his own mind of the difference between the terms chlorine and chloride; thus interchanging the terms may not be particularly detrimental for his understanding of chemical bonding. However, it is possible that the interchanging of such terms for novices may lead to alternative conceptions. To illustrate, consider another highly prevalent alternative conception revealed in this inquiry—that polar covalent compounds contain charged species (AC 8, Table 7.3). Frances, like Jason, indicated that chloroform contains a proton, Anita identified Cl minus in the same compound, whereas Kim identified charged species in the hydrogen halide series—HF, HCl, HBr and HI.

Frances. Because these two have H's in them and H with the Cl, and the highly electronegative ones like chlorides and things like that that gives the hydrogen bonding whereas they can readily donate a proton away to the hydrogen.

Anita. Yeah 'cos H is plus and Cl is minus, but I dunno why, I just know it is different but I don't know why.

Kim. That's ionic bonding isn't it?

Interviewer. That's HF you have written there.

Kim. Yeah and HCl, 'cos it's so electronegative that they cause ionic bonding.

Kim. I was thinking maybe the chloride attached to the hydrogen and share an electron, but now I am thinking maybe not [respondent laughs].

Interviewer. That's the HF is it, or is it all of them or what?

Kim. All of them.

Mary stated explicitly that she viewed the bonding in hydrogen halides as ionic in nature "I kind of think them as being ionic". Jenny articulated her views about the bonding in chloroform in greater detail drawing on previous experience about of the bonding in carboxylic acids; part of her MSc research project. However, the value of doing this seems dubious, as she confused the donation of protons in carboxylic acids with a perception of lability of the chlorine atom in chloroform (CHCl_3). The fact that she used the term chloride, rather than chlorine, is present may indicate that inappropriate nomenclature has in part contributed to her alternative conception.

Jenny. I know that to remove an atom from chloroform is quite difficult. But if you look at other organic molecules will, um...

Interviewer. Yeah, use another organic molecule if you want.

Jenny. I mean if you think, like your carboxylic acid it's quite easy to remove the proton and the same for the chloride, like a halide.

Interviewer. Right.

Jenny. It's quite easy to remove a chlorine from a long sort of carbon chain.

The fact that Jenny described the chlorine in chloroform as chloride, indicative of an ionic species, may have led her to make an inappropriate link to her own experience with the ionisation of carboxylic acids. Examination of interview transcripts revealed that it was routine across all academic levels for learners to interchange terms pertaining to halogens with the charged halide. Learners used the terminology for neutral atoms when describing the bonding in ionic compounds, and similarly described halides as halogens, as seen in Keith's description of the bonding in sodium chloride, Steve's in lithium chloride, and Alan's for chloroform.

Keith. OK the sodium has got one electron in it's outer shell. and the chlorine has got seven.

Interviewer. Right.

Keith. So the chlorine requires one more electron.

Keith. The bonds in the sodium chloride I don't think are as strong between the sodium and the chlorine so they are not attracted to each other, the sodium and the chloride ions.

Steve. Well basically it's going to be easier for the chlorines, wait a sec., um because the chlorines are still, the chlorides have still got the same size.

Alan. I guess there would be certain differences with the chlorine negative charge.

Interviewer. So the chlorine is?

Alan. Negative, being negative, more electronegative than the hydrogen.

An underlying origin of this view may be the notion of the ionic-covalent continuum (Appendix A, p. 329). Learners are usually told that there is no such thing as pure ionic bonding and that atoms in polar-covalent compounds hold partial charges. It is possible that this notion reinforces the view in learners' minds that chlorine is charged, causing confusion between the notion of a partially charged chlorine atom in a polar covalent compound and the negative chloride ion. In support of this proposition, inappropriate use of terminology seems to be influential in the formation of alternative conceptions about the bonding in pure molecular covalent substances like elemental iodine (AC 9, Table 7.3). It is perhaps more likely that learners confuse chloride and chlorine in a substance like chloroform which they are told is polar covalent and where the chlorine atom carries a partial charge. However, this is not the case for non-polar molecular covalent species like homonuclear diatomics such as molecular iodine (I_2). The fact that the same alternative conception is seen for such substances adds credence to the underlying basis of the alternative conception being confusion of nomenclature. Mary and Rose seemed to believe that the iodine atoms in I_2 carry a negative charge, although they both subsequently stated that the bonding comprised sharing of electrons, that is, a covalent bond.

Mary. Iodine well I know iodine as being I_2 , that's how I remember it. Iodine is, um, I minus so therefore it's got one extra electron I guess sitting there, that's not doing anything [respondent laughs] and it's able to pair up with another

iodine which also has a spare, and those two electrons come together and form a bond.

Rose. In iodine, well it's like two atoms of iodine, they would be equally contributing from the covalent bonds because each I minus, each iodine would be like lacking one electron.

Interviewer. What did you say? I minus one did you say?

Rose. Yep.

Interviewer. OK.

Rose. So they join together to form a more stable I₂, donating an electron each and they are shared between the two atoms.

Interviewer. So that's a combination of two I minuses is it?

Rose. Yeah.

In a similar way learners seemed to confuse ions with neutral species and nuclei in metallic bonding (AC 10-11, Table 7.3). Two alternative conceptions of this nature were identified, namely, that metallic lattices contain neutral atoms and that the positive ions present are nuclei.

Interviewer. Do you see this here as being lithium plus here?

Steve. No I don't. I just see that as just being a lithium.

Brian. The thing that appeals about B [i.e., choice B in MB01, p. 80] to me is the fact that the electrons aren't tied down to any particular atom.

Mary. I guess that's the nucleus [indicating the + symbols in MB01, p. 79].

Interviewer. So you see the electrons as not being associated with?

Kevin. Not specifically associated with any individual atoms.

Interviewer. OK what's sort holding it together?

Kevin. They share. Well my conception really anyway is the fact that the charges all the nuclei are very positively charged.

Interviewer. Right.

Kevin. The electrons are negatively charged.

Interviewer. OK.

Kevin. That will make the whole thing sort stay together.

Again the interchange of nomenclature seems inappropriate. Kevin, for example, began by describing the species present in the metallic lattice as atoms, although whether he sees atoms as neutral is perhaps questionable. However, upon probing, he stated that they are charged, but went on to identify the charged species as nuclei rather than cations. Another possible origin of this alternative

conception maybe the nature of visual clues used in the diagrams depicting the sea-of-electrons model. Diagrams like IAE focus card MB01 (p. 79) are perhaps ambiguous in that they simply show positive species, which could be interpreted as either nuclei or ions. Presentation of such diagrams is typically accompanied by textual or verbal explanations (see, e.g., Gray, 1973, p. 209). In the context of this inquiry, no such explanation was offered and this may have resulted in this alternative conception.

It is possible that another alternative conception, that electronegativity comprises attraction for a sole electron (AC 12, Table 7.3) is related to this.

Steve. It's the electron attracting ability of a species. So in the case of fluorine for instance being the most electronegative element, because it has only one space left to fill in its $2p$ orbital, then it would very strongly attract an electron to fill that orbital, to attain a stable filled valance orbital.

Frances. The chloride is electronegative which means it can give away an electron.

Claire. It's still ionic because the lithium has a stronger attraction [drawing Li and Cl enclosed by circles, lower part of Figure 6.33, p. 192]

Interviewer. Stronger attraction to what?

Claire. To the lithium. So the one electron they are sharing it will still spend most of the time around the chlorine or chloride.

Although a definition of electronegativity was not explicitly elicited, if a given learner introduced the term, he or she were asked to explain what the term meant to them. Electronegativity is not an aspect of chemical bonding *per se*. However, as seen in the views expressed by Frances and Steve above, learners' understanding of electronegativity impacts upon their understanding of bonding. Most learners produced a definition of electronegativity that was in general agreement with the scientific view. However, Steve seemed to believe that the attraction was for a single electron rather than a greater attraction for the shared pair. His statement that there is "only one space left" resulting in greater attraction suggests that the filled valence shell concept of the octet rule is influential in his view of electronegativity.

An interesting alternative concept is that I_2 is metallic in nature (AC 13, Table 7.3). Christine and Alan stated that they viewed iodine as metallic and Alan related the bonding to that of lithium which he previously encountered in IAE focus card MB01 (p. 79).

Christine. I definitely think of it as a metal.

Alan. Or perhaps even more like the structure of that lithium. I sort of see lithium-lithium bonds. It's the same in the case of the iodine.

It is possible that the implied dimeric nature of the bonding in lithium depicted on MB01 (p. 79) confused Alan and he is simply relating the dimeric I_2 to a diagram he has encountered recently, that is, MB01. However, Jason clearly considered that I_2 contains covalent bonds, and despite relating the purple colouring resulting from sublimation of the sample to the gaseous phase, he persisted with his assertion that molecular iodine is metallic in nature.

Iodine is kind of metallic, so I guess iodine certainly is a gas. Iodine will sublime when you heat it up and you will see the purple colouring in the air and that's iodine gas and iodine is I_2 . So you have one iodine covalently bonded to another iodine [drawing two Is inside circles linked together, Figure 7.6] so you have I—I like that. So my guess it's kind of metallic.

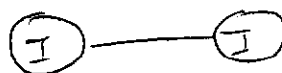


Figure 7.6 Jason's drawing illustrating the bonding in molecular iodine (I_2)

Jason stated that "iodine has some sort of metallic properties"; the origins of this view may lie in the lustrous, rather metallic, appearance of the crystalline appearance of the sample used during the interviews. Upon probing it seemed that Jason did not believe molecular iodine is a metal, yet he persisted with his statement that it will possess metallic properties.

Interviewer. What makes you say it has metallic qualities?

Jason. Just looking at it. It looks metallic it's somewhat shiny.

Interviewer. Right.

Jason. It's even gray in colour and you have sort of discrete little crystals of it. I dunno. I don't, when I say it's sort of looks like a metal, I don't expect it to behave as a metal.

Interviewer. So you are saying it is metallic in appearance?

Jason. Yeah. It obviously has some sort of metallic characteristics to it.

Again such a view may be related to Periodic trends. Although this has not been articulated by Jason, it is common to state that there is an increase in metallic character as one goes down a group in the Periodic Table (see, e.g. Chang 1991, p. 167). This, along with the metallic appearance of I_2 , may be the cause of the alternative conception.

An interesting alternative conception was related to the bonding in ionic compounds like sodium chloride (AC 14, Table 7.3). A number of learners seemed to become confused between ionic bonding and covalent bonding. Two secondary school learners, Anne and Frances, and one undergraduate, Keith, identified the bonding in ionic compounds as covalent, despite describing a process of electron transfer.

Anne. The electrons are sharing between them.

Interviewer. Between them OK. So that's between the...?

Anne. The caesium and the chloride.

Frances. OK [drawing Figure 6.21, p. 169] if there's a dimer.

Interviewer. Yep.

Frances. The chloride is electronegative which means it can give away an electron and Na plus means it can accept the electron.

Interviewer. Right.

Frances. So at one time that electron will be transferred and that makes that dipole positive and that dipole negative.

Interviewer. Right.

Frances. That forms a covalent bond, sort of sharing at any one time.

Keith. Yeah it'd be the same sort of thing.

Interviewer. OK.

Keith. Oh yeah and it's got some more electrons around here and the same sort of covalent bond [draws $Li-Cl$, with small dots around Cl, and one small x near Li, see, Figure 7.4, p. 270].

Interviewer. Between one lithium and the chlorine.

Keith. Yeah so, same thing as sodium.

Interviewer. Same as sodium OK.

Keith. And then bonding between another [draws second similar Li—Cl unit, lower part of Figure 7.4] and another, and another [draws wavy lines between units and off bottom of second unit, writes van der Waals next to wavy line].

The comments made by Frances in particular provide clues to the origins of this alternative conception. Frances mentioned electron transfer, but went on to state that the bonding is covalent in nature. Such a description is very similar to that employed to explain the ionic-covalent continuum (see, Appendix A, pp. 329-330).

In addition to the more prevalent alternative conceptions described above, there were a number of conceptions that were identified for a sole participant. Jason seemed confused about the number of nearest neighbours in copper and stated that the malleability of metallic copper involved changes to the number of nearest neighbours; he saw twelve, then six, followed by four neighbours, instead of the eight that are actually present in copper metal. Steve seemed confused about the nature of bonding in the alloy steel (AC 17, Table 7.3), viewed the bonding between the non-metal carbon and iron as electrostatic in nature rather than covalent.

Steve. Well you have still got the retention of the electrostatic forces between the iron cation and the electrons.

Interviewer. Right.

Steve. But, I am just trying to think back. With the introduction of the carbon, there's actually going to be new centres located inside the metal structure. I presume that they would be held by some sort of electrostatic interaction.

Rose seemed to believe that the shape of ions was influenced by macroscopic factors such as pressure (AC 18, Table 7.3) "like it's maybe the conditions it's under or, or something might make it somehow", such as, "metals and or high pressure things like that". Neil possessed a novel view of intermolecular forces, believing that they were affected by gravity (AC 19, Table 7.3) "it moves a little bit, but it must be that the charges on each side would not be as strong I would imagine. It may be also because it's affected more by gravity than the others". Although these views were only expressed by one individual, as mentioned above,

it is possible that these views are not idiosyncratic and were also held by other learners.

7.3 Summary

Interview data indicated that learners made considerable use of analogy to aid their conceptualisation of certain aspects of their mental models. Most frequent use of analogy was found for secondary school learners and postgraduates. The most frequent type of analogy use was simple analogy with learners drawing a single link between analog and target domains. Postgraduates made greater use of compound analogies than either undergraduates or secondary school learners. The most common target systems for which learners made use of analogy were metallic bonding and ionic bonding principally due to the models identified in the curriculum material and during interviews being analogical in nature. Likewise the data revealed prevalent alternative conceptions for chemical bonding across three levels of learning. In addition to some common alternative conceptions previously reported in the literature such as misunderstandings about intermolecular forces and molecularity of continuous lattices, the inquiry found a surprising number of alternative conceptions about simple ideas like ion size and shape.

Chapter 8 represents the conclusion of the thesis. It begins with a summary of the major findings for the inquiry, followed by a discussion of the implications of the research findings for teaching and learning. The chapter concludes with some suggestions for future research.

CHAPTER EIGHT

CONCLUSION AND IMPLICATIONS FOR TEACHING AND LEARNING

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CHAPTER EIGHT

CONCLUSION AND IMPLICATIONS FOR TEACHING AND LEARNING

Overview of the Chapter

This chapter comprises a summary of the research findings for the inquiry. It begins with a summary of methodology and the principle findings followed by a reflection of the implications of the findings for teaching and learning. The chapter concludes with some suggestions for future research.

8.1 Summary and Conclusions

8.1.1 Summary of Methodology

This inquiry was conducted from within a constructivist paradigm that utilised a research methodology ascribed to a contextual and social constructivist belief system. Development of the conceptual theme for the inquiry was based on Norman's (1983) typology and involved the identification of target systems for chemical bonding from an examination of curriculum material. According to Norman, mental models can be classified into four classes: the target system, a conceptual model, the users' or learners' mental model, and the scientists' conceptualisation. This process resulted in the identification of three target systems, namely metallic, ionic, and covalent bonding; subsequently, target models for each of the three target systems were identified. For metallic bonding the two identified target models were the *sea of electrons model* and *the band theory*. For ionic bonding the identified target models were the *electrostatic model*, and the *theoretical electrostatic model*. For covalent bonding the four identified target models were the *octet rule*, *the valence bond approach*, *the molecular orbital theory*, and the *ligand field theory*. A conceptual model was developed for these target models by the researcher and comprised a summary of the salient points of the models; these data were validated by the instructors whose students were

involved in the inquiry, and thus formed the scientists' conceptualisation for the target models.

Learners' mental models were elicited by the use of a three phase interview protocol for each of the three target systems. The translation interface developed by Johnson and Gott (1996) formed the basis of the semi-structured interviews which were audio-taped and fully transcribed. Transcriptions combined with diagrams produced by the participants formed the data corpus for the inquiry. Learners' mental models were identified by examination of interview transcripts and diagrams, and compiled into inventories for each of the target systems. Examination of inventories enabled identification of commonality of views which were subsequently summarised into a report of the research findings. The researcher's interpretation of these findings were validated by four instructors two whose students were involved in the inquiry and two independent of the inquiry.

8.1.2 Learners' Mental Models for Chemical Bonding

The data regarding learners' mental models for chemical bonding suggest that learners from all three academic levels prefer simple or realist mental models of the target systems for chemical bonding. It was not uncommon for learners to hold a number of mental models and more advanced learners typically provided more detailed explanations for the target models. In addition, more advanced learners were more critical of mental models, particularly the depicted models detailed on focus cards. The extra depth of explanation for the models of bonding by undergraduates and postgraduates compared with secondary school learners is likely a reflection of their learning experiences. Examination of curriculum material revealed that undergraduates and postgraduates have been exposed to a greater range of instruction for the topic than have secondary school learners. Interestingly, for some target systems (e.g., metallic bonding) undergraduates seemed to possess as good an understanding as postgraduates of the mental models, which may simply be due to their more recent instruction about the model(s) in question. The findings of this inquiry are consistent with those of other studies involving abstract chemistry concepts like atomic structure. For example, previous studies found that

learners preferred realist space-filling models of atoms and molecular species (e.g., Harrison & Treagust, 1996; Pereira & Pestana, 1991; Taber, 1998). The extra depth of explanations of mental models provided by more advanced learners in the present work is consistent with the findings of Kleinman et al. (1987) and, not surprisingly, suggests that older learners are capable of an increased level of abstraction and possess a greater number of mental images. Since there is considerable commonality across all three levels of learners, this suggests that learners retain mental models for considerable lengths of time, for example, it is interesting to note that final-year PhD learners retained clear images of the sea of electrons model that they encountered nearly ten years previously. Hence, it appears that the mental models preferred by the learners in this inquiry are highly stable in contrast with the assertion of Johnson-Laird (1983), but consistent with the view of Norman (1983). Nonetheless, the data revealed that learners' mental models are frequently incomplete as asserted by both Norman and Johnson-Laird. Furthermore, there was evidence that learners' ability to operate or use their mental models, for example, to explain events involving model use depicted on IAE focus cards, was limited.

8.1.3 *Learners' use of Analogy*

A number of learners struggled to describe their mental models for chemical bonding, particularly for the target systems of metallic and ionic bonding. The data indicate that when learners struggled to explain or recall aspects of mental models they encountered during previous instruction, they drew on their personal experiences and worldviews to aid their explanations. Typically this involved learners spontaneously generating an analogy to aid their explanations. In this, the findings of the present work are consistent with those reported by Dagher (1995a) and others (e.g., Jarman, 1996; Theile & Treagust, 1994b) involving science teachers' use of analogy in the classroom. Such studies found that teachers' use of analogy was idiosyncratic and that they tended to use simple analogy to aid explanations when they perceived learners were experiencing difficulty in understanding scientific concepts. The present work likewise found that learners'

use of analogy is idiosyncratic, and that their limited use of compound analogy typically consisted of models previously encountered during instruction, for example, the sea of electrons model.

8.1.4 Learners' Alternative Conceptions for Chemical Bonding

This inquiry revealed prevalent and widespread alternative conceptions for chemical bonding across all three academic levels. The most common alternative conceptions were concerned with the belief that chemical bonding is weak for metals and ionic substances and the belief that continuous lattices contained molecular species. This result, along with the related alternative conceptions that continuous lattices contain intermolecular bonds, is consistent with other studies (e.g., Boo, 1998; Peterson & Treagust, 1989; Peterson et al., 1989; Taber, 1994, 1997, 1998) that revealed widespread alternative conceptions about the nature of intermolecular bonding. One of the more surprising results is the widespread alternative conceptions for simple concepts such as the size of ionic species and presence of charged species in homonuclear diatomics.

8.2 Limitations of the Inquiry

Considerable effort has been made to ensure the trustworthiness of this inquiry; the details of which are described in Section 4.7 (pp. 95-102). Nonetheless, as in any inquiry, some limitations are present and these are described here.

The sampling for this inquiry was purposeful and comprised an even gender balance and spread of academic abilities. However, the sample contains little ethnic variety—two female ethnic Chinese undergraduates and one secondary school learner with Pacific Island ancestry being the exceptions. The most obvious omission would appear to be learners who identified themselves as Maori—a number of Maori were approached but declined to be involved in the inquiry. Likewise, the secondary school learners were chosen as a matter of convenience from two local schools both of which were rated as high-decile. Hence the sample is

not necessarily representative of the chemistry student population at the University or in New Zealand secondary schools.

The semi-structured interview protocol described in Chapter 4 (see, p. 77) imposed some restrictions on the scope of the inquiry. This likely resulted in focus on particular aspects of learners' mental models of chemical bonding and did not necessarily afford them the opportunity of expressing their views fully. The choice of some samples, for example I_2 and $CHCl_3$, may have predisposed participants to a particular model such as the Octet Rule. Furthermore, the interviews were comparatively lengthy and this restricted the interviewer's ability to probe understanding (e.g., clarifying use of terminology), particularly late in the interview. Consequently, it is possible that the length of the interviews meant that some learners' later responses were more brief than they otherwise would have been.

The principal research goal concerned learners' preferred mental models for chemical bonding whereas learners' use of analogy and alternative conceptions were subordinate goals. This was reflected in the research methodology and learners' views for analogy and alternative conceptions were not elicited explicitly. Hence, the research findings from this inquiry do not represent a comprehensive inventory of learners' alternative conceptions or use of analogy.

8.3 Implications of the Inquiry for Teaching and Learning

8.3.1 Learners' Mental Models for Chemical Bonding

The research findings from this inquiry have revealed that learners across different academic levels prefer simple or realist mental models for chemical bonding. The contrast between the models produced by learners compared with those to which they were exposed during instruction is dramatic—particularly in the case of postgraduates. For example, the rudimentary nature of the octet rule is evident upon comparison with the molecular orbital theory (cf. Appendix A, Section 1.3, pp. 330-338, and Section 1.5, pp. 343-357). It is important to note that the present work was concerned with learners' *preferred* mental models.

Hence, the finding that even able and senior learners prefer simple models does not necessarily mean that they have limited understanding of more sophisticated models; indeed the high level of their achievement revealed in their academic transcripts indicates otherwise. What the inquiry suggests is that despite competence in the description and use of sophisticated mental models for chemical bonding, learners prefer simple models and relate to more abstract models only in the context of tests or examinations. Smit and Finegold (1995) point out that the prime use of models for scientists is to "supply knowledge of reality, to promote a better understanding of nature" (p. 627), and that the "secondary functions are description, prediction and explanation" (p. 627). The learners in this work have used models for the latter purposes. However, this may simply be a reflection of the interview protocol used to probe learners' preferred mental models.

The research has shown that whilst learners prefer simple realist mental models, learners (particularly senior level learners) utilise concepts from other more sophisticated models when their simple explanations breakdown. M.U. Smith (1992) and others (e.g., Kleinman et al., 1987) maintain that it is a feature of experts that they appreciate the function of models and retain multiple images and mental models in their minds. The results of the present work show that such a situation also holds for the concept of chemical bonding; furthermore, there was evidence that senior learners appreciated the limitations of the simple models they preferred to use. For example, the preference for the cyclohexatriene-based structure for benzene (C_6H_6) is not of concern if, as was revealed, undergraduate and postgraduate learners understood the limitations of the model and choose to use it for reasons of convenience. As such, the actions of the learners in this inquiry mimic those of experts; that is, they use models as a form of verbal or visual shorthand, primarily as a means of efficient communication with other initiates (Walton, 1978; Weller, 1970).

Consequently, the observation that learners *prefer* simple models, whilst likely not the intention of their instructors, and somewhat surprising, is not necessarily cause for concern. However, these findings raise the question as to the

advisability of teaching sophisticated abstract mental models for the concept of chemical bonding. If learners across all levels prefer simple models, appreciate the limitations of these models, and are able to modify or add to these models when necessary, is there any purpose to the teaching of complex abstract models? Indeed, some authors suggest that teaching of highly abstract models at the introductory level is counter-productive. For example, Gillespie and co-workers (Gillespie et al., 1996a, 1996b) suggest that there is little point in teaching molecular orbital theory to undergraduates, and maintain that it is the concept of the orbital that proves most problematic "because the Schrödinger equation and its solution are not presented at the introductory level, the concept of an orbital can have little meaning for the beginning student" (Gillespie et al., 1996b p. 622). Ogilvie (1990) and others (e.g., Bent, 1984a; Tsapralis, 1997) support such a view "the quantitative and mathematical quantum-mechanical theory applied to molecular structure and properties is unnecessary and irrelevant in the general chemistry and undergraduate curriculum" (Ogilvie, 1990, p. 288). Similarly, Shiland (1997) asserts that the teaching of atomic structure based on quantum mechanics occurs because "the presentation of sophisticated atomic theory (quantum mechanics) is not accompanied by sufficient evidence of applications to promote its rational acceptance" (p. 535), and goes on to argue that "complex theories such as molecular orbital theory should be replaced by simpler theories like valence bonding which also explain molecular structure in an effective way" (p. 536). It is Ogilvie's (1990) contention that learners are typically presented with a plethora of theories of chemical bonding, with little attention paid to how they rationalise the use of a given model.

Ogilvie (1990) further asserts "the qualitative (hand waving) explanations of molecular structure and reactions based on orbitals and such ilk are not science (i.e., are nonsense) and should consequently be completely discarded" (p. 288). Ogilvie argues that instructors for general level chemistry should concentrate their efforts on descriptive chemistry and materials chemistry. Such a suggestion may be reasonable for undergraduates who do not intend advancing in chemistry, but

descriptive chemistry is far from cognitively challenging, and hardly seems appropriate for individuals contemplating a career as research chemists (see, e.g., Tsaparlis, 1997). Rather, it serves to place emphasis on rote learning and traditional teaching modes such as the transmissive or conduit approach. The key determinant here perhaps should be the career aims of the individual learners (Fensham, 1980; Kings, 1990; Laws, 1996; Olgilvie, 1990; Tsaparlis, 1997).

The latter part of this century has been characterised by something of a knowledge explosion in the sciences (Harding & Vining, 1997; Laws, 1996), resulting in increased technological complexity of society and increased demand for education in the sciences and related subjects. Tertiary institutions world-wide underwent a rapid expansion in the 1980s and early 1990s experiencing strong roll growth in the physical sciences, although recently there has been a shift towards Computer Sciences, Law and Management Studies. As a consequence, there has been a shift from the traditional education for specialists to education for the masses (Kings, 1990). Examination of the chemistry curricula for the tertiary institution involved in this inquiry suggests that the transition has not been addressed to any great extent. With the exception of a few applied courses the bulk of the offerings by the Chemistry Department are rather traditional in content. Furthermore, instructors use and build upon sophisticated abstract mental models, such as those for chemical bonding described in this inquiry, in order to develop other concepts such as spectroscopy and the development of reaction mechanisms or reaction schemes. Moreover, the high academic achievement of the tertiary level learners involved in this inquiry suggests that they are able to use these models for a variety of purposes. Consequently, it is not feasible to remove them from the curriculum. However, it may be advisable to limit the teaching of such models until the advanced levels of the undergraduate degree since chemistry non-majors will have little need for models in their subsequent studies.

8.3.2 *Learners' Alternative Conceptions for Chemical Bonding*

Laws (1996) points out that the vast bulk of alternative conceptions literature is concerned with secondary school science. The literature for tertiary

science education, such as it is, is mostly confined to studies of newest undergraduates. Laws further argues that university educators do not take alternative conceptions research seriously, instead believing that it is only applicable to "extremely mediocre students" (p. 56); the results of the present work suggest otherwise.

The prevalence of alternative conceptions amongst secondary school learners, whilst not desirable, is not particularly surprising considering the abstract nature of chemical bonding and the large number of other concepts that they are exposed to at this early stage of their learning (Laws, 1996; Nakhleh, 1992). These findings serve to reinforce other research reported in the science education literature, namely, that novices find the understanding of abstract scientific concepts problematic (Pfundt & Duit, 1994, 1997). This is perhaps more likely for concepts like chemical bonding in which the models used are attempting to model other models (Walton, 1978). However, it is of more concern that alternative conceptions were prevalent for undergraduates and postgraduates, particularly for relatively simple concepts. For example, it is surprising that postgraduates and undergraduates were uncertain about relative ionic size and ostensibly believed homonuclear diatomic substances contain ions.

There is a general recognition that alternative conceptions are related to prior learning experiences, although some authors have suggested that it may be more related to the learners' level of cognitive development (Heron, 1975, 1978; Craig, 1972). One factor creating alternative conceptions may be the large amount of factual material that learners are expected to memorise when developing a cognitive structure for a complex body of knowledge like chemistry (Barrow, G.M., 1994; Nakhleh, 1994; Sullivan, 1991). Contributing to this situation is confusion in the use of everyday language and scientific terminology (Garnett, Garnett, & Hackling, 1996; Garnett, Garnett, & Treagust, 1990; Harding & Vining, 1997; Laws, 1996; Nakhleh, 1992). The amount of material that a postgraduate learner has been exposed to by the end of his or her studies is formidable, for example, compare Eames and Abbott (1996, 1998) with Cotton and Wilkinson (1988). The

variety and complexity of models mentioned above, the extensive and subtle differences in nomenclature, and a variety of worldview experiences may each contribute to confusion and the generation of alternative conceptions amongst even highly able postgraduate learners. In this work, there did not appear to be any correlation between academic ability and prevalence of alternative conceptions; neither was there any obvious relationship between experience in undergraduate tutoring and prevalence of alternative conceptions. There are numerous reports in the science education literature revealing alternative conceptions across a broad range of context and academic levels (see, e.g., Carmichael et al., 1990; Novak, 1993; Pfundt & Duit, 1994, 1997). Hence, the research findings reported in the present work seem to suggest that alternative conceptions may be influenced by the complexity of the target models employed and the large amount of material that learners encounter during their studies. This suggests that instructors may need to examine the curriculum carefully and be more critical regarding the value of inclusion of some course content.

Eylon and Linn (1988) suggest that a key finding of science education research is that an in-depth coverage of relatively few topics is more beneficial than a more superficial coverage of many topics. Such a suggestion has been the cornerstone of a constructivist-based view of teaching and learning and it is possible that a constructivist-based teaching approach may prove beneficial; how feasible such a recommendation would be at the university level is debatable. At Waikato, there are two industrial and applied chemistry courses containing modules that are taught from a constructivist view of learning. The introduction of this approach was not without resistance. Indeed, there was a noticeable lack of enthusiasm amongst the learners when their views were solicited, or they were asked to engage in group activity (Coll, 1997a). Perhaps the problem relates to this course being unusual compared with other courses that continue to be taught in a conventional manner. It comes as something of an unwelcome shock for learners to find that they have to become involved and actually participate in their own learning.

The view that teaching institutions should teach less material and instead focus on developing greater learning skills is gaining increasing attention at other tertiary institutions in New Zealand (Kirkwood & Symington, 1996). Increasing ease of access to sources of information such as the internet means that educators need place much less emphasis on the mere provision of factual material and affords the opportunity of greater emphasis on higher-level cognitive skills. However, such a teaching approach may prove problematic for a number of reasons. Sanger and Greenbowe (1996) maintain that many tertiary instructors are objectivist in nature and this is automatically reflected in their teaching.

Here, then, is the crux of the problem. Most college chemistry instructors are not aware of nor do they subscribe to the constructivist philosophy of teaching and learning. Most college chemistry instructors believe that there is an objective reality and that chemists can describe, measure, and work with reality using the tools that chemistry concepts and principles provide. (p. 533)

Consequently, in order to teach from a more constructivist-based viewpoint requires a shift in role for the tertiary educator. As Bodner (1986) pointed out, this requires a major transformation in the role of the tertiary educator from "teaching by imposition to teaching by negotiation" (p. 876). This view also is supported by Herron (1978) who stated:

The major influence that research in psychology and education has had on my teaching is the proportion of time I spend telling students what I think versus the portion I spend asking them what they think. (p. 166)

Davis, McCarty, and Sidam-Tabbaa (1993) believe that such a shift would likely be traumatic for tertiary educators. Indeed, a perception amongst a number of science education researchers is that many tertiary educators are not even aware of the constructivist paradigm (e.g., Barrow, G.M., 1994; Davis et al., 1993) and this was borne out in this inquiry in informal interviews with tertiary educators. Tertiary educators perhaps even more than their secondary school counterparts are perceived to be experts and many teach by a transmissive or conduit approach

(Pope & Gilbert, 1983; Tobin, Briscoe, & Holman, 1990). The findings of this inquiry indicate that for the instructors at this institution at least, such a dramatic change in role may not be easily accomplished, although there are recent examples where constructivist learning at the tertiary level is being progressed (Henderleiter & Pringle, 1999; Kovac, 1999; Shiland, 1999; Spencer, 1999).

8.3.3 *Learners' Use of Analogy*

Learners made extensive use of simple analogy to comprehend the abstract concepts encountered in this inquiry suggesting an awareness that they were performing analogical mapping. Along with the simplicity of the analog models used, this means that it is unlikely that learners confused models with reality—the analogy of spheres with atoms and ions being a notable exception. The fact that learners generated analogies to aid their explanations and conceptual understanding suggests that they also may benefit from greater use of analogy during instruction (see, Clement, 1998; Pittman, 1999). No classroom observation was carried out during the inquiry and so it is difficult to gauge the extent of analogy use in the classroom for the learners involved in this inquiry. The curriculum material for chemical bonding did not contain extensive use of analogy, especially for the more complex models like molecular orbital theory and the valence bond approach. The secondary school teachers indicated that they made some use of analogy as part of classroom practice. In contrast, tertiary educators stated that they made little use of analogy during teaching; one tertiary instructor reported that he used an analogy to describe aspects of the Valence Shell Electron Repulsion Theory (VSEPR) (Gillespie, 1970, 1992). The mathematical complexity of the quantum mechanical-based models mitigate somewhat against this strategy. However, if, as suggested above, less content was presented during instruction, there may be scope for the use of more analogy in the teaching of chemical bonding (Clement, 1998; Glynn, Duit, & Thiele, 1995; Goh, Khoo, & Chia, 1993; Pittman, 1999).

8.4 Suggestions for Future Research

The research findings reported in this report have raised some important issues for chemistry educators, particularly at the tertiary level. Herein are reported three suggestions for future work based on the findings of the inquiry.

First, if it is considered desirable that simple models be replaced by more complex models, or that learners retain and use 'uncontaminated' models, an inquiry investigating the use of such an intervention needs to be carried out. For example, the application of a teaching intervention based on a constructivist view of learning for a complex and sophisticated mental model such as the molecular orbital theory would be of interest. The intervention could consist of more interactive classroom practice and/or the use of an innovation such as a purpose-developed interactive software package. Alternatively instruction could comprise the teaching of a sole mental model such as molecular orbital theory; an inquiry investigating if this resulted in better understanding of the target model would be of interest. Second, this inquiry has revealed that learners make use of analogy to explain their mental models, it would be interesting to investigate the implementation of an intervention in which much greater use was made of analogy during instruction, or in which learners were encouraged to generate their own analogies (Pittman, 1999). Third, the present inquiry has revealed a number of alternative conceptions and it would be interesting to extend this work by conducting a more systematic inquiry into the alternative conceptions held by senior tertiary level learners.

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APPENDIX A

TARGET MODELS OF CHEMICAL BONDING

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APPENDIX A

TARGET MODELS OF CHEMICAL BONDING

1.1 Metallic Bonding

It is common practice to treat metallic bonding as a separate class of bonding during instruction (Allen & Capitani, 1994; Anderson, W.P., Burdett, & Czech, 1994; Pauling, 1960). There has, however, been a shift away from this view in recent years (Burdett; 1997) and "modern chemical theory no longer recognises metallic bonding as a separate class of bonding since metals do not require any special bonding mechanism for their understanding" ("Metallic Bonding," 1994, p. 1965). Nonetheless, it is still common practice to treat metallic bonding separately in most New Zealand secondary schools and undergraduate chemistry courses—including those involved in this inquiry.

The elements that are classed as metals display to a larger or smaller extent certain characteristic properties including high thermal conductivity and electrical conductivity, metallic lustre, ductility and malleability, power to replace hydrogen in acids and so forth. These properties are shown most strikingly by the elements in the lower left region of the Periodic Table. In fact metallic character is closely associated with electropositive character, and in general a small value of the electronegativity of an element corresponds to pronounced metallic properties of the elementary substance (De Posada, 1999).

There are two common models used to describe the bonding in metals; the *sea of electrons* model—sometimes called the electron gas model, and the *band theory*. The sea of electrons model is rudimentary and is normally only used at an introductory level, whereas the band theory is more rigorous and involves a qualitative application of quantum mechanics (Chang, 1991; Duffy, 1974, 1990; Gray, 1973; Lagowski, 1973; Moore, W.J., 1972, 1982).

1.1.1 The Sea of Electrons Model for Metallic Bonding

In the sea of electrons model, the structure of the metal is viewed as being built up by packing like-sized metal atoms to form high symmetry lattices such as simple cubic, body-centred cubic and face-centred cubic (Figure A1)

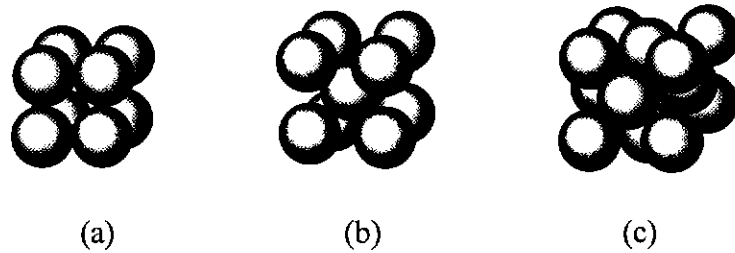


Figure A1 Common lattice structures for metallic crystals: (a) simple cubic, (b) body-centred cubic, (c) face-centred cubic

Ionisation energies for metal valence electrons are low and so they are not strongly associated with individual metal atoms; because the valence electrons are mobile they move freely throughout the metal lattice and as they move away from a metal atom an ion is formed. Hence, in this model of metallic bonding the structure consists of metal ions in an infinite array immersed in a sea of mobile, delocalised electrons (Abbott, Hume, & Cooper, 1998a, 1998b; Eames & Abbott, 1996, 1998) (Figure A2)

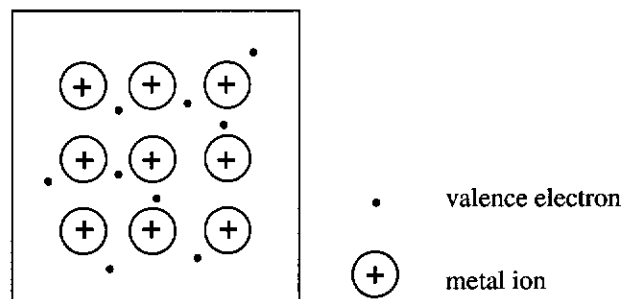


Figure A2 The sea of electrons model for metallic bonding

Powerful cohesive forces between the metal ions and delocalised electrons result in strong bonding, consistent with a metal's high mechanical strength and high melting and boiling points. Because the structure of the metallic lattice is built up by the packing together of like-sized ions, the packing efficiency in metallic lattices is high, consistent with their high densities (Bresica, Arents, Meislich, & Turk, 1988). The delocalised electrons can move freely under the influence upon application of an external electric field, hence metals are good conductors. Similarly, the delocalised electrons are able to transfer thermal energy rapidly along the metal. Because of electron delocalisation, there are few repulsive forces between layers of the metallic lattice and so the lattice layers are able to easily slip past each other when subject to an external force, explaining the high malleability of metals. Metals form two types of alloys, substitutional alloys and interstitial alloys. In substitutional alloys, alloy metal ions of like size can substitute for metal ions within the lattice. In interstitial alloys, small atoms or ions, for example, non-metals like carbon, can fit into the gaps between the metal ions.

There are, however, a number of difficulties with this simple model for metallic bonding. For example, Grigorovich (1989) points out that the model is unable to reliably predict the structure adopted by metals, and furthermore, the formation of bonds by interaction between metal atoms and free electrons seems inconsistent "strictly speaking, free electrons cannot bond atoms, since, in making the strong metallic bond, they would become bonded" (p. 110).

1.1.2 The Band Theory for the Structure of Solids

The band theory for the structure of metals (and other solids) has a number of similarities to the sea of electrons model (Duffy, 1990; Huheey, 1983). In band theory, metals also form arrays of metal ions and the valence electrons are also delocalised. However, the delocalised electrons are located in a series of energy bands formed from the overlap of atomic orbitals. The interaction between two atomic orbitals of a metal atom results in the formation of two molecular orbitals (i.e., orbitals associated with the entire piece of

metal)—one low in energy and a second higher in energy. Because atoms in a metallic lattice are in close proximity, the valence energy levels for a given atom are influenced by its immediate neighbours. This, along with the fact that there is an enormous number of metal atoms in even a very small piece of metal, means that the energy levels are spread across a finite energy interval. This collection of energy levels forms a series of energy bands as illustrated by the band formation for lithium (Figure A3)

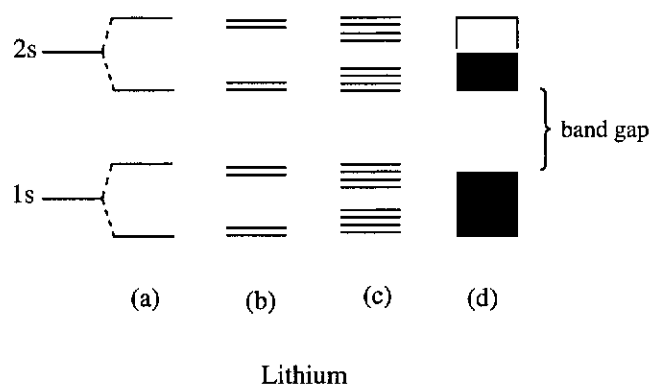


Figure A3 Formation of energy bands for lithium: (a) Li_2 (b) Li_4 (c) Li_8 (d) Li_n

The lower energy levels of the bands are filled with valence electrons and form the valence band—a non-conduction band. The upper energy levels, which in the case of lithium are only half-filled, form the conduction band and the difference between the bands is called the band gap. In order for an electron to move under the influence of an external electric field, it must be in a band that is either empty or only partially filled. In lithium the upper energy level band is only half-filled, so conduction is possible. For group-2 elements such as magnesium, all bands derived from shells are filled, including the band formed from the filled $3s$ valence orbitals. From this information, it might be expected that Mg would be a non-conductor. However, in magnesium and other group-2 elements the molecular orbitals from the $3s$ and empty $3p$ orbitals are very close in energy and blend together to form a single, partially-filled conduction band (Figure A.4)



Figure A4 Formation of energy bands for magnesium

In metals and other conductors the band gap, if it exists at all, it is very small. Hence, electrons can readily move into the conduction band and move freely throughout the lattice. As in the sea of electrons model, bond strength is a result of strong cohesive forces between the metal ions and the delocalised electrons, although there are moderate strength covalent bonds between the metal ions as a result of the presence of some electron density between the metal centres ("Metallic Bonding," 1994).

An appealing aspect of band theory is that, as well as accounting for the properties of metals, it is also able to explain why other solids are insulators or semiconductors. The electrical conductivity of a solid depends on the band gap. Insulators have full valence shells and the band gap between the valence band and conduction band is large, inhibiting electron promotion. The band gap in semiconductors falls in between that of insulators and conductors, hence they have conductivities intermediate between those of conductors and insulators.

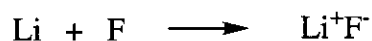
1.2 Ionic Bonding

1.2.1 Ionic Compounds and the Octet Rule: The Electrostatic Model

Ionic compounds are hard brittle solids characterised by high melting and boiling points, good solubility in polar solvents, poor electrical conductivity in the solid state, but good conductivity in solution or the liquid state (Chang, 1991; Cotton & Wilkinson, 1988; Jensen, 1984; Lee, J.D., 1991; Liptrot, 1983; Sharpe, 1981; Shriver, Atkins, & Langford, , 1994; Stranges, 1984). The formation of many simple ionic compounds is based on the *octet rule* (DeKock, 1987;

Stranges, 1984). Strictly speaking, the octet rule is more relevant for covalently bonded compounds and hence it is described in more detail in Appendix A, Section 1.3.1 (p. 331-332) where covalent bonding is discussed. However, a brief introduction is provided here in order to explain some aspects of the models used for ionic bonding.

The octet rule is based on the observation that the noble gases are stable and resistant to chemical reaction. According to the octet rule, the stability of the noble gases is due to the fact that they have filled valence shells and other elements react in such a way as to achieve the stable electron configuration, that is, to obtain an octet of electrons in their valence shells. Electropositive metals have few valence electrons with low ionisation energies; hence they obtain an octet by the loss of an electron or electrons. On the other hand, non-metals can most easily achieve an octet by gaining an electron or electrons. The formation of a simple ionic compound is thus viewed as arising from the transfer of a loosely held metal valence electron to a non-metal atom. For example, the formation of lithium fluoride can be represented as



After electron transfer, an ionic bond arises as a result of the strong electrostatic attraction between the oppositely charged ions. There are, however, many ionic compounds with more complex stoichiometries than simple M^+X^- structures, and a number of compounds do not follow the octet rule; for example, CuI and MnCl_2 . Furthermore, ionic compounds can also be formed from polyatomic ions such as NH_4^+ and CO_3^{2-} .

1.2.2 Lattice Formation

The apparently simple stoichiometry of ionic compounds is somewhat misleading. Ionic compounds do not form discrete molecular species, but large arrays of inter-penetrating close-packed lattices (Chang, 1991; DeKock, 1987;

MacKay, MacKay & Henderson, 1996). Ionic lattices can be viewed as being built up from the packing together of spheres. Anions are usually, although not always, larger than cations and thus an ionic lattice typically consists of close-packed layers of anions with the smaller cations placed in the gaps in the lattice. Because of the large difference in size between ions, the overall structure of an ionic lattice is determined by the packing of the anions in a similar manner to that described for metal ions (see Figure A1, p. 318)

The packing arrangements differ in packing efficiency, that is, the percentage of space occupied by the spheres, from 52% in simple cubic to 68% in body-centred cubic (*bcc*), to 74% in face-centred cubic (*fcc*)—also called cubic close-packing (*ccp*). There is a second close-packing arrangement, hexagonal close-packing (*hcp*). The packing arrangement in *fcc* and *hcp* lattices is illustrated in Figure A5

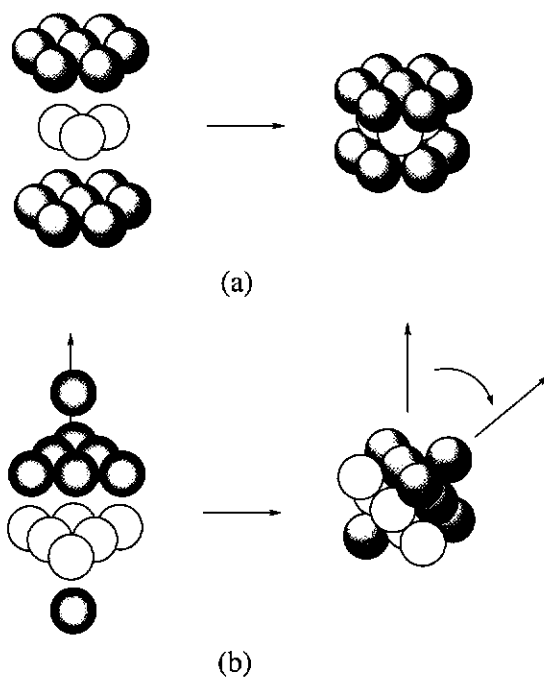


Figure A5 Close-packing arrangements: (a) hexagonal close-packing (b) cubic close-packing

Close-packed arrangements of anions, like metals, contain gaps in their structures, called interstitial holes. The interstitial holes are able to accommodate cations, whether they are metals ions or more complex polyatomic cations like the ammonium ion NH_4^+ . A view of the structure of sodium chloride is shown in Figure A6

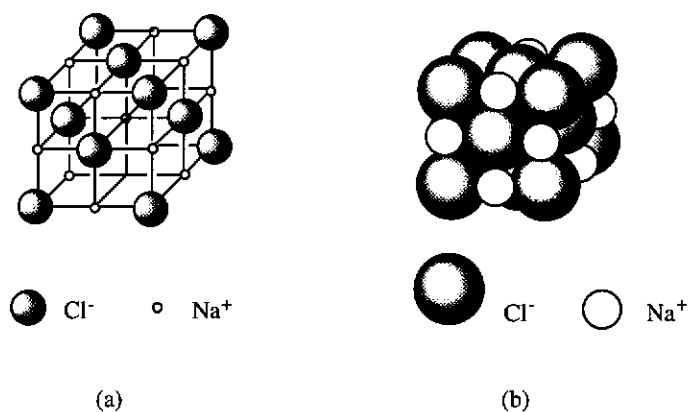


Figure A6 Structure of sodium chloride: (a) ball and stick model (b) space filling model

1.2.3 Radius Ratio & Co-ordination Number

Ionic compounds adopt the structure which maximises attractive forces and minimises repulsive forces—that is, in which the contact between oppositely charged ions is maintained and maximised. One way of viewing this is to require the cation to be sufficiently large to prevent the anions touching, yet small enough to allow efficient packing of the anions. The ability of a given structure to meet these requirements depends on the relative sizes of the ions. Because the size of the interstitial holes is fixed for a given anion and packing arrangement, there is a limit to the size of cation that can fit snugly into the interstices. Calculations of the geometry of ionic lattices suggest that ionic structures can be predicted from the ratio of cation to anion radii, $\frac{r^+}{r^-}$. For example, a face-centred cubic structure as seen in the sodium chloride lattice has a radius ratio in the range $0.4 < \frac{r^+}{r^-} < 0.7$. Application of this simple packing

approximation to other structures suggests that the various structures have the following ranges of stability in terms of the $\frac{r^+}{r^-}$ ratio (Table A1)

Table A1 Radius ratios and structures for some ionic compounds

Structure	Radius Ratio ($\frac{r^+}{r^-}$)	Coordination Number
CsCl and CaF ₂ structures	> 0.7	8
NaCl and rutile structures	0.4-0.7	6
ZnS structures	0.1-0.2	4

The predictive power of these values are more reliable for the lower than the upper limit, and there are many exceptions to these rules. Nonetheless, they provide a rough guide to the likely co-ordination number and structure (Shriver et al., 1994). It is important to note that ionic radii are not easily estimated reliably which complicates the rules (Shriver et al., 1994). In addition, breakdown of this model occurs when there is significant covalency within arising from polarisation of ions, or non-spherical ions (DeKock, 1987), this point is discussed further in Appendix A, Section 1.2.6 (pp. 329-330).

The co-ordination number for a cation depends on the packing arrangements adopted by the anions. By examination of the interstices in the packing arrangements, it is possible to deduce the co-ordination number of the ions. In some packing arrangements there are several interstitial sites with different co-ordination numbers, for example, in *hcp* and *fcc* close-packing arrangement there are both tetrahedral holes (i.e., with four nearest neighbours) and octahedral holes (i.e., with eight nearest neighbours).

1.2.4 Lattice Energy and the Born-Haber Cycle

Since the formation of an ionic lattice involves the formation of ions it might be expected that calculations using ionisation energies (IE) and electron affinities (EA) would provide a guide as to the stability of ionic compounds. Such calculations are, however, somewhat limited since IE and EA values are

based on experiments in the gas phase, and assume little or no interaction between the particles—in marked contrast to the situation in an ionic lattice. For example, caesium has the lowest ionisation energy, but still requires more energy to remove its outer electron than is released by fluorine, the element with the highest electron affinity (Chang, 1991). The stability of an ionic lattice can be estimated by the determination of the lattice energy (U), that is, the energy required to completely separate one mole of a solid ionic compound into gaseous ions



Lattice energy cannot be measured directly but can be determined indirectly in two ways—calculated from the electrostatic interactions in the lattice, and determined from experimental data indirectly via the Born-Haber cycle (Figure A7)

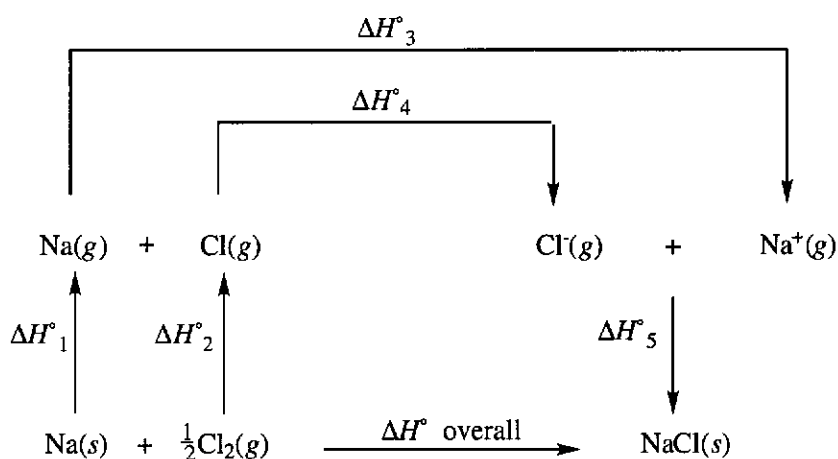


Figure A7 Born-Haber cycle for sodium chloride

In the Born-Haber cycle the lattice energy is deduced by envisaging that the ionic lattice is formed in a series of steps. Because the energy changes associated with each step can be determined, then by using Hess's law the value for the lattice

enthalpy (ΔH_L i.e., $-\Delta H_s^\circ$ in Figure A7) can be determined for any ionic compound. The lattice enthalpy and lattice energy are not exactly the same, but are related by

$$\Delta H_L = U + 2RT$$

Since typically U varies little with temperature, the difference between lattice energy and enthalpy is low, ca. 1-2 kJ mol⁻¹.

1.2.5 *A Theoretical Electrostatic Model for Ionic Bonding: Calculation of Lattice Energies*

The assumption that ionic lattices are made up from arrays of anions and cations in fixed geometrical arrangements means that lattice energy can be calculated from the attractive and repulsive forces present in the lattice, using what in this thesis has been termed the *theoretical electrostatic model* (Huheey, 1983). The total coulombic potential energy for (V_{AB}) for the lattice can be calculated from the sum of the individual coulombic interactions

$$V_{AB} = \frac{z_A z_B e^2}{4\pi\epsilon_0 r_{AB}}$$

where z_A and z_B are the charges on ions separated by distance r_{AB} , and ϵ_0 is the vacuum permittivity. For example, examination of the geometry of the sodium chloride lattice (Figure A6, p. 324), reveals that each cation is surrounded by 6 anions at a distance d , 12 cations at a distance $d\sqrt{2}$, 8 anions at distance $d\sqrt{3}$, six cations at $d\sqrt{4}$, and so forth, that is, each cation experiences alternating attractive and repulsive forces at certain fixed distances which are determined by the geometry of the lattice. Thus, the total energy of interaction between the (univalent) ions in the structure can be calculated from a sum of these alternating attractive and repulsive terms

$$\begin{aligned}
 V &= -\left(6 \frac{z_+ z_- e^2}{4\pi\epsilon_0 d}\right) + \left(\frac{12}{\sqrt{2}} \frac{z_+ z_- e^2}{4\pi\epsilon_0 d}\right) - \left(\frac{8}{\sqrt{3}} \frac{z_+ z_- e^2}{4\pi\epsilon_0 d}\right) + \left(\frac{6}{\sqrt{4}} \frac{z_+ z_- e^2}{4\pi\epsilon_0 d}\right) \dots \\
 &= -\frac{z_+ z_- e^2}{4\pi\epsilon_0 d} \left(6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} \dots\right)
 \end{aligned}$$

The dimensionless quantity in parenthesis is a constant for a given lattice geometry and forms an infinite series. This series converges for a given lattice geometry and is known as the Madelung Constant (A) for the structure. The potential energy of the lattice for one mole (N_A) of sodium chloride is

$$V = -N_A \frac{z_+ z_- e^2}{4\pi\epsilon_0 d} A$$

The calculations of lattice energies described here assume the ions behave as point charges and make no allowance for repulsive forces between the ionic electronic shells. Allowing for repulsive forces necessitates a further term in the calculations

$$V = -N_A \frac{z_+ z_- e^2}{4\pi\epsilon_0 d} A + N_A C e^{-d/d^*}$$

where C is a constant, and d^* is a constant related to the compressibility of the ion. The repulsion terms will be at a minimum at the equilibrium internuclear distance, that is, when V is at a minimum, in which case the lattice energy U becomes

$$U = N_A \frac{z_A z_B e^2}{4\pi\epsilon_0 d} \left(1 - \frac{d^*}{d}\right) A$$

This expression, known as the *Born-Mayer Equation*, is a theoretical model. Kapustinskii devised an empirical model that is independent of structure, by noting that if the Madelung constant for a number of structures was divided by n (the number of ions per formula unit), then approximately the same value was obtained for them all (Moore, W.J., 1972). Kapustinskii proceeded to derive an equation for calculating the lattice enthalpy from the Madelung constant and ionic radii without knowledge of the lattice structure

$$\Delta H_L = -\frac{nz_A z_B}{d} \left(1 - \frac{d^*}{d}\right) K$$

where $d = r_A + r_B$, $K = 1.21 \text{ MJ } \text{\AA} \text{ mol}^{-1}$ and n is the number of ions in each formula unit. Remarkably, for such a simple model, there is reasonable agreement between calculated and experimental values, within 2-3% in ideal cases.

1.2.6 *Limitations of Models for Ionic Bonding: The Ionic character of a Bond*

The octet rule and electrostatic models of ionic bonding presented here assumes that there is complete transfer of an electron or electrons from the metal to the non-metal atom, resulting in the formation of charged species. However, such a view is overly simplistic—even for compounds containing highly electropositive metals and highly electronegative non-metals (DeKock, 1987; Gillespie, 1998; Madden & Wilson, 1996; Sacks, 1986). One way of deciding if a bond formed between two atoms possesses ionic character is by calculating the electronegativity difference. A useful guide is that if the difference in electronegativities on Pauling's scale is greater than 2.0, the compound is ionic in character, if it is lower than 2.0, the compound is described as polar-covalent. The cations in an ionic lattice exert a polarising influence on the neighbouring anions. Small and/or highly charged cations like Li^+ and Al^{3+} polarise the electron cloud of anions, causing a shift of electron density towards the cation, resulting in a build-up of electron density between the ions—thus increasing the covalent character of the bond. Covalent character is favoured by the following factors;

(i) high charge on the cation or anion, for example, Al^{3+} , (ii) small sized cations, for example, Li^+ , and (iii) large sized anions, such as, I^- . These rules, known as Fajan's rules, are a useful guide to the factors that influence the ionic-covalent character of a compound.

1.2.7 *Important Properties of Ionic Compounds*

The models used here to describe the structure of ionic compounds are able to account for their properties quite well. The efficient packing of the ions is consistent with the relatively high densities of many ionic compounds. The values for lattice energies are high (range $800\text{-}3900\text{ kJ mol}^{-1}$), consistent with the high melting points and boiling points of ionic compounds. The strong attractive forces present in the ionic lattice are consistent with their hard, brittle nature. Dislocation of the lattice brings like charges into close proximity resulting in the formation of repulsive forces; thus, explaining the friability of ionic substances. Ionic compounds in the solid phase do not conduct electricity well. This is in agreement with models of their structure since there are no free or delocalised electrons as proposed for metallic bonding. However, when ionic compounds are heated strongly the attractive forces are broken to form a liquid containing mobile ions. Similarly, solutions of ionic compounds contain charged species which can move under the influence of an external electric field.

1.3 **Covalent Bonding**

In this Section, the bonding in molecular covalent compounds, giant covalent networks and transition metal complexes is described. There is an enormous variety of covalently bonded compounds and there are a number of models employed to account for their properties. Because covalently-bonded molecular compounds are so numerous and so varied in structure, their properties vary, but they share some general features. Covalently bonded substances tend to be non-conductors in any phase or in solution, possess low melting and boiling points and are usually gases, liquids, or soft solids at room

temperature—except giant covalent networks. There are a number of models proposed to describe the bonding in covalent compounds: the *octet rule*, the *valence bond approach*, the *molecular orbital theory* and the *ligand field theory*.

1.3.1 Lewis structures and the Octet Rule

Lewis proposed that *s* and *p*-block elements form chemical bonds by sharing a pair of electrons (Jensen, 1984; Pauling, 1984; Stranges, 1984). The driving force for bond formation is, as described previously (see, pp. 321-322), a desire to obtain a octet in order to achieve the noble gas configuration. An complete octet implies full occupancy of the *s* (2e) and *p* (6e) orbitals of the valence shell. Hydrogen, however, requires only two electrons to complete the *1s* valence shell—the so called *duet rule*. Elements of the third and subsequent period can expand their octet by using *d* orbitals and commonly break the octet rule (Gillespie & Robinson, 1995b). It is energetically unfavourable for atoms of main group elements in the middle of the Periodic Table to lose or gain the number of electrons needed to obtain an octet, because the energy cost in terms of IE and EA would be too high. However, these elements can obtain an octet by sharing electrons with another atom so that the total number of electrons in the valence shell is eight (Figure A8)

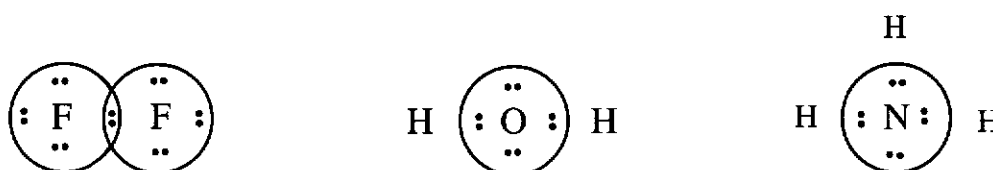


Figure A8 Lewis structures for molecular fluorine (F_2), water (H_2O), and ammonia (NH_3)

Multiple bonds involve sharing several pairs of electrons; two pairs resulting in a double bond, and three pairs in a triple bond (Figure A9)

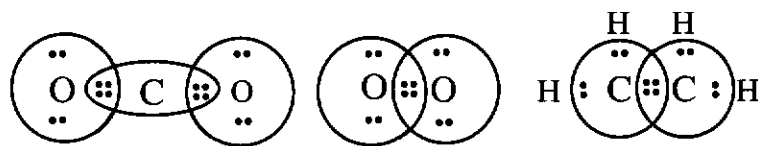


Figure A9 Lewis structures for carbon dioxide (CO₂), molecular oxygen (O₂) and ethene (C₂H₄)

Rather than showing electrons explicitly as in Figures A8 and A9, it is common to draw bonded electron pairs using a single line linking the atoms.

There is a four-step procedure used for constructing Lewis structures (Chang, 1991; Pardo, 1989)

- (i) identification of the molecular skeleton, with the least electronegative atoms the central atom
- (ii) calculation of the total number of valence electrons including allowing for charge on the molecule
- (iii) drawing a single covalent bond between atoms of the molecule, and completing the octets of all atoms
- (iv) if steps (i) to (iii) fail to produce a structure in which the atoms have attained an octet, the use of multiple bonds is invoked

Using this procedure it is possible to devise Lewis structures for many simple compounds of the main-group elements.

1.3.2 Resonance and Formal Charge

The formal charge for a atom is the difference between the number of valence electrons in an isolated atom and in a given Lewis structure. The purpose of formal charge is as an aid in assignment of Lewis structures. The formal charge for a given atom in a Lewis structure is given by

$$\text{formal charge} = \left(\begin{array}{c} \text{valence electrons} \\ \text{in isolated atom} \end{array} \right) - \left(\begin{array}{c} \text{nonbonding} \\ \text{electrons} \end{array} \right) - \frac{1}{2} \left(\begin{array}{c} \text{bonding} \\ \text{electrons} \end{array} \right)$$

The Lewis structure for the ozone molecule indicating the formal charge for the oxygen atoms is shown in Figure A10

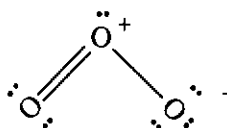


Figure A10 Formal charges for the ozone (O₃) molecule

Lewis structures with no formal charges are likely to be more stable, as are those with low formal charges and structures in which the negative formal charges are on the most electronegative atoms (e.g., oxygen and fluorine) (Laing, 1996). It is important to realise that formal charge is essentially an exercise in electron bookkeeping helpful in satisfying the octet rule, but does not necessarily indicate that there is a charge on an atom in a given Lewis structure. As mentioned previously, there are many compounds for which we are able to write Lewis structures of equal plausibility (Laing, 1996). For example, it is possible to draw two equally plausible Lewis structures for the hydrocarbon benzene (C₆H₆) (Figure A11)

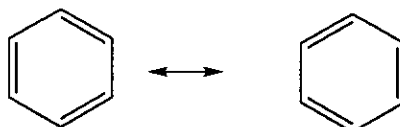


Figure A11 Lewis structures for benzene (C₆H₆)

However, neither of the individual Lewis structures are consistent with known structural data, or the chemical reactivity of benzene. For instance, the Lewis structures in Figure A11 suggests that the carbon-carbon bond lengths are different—that is, alternating single and double bonds. However, structural and

spectroscopic data indicate that the carbon-carbon bond lengths are identical. The presence of multiple bonds in the Lewis structures also suggests that benzene would exhibit chemical reactivity similar to that of alkenes: however, no such reactivity is observed. In cases like benzene for which it is possible to draw a number of plausible structures, the structure is viewed as being a weighted average of the contributing or *resonance* forms—the presence of resonance indicated by the use of double headed arrows (Figure A11) (McMurray, 1996; Purser, 1989; Solomons, 1984). It is important to emphasise that neither resonance structure alone adequately represents the structure for benzene and it is not intended to suggest that there is any type of dynamic equilibrium or switching between the resonance forms. Interestingly, although this latter point is invariably strongly emphasised during instruction, in the interests of simplicity it is normal practice to use only a single resonance structure when representing a molecule in chemical equations. The example of buckminsterfullerene (C_{60}), a recently discovered allotrope of carbon, emphasises the reason for this: for this allotrope of carbon there are a total of 12,500 equivalent resonance forms (Billups & Ciufolini, 1993; Klein, Schmalz, Hite, & Seitz, 1986).

1.3.3 *Expanded Octets, Incomplete Octets, and Co-ordinate Covalent Bonds*

There are a few stable compounds in which the central atom has less than a complete octet, for example, compounds containing beryllium, boron and aluminium (Curnow, 1996, 1998). The usual explanation offered for this observation is that the small size of the co-ordination centre in such compounds precludes higher co-ordination on steric grounds. There also are many *hypervalent* molecules, that is, molecules which have more than eight valence electrons around the central atom—particularly for elements of the third period and beyond (Burdett, 1997; Curnow, 1996; Gillespie & Robinson, 1995b). It is in the expanded octet case that the rule becomes most cumbersome. The case of buckminsterfullerene may be an extreme example, but even relatively simple examples like SO_4^{2-} comprising 11 plausible forms (Straub, 1995) and SO_2 with

nine (Purser, 1989), prove problematic. In such cases it is usually proposed that the *d* orbitals are part of the valence shell allowing for an expanded octet—although this has been disputed (Purser, 1989) and the value of discussing expanded octets at the introductory level has been argued recently (Straub, 1995).

In producing the Lewis structures described here, it has been assumed that each atom contributes one electron to the shared pair. However, in some cases both electrons in the shared pair are contributed from the same atom. In thionyl chloride (SOCl₂), for example, there is already an octet around the sulfur atom before co-ordination of the oxygen atom, hence the oxygen atom is able to complete its octet without contributing an electron to the bond (Figure A12)



Figure A12 Lewis structures for thionyl chloride (SOCl₂)

This structure satisfies the octet rule for all three main group atoms, and the bond between sulfur and oxygen is called a dative, or co-ordinate covalent bond, often indicated by an arrow indicating donation of an electron pair (Figure A12).

1.3.4 Electronegativity and Bond Polarity

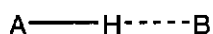
Electronegative elements are elements that have a greater attraction for the shared electron bond pair in a covalent compound (Chang, 1991; Gillespie et al., 1996a). Electronegativity is related to EA and the IE, particularly EA. The EA is defined as the attraction that an isolated atom (e.g., gas phase) has for an electron, whereas the electronegativity refers to the attraction an atom has for the shared electron pair. Electronegativity is not an absolute parameter like IE and EA, but is measured on a relative scale, most commonly the Pauling scale (Gillespie et al., 1996a). As mentioned previously the electronegativity

difference between atoms can be used as a guide to the amount of covalent character of a bond—the greater the difference in electronegativity, the less covalent character and the greater the ionic character of the bond (Appendix A, Section 1.2.6, pp. 329-330).

1.3.5 Intermolecular Bonding

The covalent bonding described here consists of strong bonds within a molecular species. Because many molecular species are polar, there is also the possibility of intermolecular bonding, that is, bonding between molecules. Intermolecular forces, commonly referred to as van der Waals forces, are much weaker than intramolecular forces, with bond strengths ca. 40 kJ mol^{-1} cf. $300\text{--}400 \text{ kJ mol}^{-1}$ for intramolecular covalent bonds (Chang, 1991; Tykodi, 1989). These forces result from interaction between polar species and are due to dipole-dipole, ion-dipole, or induced dipolar interactions (Tykodi, 1989). In dipole-dipole and ion-dipole interactions there is a small electrostatic attraction between the polar species. For non-polar species like hydrocarbons that do not possess a permanent dipole, the proximity of a charged species may induce a temporary dipole as a result of polarisation of the electron cloud. Because this effect depends on the amount of polarisation, induced-dipolar interactions increase with increasing molar mass since larger molecules have more electrons which are usually less strongly bound.

A special case of dipole-dipole interaction of particular importance is the hydrogen bond. Hydrogen bonding occurs when hydrogen is bound to a strongly electronegative atom (A) such as fluorine, oxygen, or nitrogen



where the dashed line represents the hydrogen bond to atom B. Hydrogen bonding is important in water and many biological compounds and can have a marked influence on structure and physical properties (Chang, 1991; Solomons, 1984; Tykodi, 1989). A dramatic example of the effect of hydrogen bonding can

be seen in the comparison of boiling points for a series of related hydrides (Figure A13)

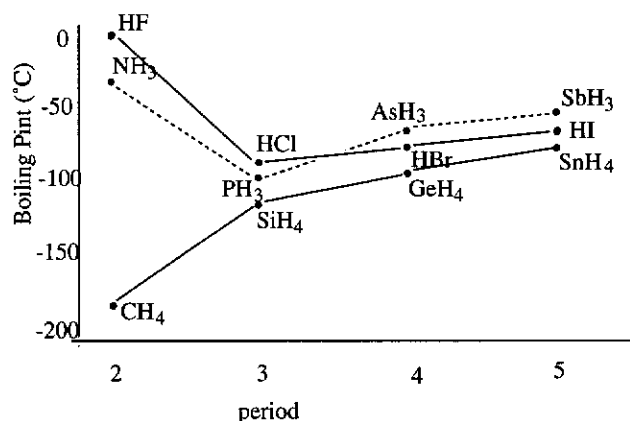


Figure A13 Boiling points for related hydride compounds

The stronger intermolecular attraction as a result of hydrogen bonding in HF and NH₃ results in much higher boiling points than would be expected based on dispersion forces alone.

1.3.6 Giant Covalent Networks

Most covalently bonded compounds exist as discrete molecules. However, there are some compounds (e.g., silica SiO₂) and allotropes of some elements (e.g., diamond) which exist as giant covalent networks (Figure A14)

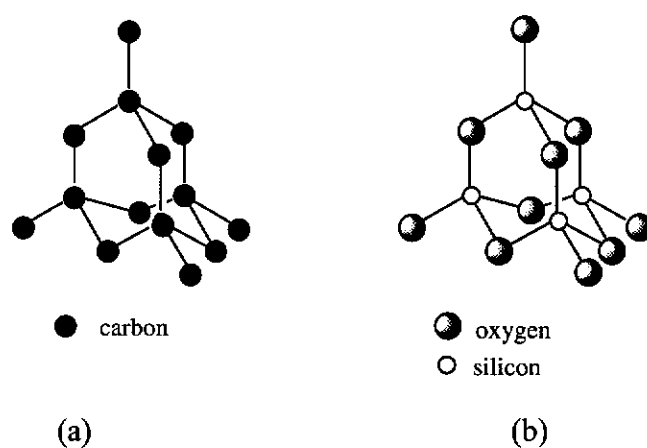


Figure A14 Structure of giant covalent networks: (a) diamond (b) silica (SiO₂)

In these substances because the strong covalent bonds extend in all three dimensions, their properties are very different to those of most molecular covalent compounds—for example, they have very high melting and boiling points and high mechanical strength.

1.4 The Valence Bond Approach

1.4.1 *Valence Bond Approach and Orbital Overlap*

The valence bond (VB) approach is one of two models of chemical bonding which has its origins in quantum mechanics: the other model being the molecular orbital theory (MOT) (Klein & Trinajstić, 1990; Ogilvie, 1990). In the valence bond approach the bonding wavefunction resulting from a combination of atomic orbitals can be viewed as linking the two atoms together in a bond. This approach is in many ways similar to the Lewis model and the electrons are assumed to be localised in atomic orbitals. A calculation of the electron's probability density reveals that there is a build-up of electron density in the internuclear region for the bonding interaction that exceeds the density normally present in the separated atoms. Electrons described by bonding wavefunctions; that is, those that occupy bonding orbitals, are thus more energetically stable than those described by atomic orbitals in the separated atoms. The results of the combination of atomic orbitals can be envisaged using a qualitative model by considering the energy changes associated with the bringing together of two atoms (Figure A15). As the internuclear distance decreases the energy drops markedly since each electron experiences an attraction from the nucleus of the other atom and at the same time the electrons and nuclei repel each other. While the atoms are some distance apart the attractive forces are greater in magnitude than the repulsive forces and the potential energy of the system decreases.

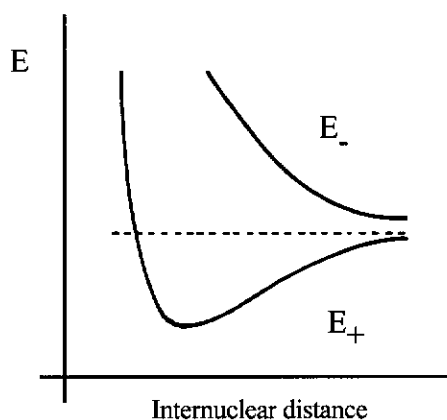


Figure A15 Potential energy (E) for the bonding orbital (E_+) and antibonding orbital (E_-) as a function of internuclear distance for a single-electron homonuclear diatomic

This trend continues until the potential energy reaches a minimum value—representing the most stable situation. If the distance between the nuclei is reduced further, the repulsive forces outweigh the attractive forces resulting in an increase in potential energy.

The electron arrangement is depicted using two types of diagrams; one which shows the electron configuration (Figure A16a), and the other which shows the orbital overlap pictorially (Figure A16b). As a simple visualisation, the bonding between atoms is envisaged as arising from the overlap of two half-filled atomic orbitals (where like colour indicates like phase) and the greater the degree of overlap the stronger the bond (Figure A16b). Orbital overlap is also possible between empty and filled atomic orbitals, and may include overlap of filled π -orbitals with empty atomic orbitals.

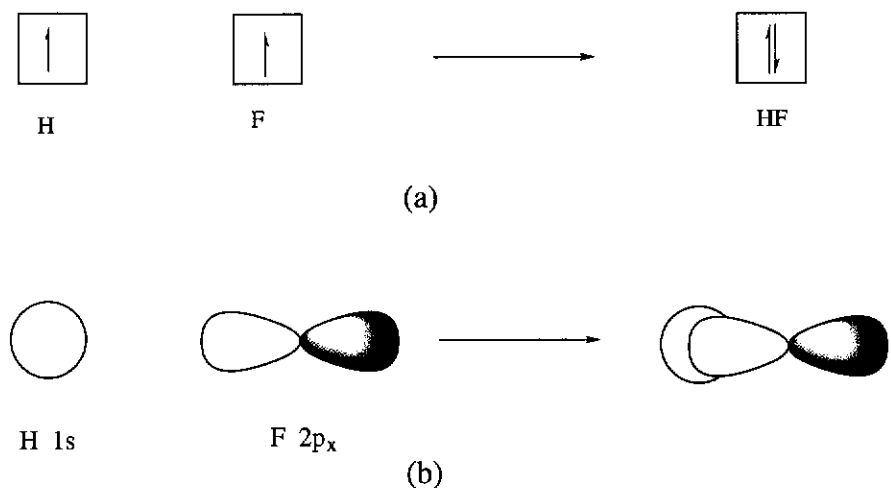


Figure A16 Valence bond approach showing formation of a bond in the hydrogen fluoride molecule: (a) electron configuration (b) orbital overlap

1.4.2 Hybridisation of Atomic Orbitals

The valence bond approach is unable to predict the structure and geometry for even simple molecules without some modification; a classic example being methane (Curnow, 1998; King, 1996). The ground state electron configuration for the carbon atom in methane (Figure A17a) suggests that it would only form two bonds with hydrogen. Promotion of one of the *s* electrons costs some energy, but produces four orbitals that are only partially filled, enabling the formation of bonds to four hydrogen atoms (Figure A17b)

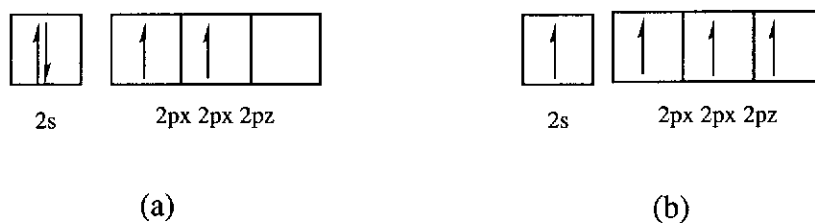


Figure A17 Electron configuration for carbon in the methane molecule: (a) ground state (b) valence state

However, the geometry of the carbon atom p orbitals suggests that the H-C-H bond angles would be 90° , whereas experimental data indicates that the angle is in fact 109.5° , that is, the tetrahedral angle. The geometry in methane and similar molecules can be rationalised by the concept of hybridisation. Hybridisation consists of the mixing together of atomic orbitals to produce new hybridised atomic orbitals. The number and geometry of the hybridised orbitals depends on the specific atomic orbitals combined. For example, two sp hybrid orbitals are formed by the combination of one s orbital and one p orbital, three, sp^2 orbitals are formed by combining one s orbital and two p orbitals and four sp^3 orbitals from combination of one s orbital and three p orbitals. The geometry of the s and p orbitals means that the sp^3 orbitals are tetrahedral, the sp^2 hybrid orbitals are trigonal planar, and sp hybrid orbitals are linear (Figure A18)

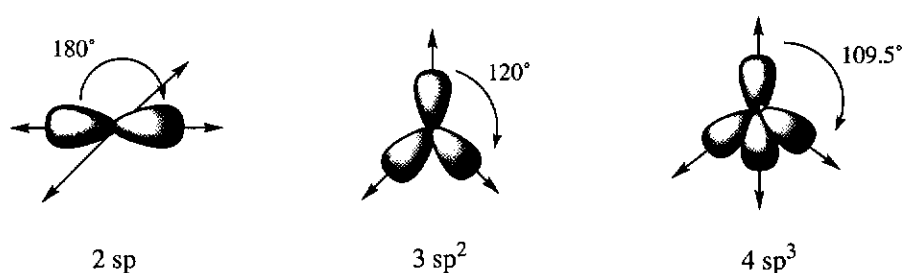


Figure A18 Some hybridised atomic orbitals and their geometrical arrangement

Other hybridised orbitals are also possible, for example, dsp^3 (trigonal bipyramid) and d^2sp^3 (octahedral). In the case of the carbon atom in methane, there are four equivalent sp^3 hybrid orbitals on the carbon atom and four covalent bonds are formed by overlap of sp^3 hybridised orbitals with $1s$ orbitals of the hydrogen atoms (Figure A19)

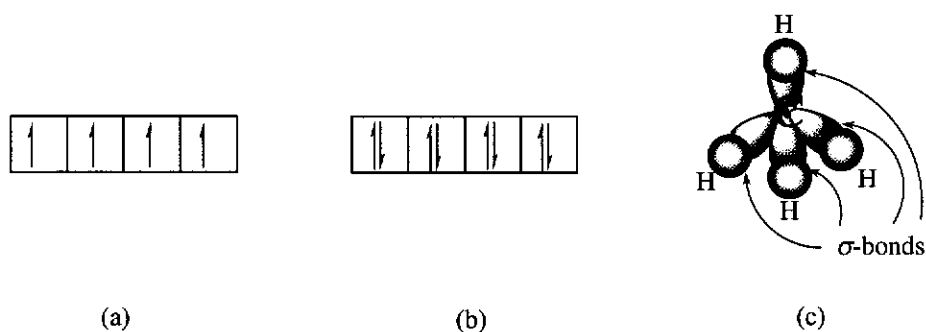


Figure A19 Covalent bond formation in methane: (a) carbon— sp^3 hybridised orbitals, (b) methane— sp^3 hybridised orbitals, (c) orbital overlap between hydrogen $1s$ and carbon sp^3 orbitals

The valence bond approach may also be used to describe multiple bonding, with or without the use of hybridisation. For example, the double bond in alkenes is formed by the overlap of two sets of mutually perpendicular orbitals; $2p_z$ orbitals and sp^2 hybridised orbitals (Figure A20a), and in a similar way the triple bond in alkynes from the overlap of sp hybridised orbitals and two mutually perpendicular $2p$ orbitals, $2p_y$ and $2p_z$ (Figure A20b)

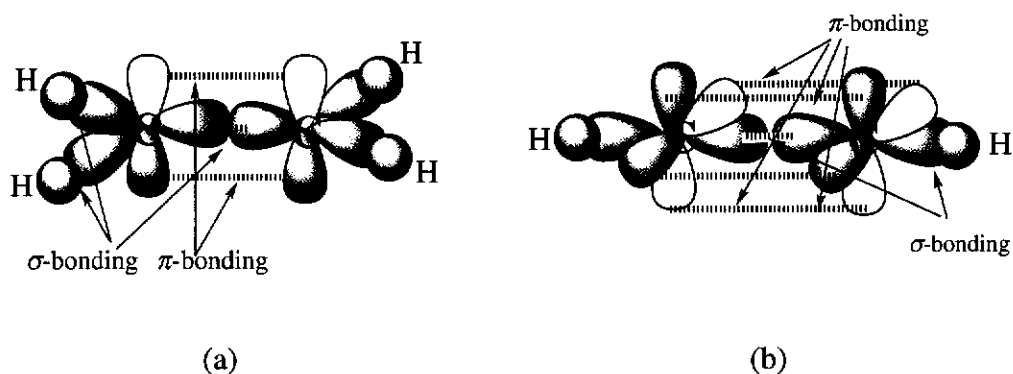


Figure A20 Covalent bond formation in unsaturated hydrocarbons: (a) ethene (b) ethyne

Bonds formed by end-on overlap resulting in the build up of electron density centred on the line between the atoms are called σ -bonds (Figure A19 & 20), whereas bonds formed by side-on overlap resulting in build up of electron

density between the atoms, but above and below the plane of the nuclei, are called π -bonds (Figure A20).

The strength of the bond depends on the degree of overlap of the orbitals. End-on overlap is highly efficient, but sideways overlap is less efficient and is only of significance for $2p$ - $2p$ interaction because the interatomic distances are small. Overlap of $2p$ with $3p$ orbitals does occur, but is rare since the extra node of the $3p$ orbital, along with the internuclear separation mitigate against efficient overlap. Similarly, $3p$ - $3p$ overlap is virtually unknown, but atoms with low-energy d orbitals (group 14-18) can form $d\pi$ - $p\pi$ bonds, since two lobes of the d orbital point directly towards the π orbital, hence overlap can be efficient even at relatively large internuclear distances (Figure A21)

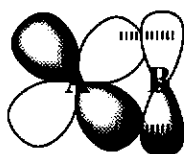


Figure A21 π -bond formation from $d\pi$ - $p\pi$ overlap

Barth (1995) and others (e.g., Martin, 1988) caution that there is a problem with the pictorial representations of orbital overlap in many diagrams of p and d orbitals. Many diagrams are seriously misleading implying that there is substantial electron density in the region of the nucleus. In fact there are nodes as a result of the phase change of the wavefunction at the nucleus, and thus zero electron density. Hence, it is necessary to exercise care when estimating orbital overlap based on pictorial representations of atomic orbitals.

1.5 The Molecular Orbital Theory

The molecular orbital theory (MOT) is a quantum-mechanically based model used to describe the behaviour of electrons in molecules (Curnow, 1998;

Anderson, W.P., et al., 1994; Dunne, Morris, & Orpen, 1991; Dykstra, 1988; Gallup, 1988; Laing, 1996; Olgilvie, 1990). The essence of the approach is that combination of wavefunctions from the familiar *s*, *p*, *d*, and *f* atomic orbitals result in the formation of new orbitals that are associated with the *whole molecule* rather than individual atoms. Whilst exact solutions for the Schrödinger wave equation can only be found for very simple molecular systems, there are a number of approximation models which provide useful picture of the bonding in molecular systems: the most common being the linear combination of atomic orbitals (LCAO) approach (Anderson, W.P., et al., 1994; Comba & Hambley, 1995; Dykstra, 1988; Gallup, 1988; Murrell, Kettle, & Tedder, 1985). Whilst the LCAO approach has as its basis a simplification of the complex mathematics involved in producing approximate solutions to the Schrödinger wave equation, there are sound physical grounds to the approach (Gallup, 1988; Murrell, Kettle, & Tedder, 1985). There are two main physical grounds for the LCAO approach. Firstly, imagine that a molecule is pulled apart into its component atoms—then the molecular orbitals must go smoothly into the set of atomic orbitals of the atom. Secondly, the effective potential for an electron in a molecule when it is close to one nucleus is so dominated by the potential due to that nucleus, that all other potentials are negligible in comparison. Thus, it is evident that the functional form of a molecular orbital near to a nucleus must be similar to the functional form of an atomic orbital of that atom.

1.5.1 *The Linear Combination of Atomic Orbitals (LCAO) Approach*

In the LCAO approach the linear combination is represented as a sum (rather than a product) of normalised atomic wavefunctions (ψ) and the number of molecular orbitals produced is given by the number of atomic orbitals combined. Only two linear combinations are possible; the sum (ψ_+)—viewed as arising from constructive interference of the wavefunctions and the difference (ψ_-)—arising from destructive interference

$$\psi_+ = \psi_1 + \psi_2$$

$$\psi_- = \psi_1 - \psi_2$$

The lower energy molecular orbital (Ψ_+) represents a more stable arrangement, and is called a bonding molecular orbital (σ). The higher energy molecular orbital (Ψ_-) corresponds to a less stable arrangement and is called an antibonding orbital (σ^*) (Figure A22)

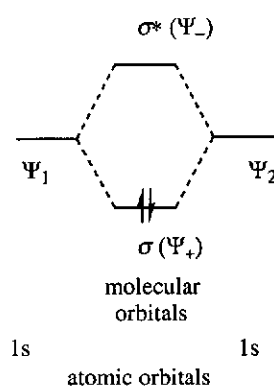


Figure A22 Energy level diagram for the hydrogen molecule

The Aufbau process also applies to molecular orbitals and the electrons fill the molecular orbitals in a similar manner to atomic orbitals, that is, in accord with the Pauli exclusion principle and Hund's rule (Melrose & Scerri, 1996). The diagram shown in Figure A22 is a qualitative energy level diagram for homonuclear diatomics of up to four electrons. Because the σ orbital is the molecular orbital associated with the bonding interaction of the atomic orbitals, the ground state of the H_2 molecule may be described by placing two electrons in the molecular orbital with one spin up and the other down, resulting in a molecular electron configuration $1\sigma^2$. The next two electrons would then be placed in the σ^* antibonding molecular orbital.

The combination of two atomic orbitals produces two molecular orbitals. There are a number of ways that the resultant molecular orbitals can be depicted in a way as to provide a link between their wavefunction and relative energies. It is easy to see why ψ_+ is a bonding function when the value of the function, or more importantly, the value of the function squared (i.e., the probability) is plotted as a function of internuclear distance. In this case, a build-up or decrease of internuclear electron density is immediately apparent (Van Houten, 1988) (Figure A23)

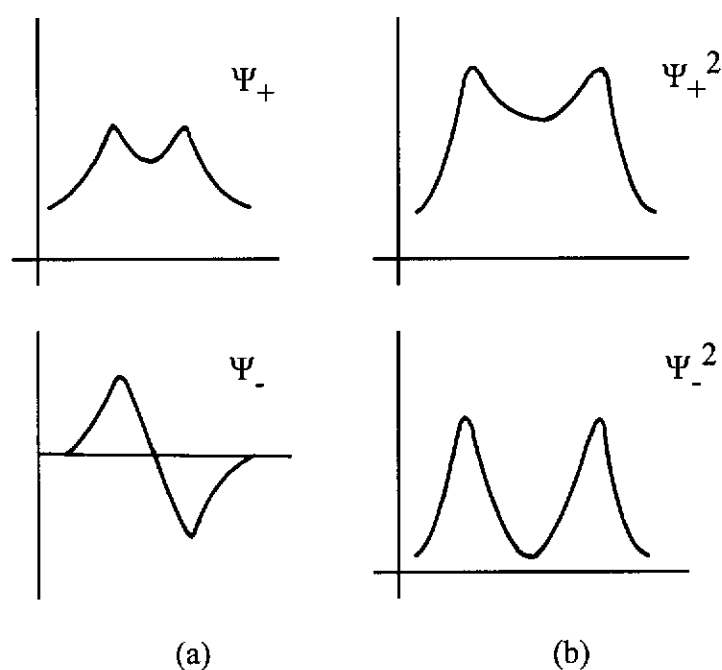


Figure A23 Plot of energy as a function of internuclear distance for a single electron homonuclear diatomic: (a) wavefunction (b) square of the wavefunction

For the bonding molecular orbital (Figure A23a) there is a build-up of electron density between the nuclei drawing them together. In the case of the antibonding molecular orbital there is a node between the nuclei, resulting in internuclear repulsion (Figure A23b).

The most conventional pictorial representation for wavefunctions is the boundary surface and in a similar way to described for the valence bond

approach, it is used to give a three-dimensional representation of the bulk of the electron density in an orbital. The different shading (Figure A24), or in some representations + and - signs, represent different phases of the Schrödinger wavefunctions—in phase combination (+) suggesting constructive interference of classical waves and leading to bonding orbitals and out-of-phase combination (-) indicative of destructive interferences leading to antibonding character. The build up of the electron density in the internuclear region of the ψ_+ orbital shows the connection of the atoms (Figure A24)

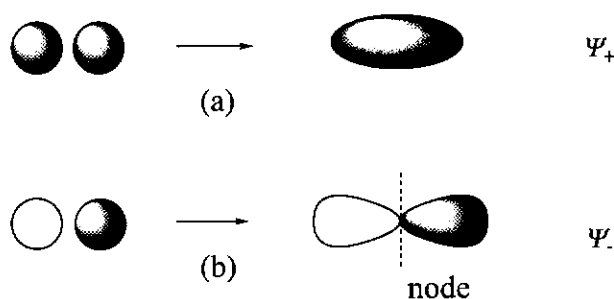


Figure A24 Pictorial representation of formation of molecular orbitals for the hydrogen molecule

It is evident from Figures 23 and 24 that the bonding molecular orbital is more stable than the antibonding orbital since the latter possess a node (i.e., a point of zero electron density). For more complex molecules there may be several nodes. The more nodes a molecular orbital possesses, the higher is its energy. Hence, bonding molecular orbitals are those with few or no nodes, whereas, antibonding molecular orbitals typically have several nodes.

Molecular orbital energy level diagrams like Figure A22 (p. 345) can be used to deduce bond order and thus provide a guide as to the likely stability of molecular species. For example, construction of a similar energy level diagram for helium shows why He_2 does not exist under normal conditions (Figure A25)

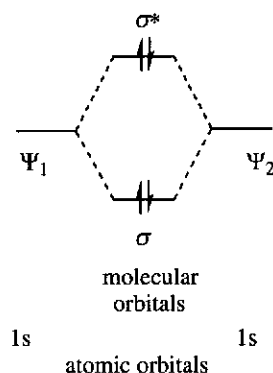


Figure A25 Energy level diagram for helium

Electrons in bonding molecular orbitals hold the atoms together and the molecular orbital theory is able to predict the bond order for a molecule—given by the number of net bonding pairs (Sannigrahi & Kar, 1988)

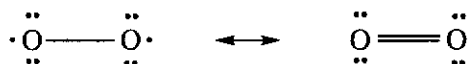
$$\text{bond order} = \frac{\left(\begin{array}{c} \text{number of bonding} \\ \text{electrons} \end{array} \right) - \left(\begin{array}{c} \text{number of antibonding} \\ \text{electrons} \end{array} \right)}{2}$$

Hence, the bond order in H₂ is one (Figure A22), whereas in He₂ it is zero (Figure A25) and so H₂ is predicted to exist as a stable molecular species, whereas He₂ is predicted to be unstable.

1.5.2 Application of Molecular Orbital Theory to Homonuclear and Heteronuclear Diatomics

Molecular orbital theory, like Lewis structures (Gallup, 1988), can be applied to a wide variety of compounds, such as homonuclear diatomic molecules, heteronuclear diatomics, polyatomics, and transition metal complexes (Curnow, 1998; Dias, 1989). Whilst there is less conflict between the Lewis model of bonding and the molecular orbital theory than many chemist realise (Gallup, 1988), the power of molecular orbital theory as a model for chemical bonding is well illustrated by its' application to problematic molecules like molecular oxygen O₂. Experimental evidence indicates that the molecule contains

a double bond and is paramagnetic with two unpaired electrons. It is possible to draw two Lewis structures in an attempt to explain the properties of the molecule



However, neither of these structures is particularly satisfactory: one structure predicts a paramagnetic species with a single O—O bond but does not satisfy the octet rule. The other structure suggests the molecule has a double bond, but suggests that the molecule would be diamagnetic, hence it is necessary to invoke resonance in order to explain the properties of molecular oxygen. Molecular orbital theory provides an elegant explanation for the properties of the oxygen molecule without the need for resonance (Figure A26)

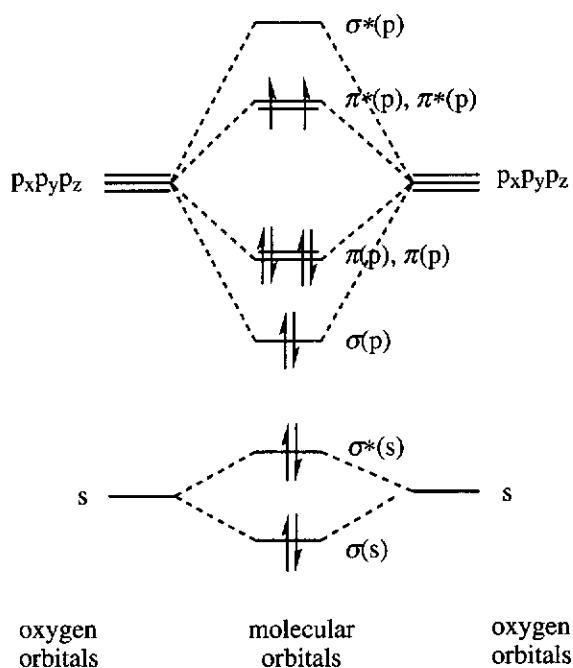


Figure A26 Energy level diagram for the oxygen molecule

The twelve valence electrons fill the molecular orbitals beginning with the lowest energy orbitals and since the two π^* -orbitals are degenerate, the last two electrons go into separate orbitals in accordance with Hund's rule. The result is a bond order of two, with two unpaired electrons—hence the molecule is predicted to have the equivalent of a double bond and to be paramagnetic.

The molecular orbital diagrams for heteronuclear diatomics are similar to homonuclear diatomics and molecular orbital theory is able to explain bond length data and chemical reactivity that is difficult using simpler models. For example, the odd electron species nitrogen(II)oxide (NO) is difficult to represent adequately using Lewis structures or the valence bond approach (Cotton & Wilkinson, 1988; Greenwood & Earnshaw, 1984). However, the bond order of two and a half is easily explained by molecular orbital theory (Figure A27)

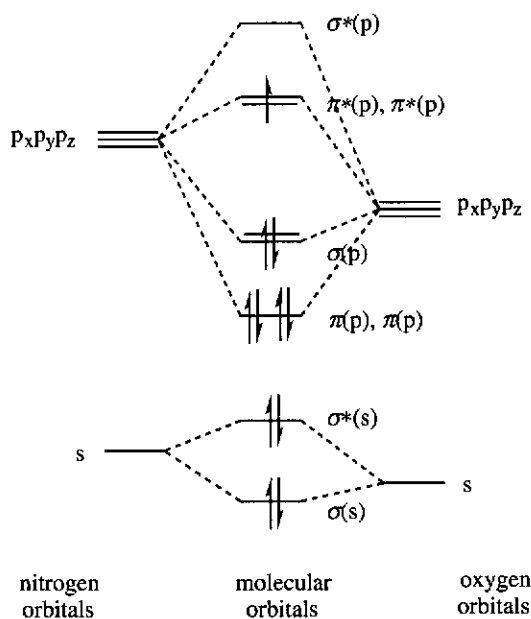


Figure A27 Energy level diagram for nitrogen(II)oxide (NO)

The bond order of two and a half arises from the fact that there are three pairs of electrons in bonding orbitals and a single electron in an antibonding orbital.

The atomic energy levels for electronegative atoms are lower in energy than for less electronegative atoms. The more divergent the energy of the atomic orbitals, the less strong the interaction and the less energy saving accrued. However, this does not necessarily mean that the bond strength for heteronuclear diatomics is always less than that of homonuclear diatomics as there are other factors of influence, for example, orbital size and distance of approach. If the interaction is low, the orbitals may be described as being as belonging substantially to one or other of the atoms (e.g., oxygen or nitrogen in Figure A27).

A comparison of Figure A27 (p. 350) with Figure A26 (p. 349) shows that the order of the $\sigma(p)$ and $\pi(p)$ orbitals is reversed. The $2s$ and $2p_z$ orbitals have similar energies and both have cylindrical symmetry about the z axis. Hence, in some cases the s and p_z orbitals may interact, causing the energy levels to move apart—a process called s - p mixing. The magnitude of interaction is dependent upon the similarity in energies of the s and p orbitals and the net effect is to reverse the order of the energy levels. In molecular oxygen, the $2s$ and $2p$ energy levels are widely different in energy and there is little interaction between the orbitals. This is also the case for other homonuclear diatomics of the second period excepting C_2 and B_2 . For these elements, there is reversal of energy levels and the molecular orbital energy level diagram resembles that of nitrogen(II) oxide.

1.5.3 *Application of the Molecular Orbital Theory to Polyatomic Molecules*

Molecular orbital theory can also be applied to polyatomics, although the energy level diagrams and pictorial representations become increasingly complex (Dias, 1989). The same basic approach used for diatomics is applied to polyatomic molecules, but the molecular orbitals extend over a greater number of atoms. A good example of the application of the model is the benzene molecule (Figure A28)

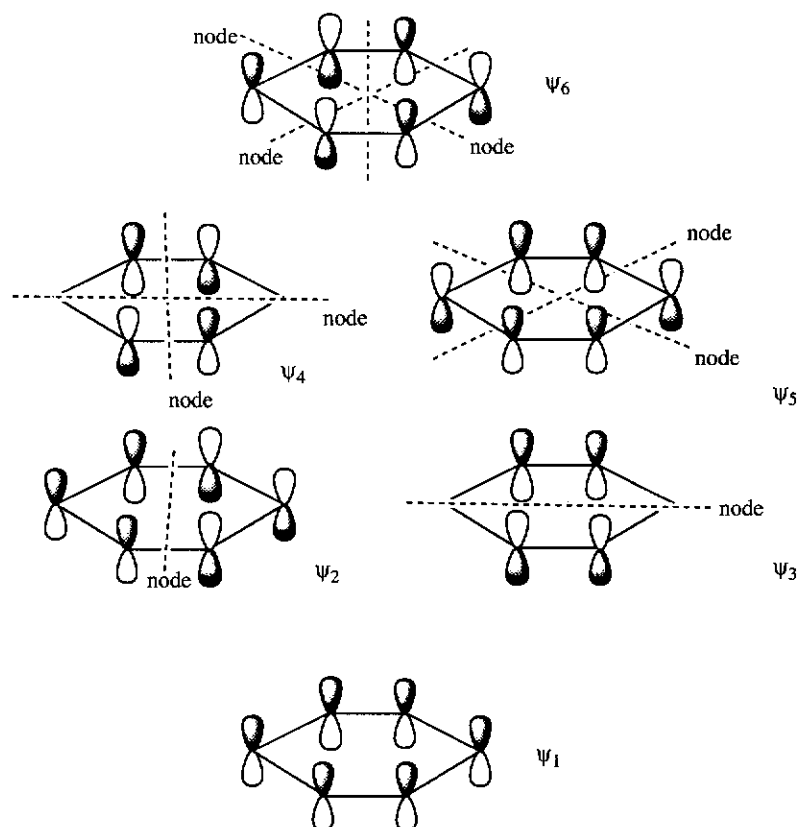


Figure A28 Boundary surface representation of the molecular orbitals for benzene (C_6H_6)

The six-membered ring contains σ -bonds between each carbon arising from the linear combination of sp^2 hybridised orbitals. Further σ -bonds are formed between the carbon atoms and hydrogen atoms from combination of sp^2 hybridised orbitals with hydrogen $1s$ orbitals. This leaves the p_z orbital of each carbon, perpendicular to the plane of the molecule, that is, a total of six atomic orbitals. The combination of the six atomic orbitals produces six molecular orbitals, three of which are bonding in nature (Ψ_1 , Ψ_2 and Ψ_3) and three antibonding (Ψ_4 , Ψ_5 and Ψ_6) (Figure A28). Note that the bonding orbitals are those with zero or one node, whereas the antibonding orbitals are those with two or three nodes.

The sum of six electrons in three bonding molecular orbitals gives rise to a net of three π -bonds, delocalised across the six carbon atoms (Figure A29)

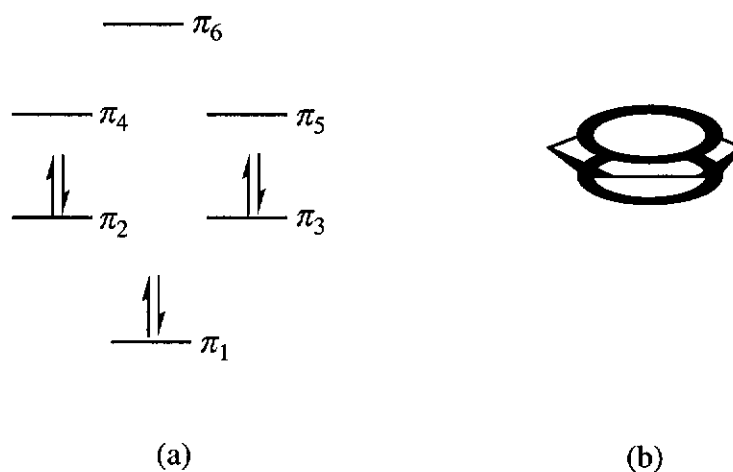


Figure A29 Structure for benzene (C_6H_6) as predicted by molecular orbital theory: (a) partial energy level diagram, (b) orbital diagram showing delocalisation of π -orbitals

Hence, molecular orbital theory is able to offer an explanation for the properties of the benzene molecule without the use of the concept of resonance.

1.5.4 *The Use of Group Theory with Molecular Orbital Theory*

It is sometimes possible to decide which atomic orbitals are able to be combined together to form molecular orbitals by inspection. However, in order to extend the process of drawing qualitative molecular orbital diagrams and energy level diagrams it is necessary to consider the symmetry relationships of atomic orbitals (Cotton & Wilkinson, 1988; Dias, 1989; Murrell et al., 1985). The symbols σ and π have already been used to indicate molecular orbitals that are symmetric and antisymmetric with respect to a C_2 rotation about the internuclear axis—referred to previously as end-on and side-on overlap (Appendix A, Section 1.4.2 pp. 342-343). For other orbitals in more complex molecules, other symmetry relationships are possible, for example, C_n rotations, reflections through planes, inversion centres, or a combination of symmetry elements. All objects (including atomic orbitals) can be categorised by the list of symmetry elements they contain. The complete list of symmetry elements for a molecule identifies its point group classification: the term point group referring to the fact

that all the planes, inversion points, rotational axes, and so forth, pass through a single point. There are nearly 50 point groups ranging from those with little symmetry, for example, C_v which has only the identity element and a vertical mirror plane, to high symmetry groups like the tetrahedral group (T_d) which possesses 24 separate symmetry elements. The entire list of information that details all of the symmetry elements for a given point group is called the reducible representation. These representations may be factored, or reduced, into smaller groups to produce irreducible representations, a detailed representation of which is called a character table (Figure A30)

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma'_v(yz)$	
A_1	1	1	1	1	z
A_2	1	1	-1	-1	
B_1	1	-1	1	1	x
B_2	1	-1	-1	-1	y

Figure A30 Character table for the C_{2v} point group

In the C_{2v} point group, there are four irreducible representations, with the labels or names A_1 , A_2 , B_1 , and B_2 (i.e., the four rows in Figure A30). These representations designate the type of symmetry that an object has. For example, in the case of the C_{2v} point group (Figure A30) an orbital or object labelled A_1 is totally symmetric with respect to the symmetry elements of the group, that is, each of the symmetry elements turns the object into itself. The letters A and B are used to designate singly degenerate representations, while E and T (not used in this character table) are used to designate doubly and triply degenerate representations respectively.

Similar character tables are available for all of the common point groups (see, e.g., Cotton & Wilkinson, 1988), and it can be shown that the total wavefunction for molecule and all the molecular orbitals in a given point group can be expressed by these irreducible representations. The numbers in the table (i.e., the characters) describe the effect of the symmetry operation at the top of the column on each representation at the front of the row; the number 1 indicating that the object is symmetric with respect to that symmetry operation whereas the number -1 indicates antisymmetry. For example, in Figure A30 the mirror plane $\sigma_v(xz)$ leaves an orbital of B_1 symmetry unchanged (symmetric), whereas a C_2 operation on the same orbital changes the sign of the wavefunction (antisymmetric). Once the atomic orbitals have been labelled by their symmetry behaviour, a qualitative molecular orbital energy level diagram can be constructed and orbitals of like symmetry interact to produce molecular orbitals of the same symmetry.

1.5.5 *Application of Molecular Orbital Theory to Transition Metal Complexes*

Molecular orbital theory may also be applied to transition metal complexes. This is illustrated here by its application to an octahedral complex, ML_6 . Consider the case of a first row transition metal, that is, from the $3d$ series. In this case, molecular orbitals are produced by combination of metal valence orbitals ($3d$, $4s$ and $4p$) and ligand atomic orbitals of appropriate energy and geometry. The energy level diagram for a ML_6 complex assuming σ -only bonding is shown in Figure A31

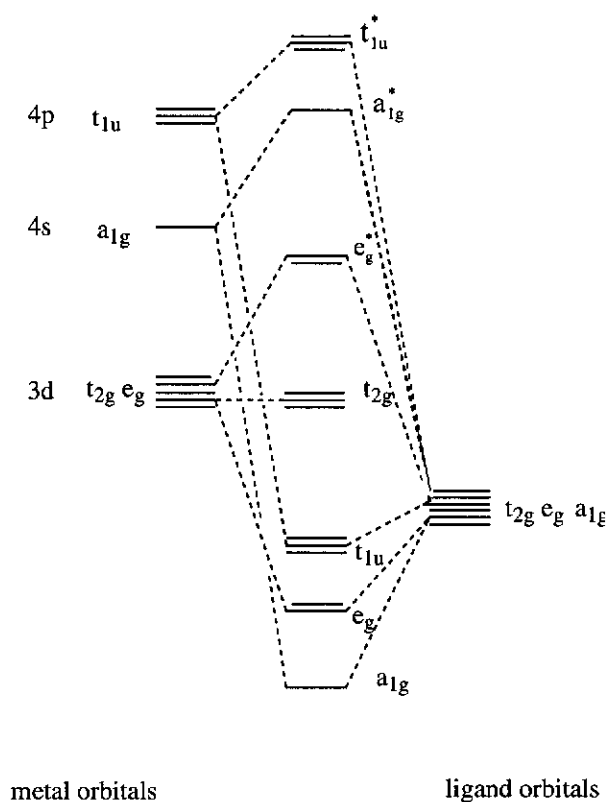


Figure A31 Energy level diagram for an octahedral ML_6 complex assuming σ -only bonding

Of the nine metal valence orbitals, only six possess symmetry suitable for interaction with the ligand orbitals, that is, oriented along the co-ordinate axes; the remaining three orbitals are interaxial and are thus non-bonding. The combination of six metal orbitals with six ligand orbitals produces a total of twelve molecular orbitals, six bonding and six antibonding. The six bonding molecular orbitals are labelled a_{1g} , e_g and t_{1u} using group theoretical symbols used to specify the symmetry properties of the functions. It is conventional to designate orbitals, which are single-electron wavefunctions using lower case symbols, and states, which are many-electron wavefunctions, using upper-case symbols. In either case, they designate irreducible representations of the octahedral (O_h) point group, corresponding to single, doubly and triply degenerate energy states. The subscripts g and u for O_h signify respectively, symmetry or antisymmetry with respect to a centre of symmetry. The

antibonding orbitals are similarly designated a_{1g}^* , e_g^* , and t_{1u}^* . The non-bonding orbitals are designated t_{2g} —indicative of their triply degenerate state. The non-bonding orbitals correspond to the interaxial metal d_{xy} , d_{xz} and d_{yz} interaxial orbitals.

There are many metal complexes for which metal and ligand orbitals are at a suitable orientation for π -interaction to occur (i.e., side-on overlap). When π -interaction occurs this involves the non-bonding t_{2g} molecular orbitals and there are two possible scenarios; the ligand π -orbitals lie lower in energy than the metal t_{2g} orbitals, or they are higher in energy than the metal t_{2g} orbitals. Interaction of the ligand orbitals with the metal t_{2g} orbitals results in the formation of new molecular orbitals. The energy level diagrams for the two possibilities are given in Figure A32

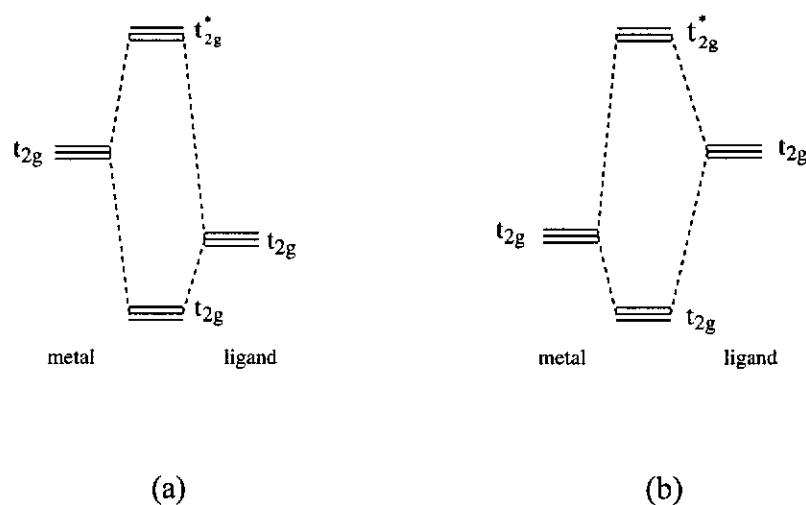


Figure A32 Effect of π -interaction in an octahedral ML_6 complex:
 (a) ligand π -orbitals lower in energy than metal $3d$ orbitals
 (b) ligand π -orbitals higher in energy than $3d$ metal orbitals

1.6 Ligand Field Theory

The term crystal field theory (CFT) is used almost interchangeably with the term ligand field theory (LFT); although strictly speaking crystal field theory

refers to an early version of what inorganic chemists now understand to be ligand field theory (Moore, E.A., 1990; Smith, D.W., 1994). To illustrate the principles of ligand field theory, its application to an octahedral complex ML_6 is described here.

An isolated metal atom contains a set of five degenerate d orbitals; that is, the $d_{x^2-y^2}$, d_{xy} , d_{xz} , d_{yz} , and d_{z^2} (Figure A33). The ligand field theory is based on the fact that these orbitals have different orientations with respect to the co-ordinate system. The orbitals form two sets; those that are oriented along the axes of the co-ordinate system, that is, the d_{z^2} , and $d_{x^2-y^2}$, and those that are interaxial, that is, the d_{xy} , d_{xz} , and d_{yz}

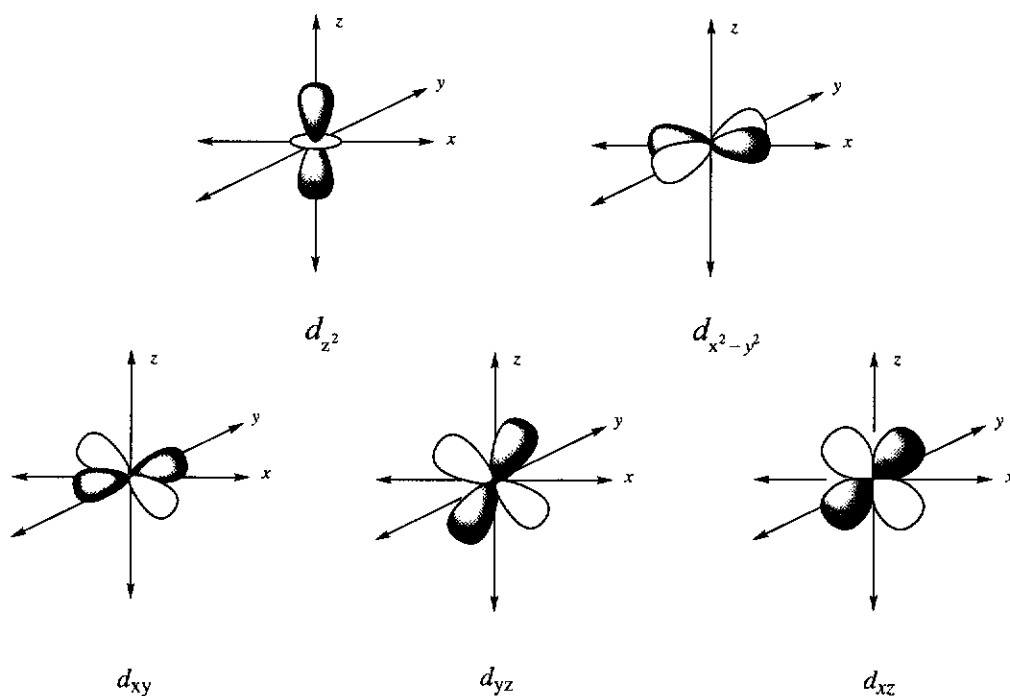


Figure A33 The five d -orbitals for a free metal ion

It is possible to imagine the influence the six ligands exert by considering what would happen when they are placed at infinity and moved towards the metal centre until they reach the normal M—L distances (Figure A34)

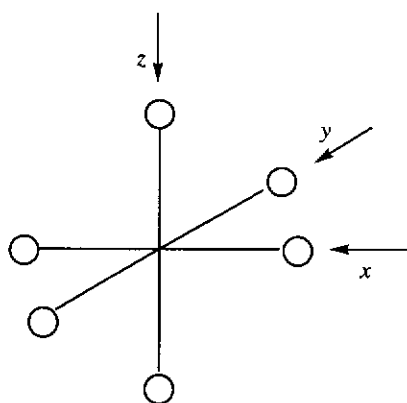


Figure A34 Negative point charges approaching ligand positions for an octahedral complex

In the simplest approach, the ligands are considered to be negative point charges and the interaction between the ligands and the metal centre is purely electrostatic in nature, that is, no covalency is considered. Because the ligands are either negatively charged or electron-rich species, the metal comes under the influence of an external negative electric field as this process occurs. If the electric field arising from the influence of the ligands were perfectly spherical, then each metal d -orbital would experience the same effect and the energy level of all five orbitals would be raised to the same extent. However, the orbitals that lie along the axes (i.e., the d_{z^2} , & $d_{x^2-y^2}$) are perturbed more than those that lie between the axes (i.e., the d_{xy} , d_{xz} , & d_{yz} Figure A33). Thus, in an octahedral field the five degenerate d orbitals are split into two groups (Figure A35)

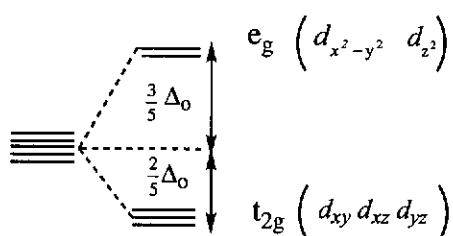


Figure A35 Energy level diagram showing splitting of d orbitals in an octahedral field

This result, achieved in an intuitive manner here, can be more rigorously obtained by the application of group theory to the symmetry of the d orbitals (Smith, D.W., 1994). Using group theory nomenclature, the doubly degenerate higher energy set of orbitals are labelled e_g , and the triply degenerate lower energy levels t_{2g} . The energy difference between the two sets of orbitals (designated, Δ_o or $10Dq$) is termed the splitting energy. Perturbation theory requires that the sum of the energies in the orbitals in a non-spherical external field must be equal to the energy of the spherical field—hence a centre-of-gravity rule applies. Thus under the influence of an electrostatic field the average energy of the perturbed orbitals is zero and so the e_g orbitals must be raised in energy by $\frac{3}{5}\Delta_o$, and the t_{2g} orbitals lowered by $\frac{2}{5}\Delta_o$. The gain in energy when electrons occupy the t_{2g} orbitals, along with allowance for any inter-electron repulsion terms, compared with the energy they would have if they occupied orbitals corresponding to the average energy, is called the crystal field stabilisation energy (CFSE).

The discussion of crystal field effects described here assumes that the ligands are identical and that they are the same distance from the metal centre. However, the relative influence of the ligands varies depending on their charge and distance from the metal centre. Hence, their effect on the energy of the d orbitals varies also. Crystal-field effects on metal d orbitals surrounded by any number of ligands can also be deduced by intuitive or group theoretical considerations in a similar manner to that described for the octahedral case, for example, linear, tetrahedral, and square planar; the most important other coordination geometry being tetrahedral (T_d) (Smith, D.W., 1994) (Figure A36). In contrast with an octahedral field, the interaxial orbitals experience greater repulsion, hence, their energy level is raised compared with the axial orbitals. Furthermore, the splitting energy for the tetrahedral field is smaller than for the octahedral field ($\Delta_t \approx \frac{4}{9}\Delta_o$) since the orbitals point less directly at the ligands. Note also that there are no subscripts g and u as seen for the O_h case, since the T_d has no centre of symmetry.

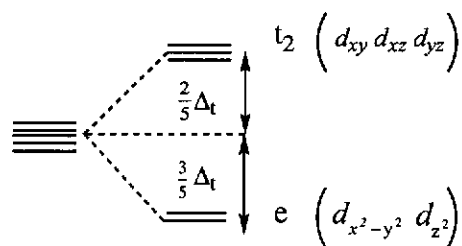
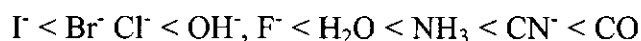


Figure A36 Energy level diagram showing splitting of d orbitals in a tetrahedral field

The value of Δ can be deduced from electronic absorption spectra (EAS) assuming band assignments are made and a major use of LFT is in the interpretation of EAS. The value of Δ depends on the ligand, and a ligand that produces a high value of Δ is termed a high-field ligand. The field strength of ligands is related to their ability to bind strongly to a given metal centre. The list of ligands arranged in order of their ability to split the d orbital energies is called the spectrochemical series, a portion of which is shown below



\longrightarrow
 increasing Δ

The magnitude of Δ also determines the magnetic properties of a complex. So for example, iron(III) (d^5) if co-ordinated to a low field ligand (i.e., small Δ) like fluoride will be high spin, that is, maximum unpaired electrons, but if co-ordinated to a high field ligand like cyanide (large Δ) will be low spin (i.e., with a minimum of unpaired electrons). The actual arrangement of electrons is determined by the amount of stability gained by having maximum parallel spins, taking into account the cost of energy required to promote electrons into the higher energy level (Figure A37).

There is much evidence to suggest that the ligand field theory model of bonding in transition metal complexes is inadequate. The simplest example

relates to the failure of ligand field theory to explain the spectrochemical series. Assuming purely electrostatic interactions, we would expect negatively charged ligands (e.g., halides and OH⁻) to be high field ligands; however, the experimental evidence shows that this is not the case. But perhaps the most serious limitation of ligand field theory is that the purely ionic model assumes localisation of electrons in metal *d* orbitals. However, electron spin resonance (ESR) evidence indicates that electrons in *d* orbitals are in fact delocalised over the molecule and this delocalisation is further supported by nuclear magnetic resonance (NMR) evidence

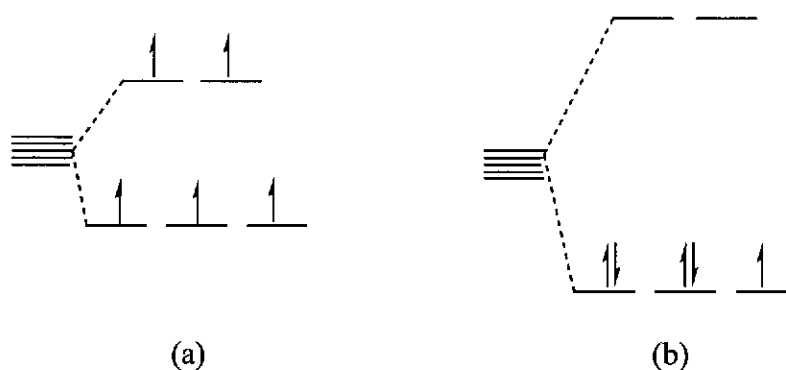


Figure A37 Electron arrangement of iron(III) complexes: (a) in $[\text{FeF}_6]^{3-}$ low field, high spin (b) in $[\text{Fe}(\text{CN})_6]^{3-}$ high field, low spin

Interestingly, despite its obvious limitations, ligand field theory is still widely used, simply because in many instances it is able to correlate experimental data adequately, in other words, the LFT gives the basis for many predictions even if it is not physically realistic.

APPENDIX B
CONCEPT PROFILE INVENTORIES FOR LEARNERS' ALTERNATIVE
CONCEPTIONS

APPENDIX B
CONCEPT PROFILE INVENTORIES FOR LEARNERS' ALTERNATIVE
CONCEPTIONS

Alternative Conception 1

Metallic bond is weak bonding

Keith. I think sort of...as it goes through.

Interviewer. Yep.

Keith. Through the rollers, um...the...the copper like, copper atoms.

Interviewer. Yep.

Keith. Um, just spread out like, the bonding, the bonding between them isn't so strong that it doesn't, doesn't not let them roll on [MB03]

Alternative Conception 2

Intramolecular covalent bonding is weak bonding

David. It must be letting off some hydrogens and stuff, so I don't think it would be that strong [chloroform]

Alternative Conception 3

Ionic bonding is weak bonding

Anne. Um, sodium chloride is weak [sodium chloride]

Neil. In the sodium chloride it can yeah, the force can just break it, the bonds are not very strong [IB03A]

Keith. The bonds in the sodium chloride I don't think are as strong [IB03A]

Richard. I would see them a lot weaker than the diamond [IB03A]

Steve. The ionic bonding that is holding this crystal together here is weaker than is the case of the covalent [IB03B]

Kim. Would it be like the sodium chloride's got weaker bonds than silicon oxide? [IB03B]

*Jane....*Um...'cos...yeah I don't know, I mean it's really that it's stronger [IB03B]

Grace. Not as strong I don't see that attraction as being as strong as the bond in the silica [IB03B]

Brian. It's much harder to break bonds, actual direct covalent bonds like this then it is to break, um, weak ionic bonds [IB03B]

Rose. Like stronger bonds.

Interviewer. Stronger, ok.

Rose. Yeah, um, yeah than the sodium [IB03B]

Alternative Conception 4

Continuous metallic or ionic lattices are molecular in nature

Frances. When you are heating it up it's making the, um, solid molecules move around more giving them more energy from the heat.

Interviewer. yep.

Frances. That, um, allows the electrons to, some of them to be released into the circuit to make the bulb glow where this is a, all the molecules can only move a little bit side to side so it can't move and make the bulb glow [IB02]

Keith. And the copper molecule and, so it's flowing. Like it's going from positive to negative so the electrons can flow along [MB02]

Keith. The sort of bonds are...are rigid and aren't allowing the sodium chloride to sort of ionise and holds, um, the electrons from flowing on through the sodium 'cos the ah the molecules are held like tightly together by the bonds in the sodium chloride so they can't move around [IB02]

Interviewer. Can you just look at what you have drawn there. You have drawn circles for the sodium and then the, ah, chloride, can you just tell me how you would imagine the shape would be of those ions.

Richard. The shape of the whole molecule? [sodium chloride]

Interviewer. Can you tell me what appeals to you most about D?

Bob. The, um, the packing together of the molecules in a regular fashion [MB01]

Alan. All the ions would just be I assume it's a regular lattice, so the ions would be paired so

Interviewer. Oh, yeah.

Alan. So it'd have a neutral charge on it [IB02]

Alan. It shows how the caesium atom and the makes contact with all the, and these the chloride in the middle of the caesium is.

Interviewer. oh yeah ok.

Alan. That sort of interaction between the caesium and chloride, like how you are taught NaCl the NaCl molecule [IB01]

Interviewer. The attraction in this case you are referring to as what?

Grace. As within the actual molecule [sodium chloride]

Brian. Ah well ok each, um, each sodium is effectively surrounded by chlorines

Interviewer. Right.

Brian. The chlorines are very large molecule, and sodium is quite small [sodium chloride]

Alternative Conception 5

The bonding in metals and ionic compounds involves intermolecular bonding

Interviewer. Ok so between that Al and that Al, do you see anything between there at all?

David. Oh, um, I suppose, I suppose there is always the van der Waals things with a, the just the attraction of the electro, electrostatics and stuff, maybe, I am not sure about the actual metal [aluminium foil]

Kim. With van der Waals in between.
Interviewer. Ok that's in between what?
Kim. Between the atoms [aluminium foil]

Alternative Conception 6

The ionic radius of the sodium ion is greater the chloride ion

Anita. The sodium, would be bigger than chlorine [sodium chloride]

Neil. Ok lithium's smaller than sodium and, and chloride is smaller than sodium [sodium chloride]

David. Um...ah I would say the Na would be bigger and the Cl would be smaller [sodium chloride]

Richard. Oh well I say the sodium is the large one.

Interviewer. Ok.

Richard. And then the smaller ones would be the chloride [sodium chloride]

Jenny. Well I know that they are different, but when I visualise them I see the being the same

Interviewer. Being the same?

Jenny. I know that chloride is smaller, or is it large, chloride might be larger yeah I don't really know [respondent laughs] I know they are different but when I visualise them they are the same [sodium chloride]

Rose. Yeah the sodium's larger and the chloride is sort of packed around it [sodium chloride]

Alternative Conception 7

The ionic radius of the lithium ion is greater the sodium ion

Neil. Because lithium would be bigger it'd have more protons and electrons it'd be bigger.

Alan. Oh yeah I basically see the bonding to be the same but I would consider lithium to slightly larger than the sodium [lithium chloride]

Mary. Yeah, um, yeah I just, yeah to me I see it just the same, because it's exactly the same charge.

Interviewer. Right.

Mary. Um, yeah, maybe it could be a little bit bigger maybe.

Interviewer. Sorry what would be bigger?

Mary. Um, the, I am just trying to work it out here, um, maybe a little bit bigger than sodium, the lithium [lithium chloride]

Alternative Conception 8

Polar covalent compounds contain charged species

Frances. Because they, these two have H's in them and H with the Cl, and the highly electronegative like chlorides and things like that that gives the hydrogen bonding whereas they can readily donate a proton away to the hydrogen [**chloroform**]

Anita. Yeah 'cos H is plus and Cl is minus, but I dunno why, I just know it is different but I don't know why [**chloroform**]

Kim. That's ionic bonding isn't it.

Interviewer. That's HF you have written there.

Kim. Yeah and HCl 'cos it's so electronegative that they cause ionic bonding [**CB03B**]

Kim. I was thinking maybe the chloride attached to the hydrogen and share an electron, but now I am thinking maybe not [respondent laughs] [**CB03B**]

Interviewer. That's the HF is it, or is it all of them or what?

Kim. All of them [**CB03B**]

Mary. I kind of think of them, I kind of think them as being ionic [**CB03B**]

Jason. Chloroform is a tetrahedral molecule in which, um, a central carbon atom is covalently bonded to three chlorine atoms and a proton [**chloroform**]

Jenny. I know that to remove an atom from chloroform is quite difficult.

Interviewer. Right.

Jenny. But if you look at other organic molecules will, um....

Interviewer. Yeah, use another organic molecule if you want.

Jenny. I mean if you think, like your carboxylic acid it's...

Interviewer. Yes?

Jenny. Quite easy to remove the proton from.

Interviewer. Right.

Jenny. From sort of thing, and the same for, um...the chloride, like a halide.

Interviewer. Right.

Jenny. It's quite easy to remove the, um, a chlorine from a long sort of carbon chain [**chloroform**]

Alternative Conception 9

Molecular iodine contains I minus ions

Mary. Iodine well I know iodine as being I₂, that's how I remember it.

Interviewer. Ok.

Mary. Iodine is, um, I minus so therefore it's got um, one extra electron I guess sitting there, that's not doing anything [respondent laughs].

Interviewer. ok.

Mary. And it's able to pair up with another iodine which also has, um, spare, and those two electrons come together and form a bond [**iodine**]

Rose. In iodine, um, well it's is like two atoms of iodine, um, just they would be equally contributing from, the like, um, covalent bonds, um, because like each I minus one each iodine would be like lacking one electron.

Interviewer. What did you say? I minus one did you say?

Rose. Yep.

Interviewer. Ok.

Rose. And so they like when they join together to form a more stable I₂ donating an electron each and they are shared between the two atoms.

Interviewer. So that's a combination of two I minuses is it?

Rose. Yeah [iodine]

Alternative Conception 10

The charged species in metallic lattices are nuclei rather than ions

Mary. I guess that's the ah, the nucleus [MB02]

Interviewer. So you see the electrons as not being associated with?

Kevin. Not specifically associated with any individual atoms.

Interviewer. Ok what's sort of holding, holding it together if you like?

Kevin. Ah the share, well my conception really anyway is the fact that the charges all the nuclei are very positively charged, the electrons are negatively charged, that will make the whole thing sort stay together [aluminium foil]

Alternative Conception 11

Metallic lattices contain neutral atoms

Interviewer. Do you see this here as being lithium plus here?

Steve. No, no I don't. So I just see that a, as just being a lithium [MB01]

Brian. that's sort of a, um, shear there the metal atoms have [aluminium foil]

Brian. The thing B that appeals to me is the fact that the electrons aren't tied down to any particular atom [MB01]

Alternative Conception 12

Electronegativity comprises attraction for a single electron

Frances. The chloride is electronegative which means it can give away an electron [sodium chloride]

Claire. It's still ionic because the lithium has a stronger attraction [drawing Li and Cl enclosed by circles].

Interviewer. Stronger attraction to what?

Claire. To the lithium. So the one electron they are sharing it will still spend most of the time around the chlorine or chloride. But it'll spend more time around here as well [draws small circle between Li and Cl and draws lines linking the "e" to Li circle] [lithium chloride]

Steve. Ah it's the electron attracting ability of, of a species.

Interviewer. Right.

Steve. So, um, in the case of fluorine for instance being the most electronegative element

Interviewer. Yep.

Steve. Because it, it has only one space left.

Interviewer. Yep.

Steve. To fill in it's, in it's two p orbital, then it would very strongly, um, attract an electron to fill that orbital, attain a stable filled.

Interviewer. Yep.

Steve. Valance orbital [CB03B]

Alternative Conception 13

Molecular iodine is metallic in nature

Alan. Or perhaps even sort of more like the, um, the structure of that lithium.

Interviewer. Oh yeah, yeah [respondent draws Li—Li] yep, yep.

Alan. I sort of see lithium-lithium bonds. It's the same in the case of the iodine [iodine]

Jason. Um, iodine is kind of metallic, um...so I guess iodine certainly is a gas. Iodine will sublime.

Interviewer. yep

Jason. When you heat it up and you will see the purple colouring in the air and that's iodine gas and iodine is I₂.

Interviewer. Ok.

Jason. So you have one iodine covalently bonded to another iodine [drawing I's inside circles linked together] so you have I, I.

Interviewer. Yep.

Jason. Like that, so my guess is so because it's kind of metallic [iodine]

Jason. I would say but iodine has some sort of metallic properties [iodine]

Christine. I definitely think of it as a metal [iodine]

Alternative Conception 14

Ionic bonding comprises sharing of electrons

Anne. The electrons are sharing between them.

Interviewer. Between them ok. So that's between the?

Anne. The caesium and the chloride [IB01]

Frances. Ok [drawing] if there's a dimer ...

Interviewer. Yep.

Frances. The chloride is electronegative which means it can give away an electron, and Na plus means it can accept the electron.

Interviewer. Right.

Frances. So at one time that electron will be transferred to the, that and that makes that dipole positive and that dipole negative.

Interviewer. Right.

Frances. That's sort forms a covalent bond sort of sharing at any one time [sodium chloride]

Keith. Yeah it'd be the same sort of thing.

Interviewer. Ok.

Keith. [draws Li—Cl, with small dots around Cl, and one small x near Li] oh yeah and it's got some more electrons around here and the same sort of covalent bond.

Interviewer. Between one lithium and the chlorine.

Keith. Yeah so, same thing as sodium.

Interviewer. Same as sodium, ok.

Keith. And then bonding between another [draws second similar Li—Cl unit] and another, and another [draws wavy lines between units and off bottom of second unit, writes van der Waals next to wavy line] [**lithium chloride**]

Alternative Conception 15

Ionic and metallic bonding contains an element of directionality

Interviewer. Do you think it would have any difference or any influence on the bonding at all?

Phill. Not really, it might...um, it might change the angles [**lithium chloride**]

Jason. But again it goes back to like the fact that you see hexagonal and cubic close-packing.

Interviewer. Right.

Jason. Like there must be an element of directionality [**aluminium foil**]

Jason. Because the directionality isn't too strong it can endure going from twelve, ah, six nearest neighbours, to four [**MB03**]

Alternative Conception 16

Ions in close-packed metal lattices possess other than eight nearest neighbours

Jason. Each one has sort of twelve nearest neighbours [**MB03**]

Jason. It can endure going from twelve, ah, six nearest neighbours to four [**MB03**]

Grace. I guess it's yeah if you like obviously, caesium chloride is CsCl_8 but it shows you that the eight chlorine's are each interacting with the caesium [**IB01**]

Alternative Conception 17

Metal to non-metal bonding in alloys is electrostatic in nature

Steve. Um, well you have still got, it's still the retention of the electrostatic forces,

Interviewer. Right.

Steve. Between the iron cation and the electrons.

Interviewer. Bight.

Steve. But, um, I am just trying to think back, with the introduction of the, of the carbon's actually going of new centres located inside the metal structure and um I presume that they would be held in there as well by some sort of electrostatic interaction [**steel wool**]

Alternative Conception 18

Ionic shape and packing is influenced by pressure

Rose. Yeah. Like it's maybe the conditions it's under or, or something might make it somehow.

Interviewer. Do you have any ideas of what sort of things might influence it?

Rose. Um, metals and or high pressure things like that [sodium chloride]

Alternative Conception 19

Intermolecular forces are influenced by gravity

Neil. Yeah it moves a little bit, but it must be, um, the charges on each side would not be as strong I would imagine or also it maybe because it's affected more by gravity than the others [chloroform]

Alternative Conception 20

Glass is an ionically bound crystalline substance

Alan. The glass rod is more like a crystalline structure [MB02]

APPENDIX C
INFORMATION FOR PROSPECTIVE PARTICIPANTS
PARTICIPANT CONSENT FORMS

Learners' Mental Models of Chemical Bonding

*Richard K. Coll
The University of Waikato
Hamilton, new Zealand*

Information for Prospective Participants

Purpose of the Study

One of the most important concepts for the teaching of chemistry is chemical bonding. Chemical bonding is a complex concept and there are many reports in the literature describing difficulties encountered during teaching chemical bonding. Recent research in science education has established that learners create or construct their own mental models of abstract scientific concepts. A key aspect of this research is that learners' mental models are very real to them, and are often highly resistant to change. Because learners' mental models are tenacious, and in some instances used inappropriately, it is of interest to understand the nature of mental models used by learners at various stages of their educational development. The overall purpose of this study is to gain an understanding of mental models learners hold for the concept of chemical bonding. It is intended that the findings from this investigation will provide chemistry educators with an understanding of the preferred mental models for the concept of chemical bonding, and enable them to teach the appropriate use of mental models.

Methodology

Student participants will be interviewed and tape-recordings made of the interviews. These recordings will be transcribed and made available to the participants upon request. Interviews will be conducted at mutually agreed times and at a mutually agreed venue. The results of the findings and interpretation of the data will be made available to the participants. The interviews will be semi-structured and should take about one hour to complete. It is possible that a follow-up interview may be required in some instances. Participation in the study will also involve reading transcripts of interviews to check for accuracy.

Part or all of the dialogue may be modified or deleted at your request at this time. As part of the investigation the investigator will also observe some classroom lessons. This observation will be carried out in an unobtrusive manner and will not involve any significant interaction between the investigator and either teacher or students.

Participant Confidentiality

All efforts will be taken to assure participant confidentiality. Confidentiality of your participation is covered under the provisions of New Zealand Privacy Act (1993). In addition the following measures will be undertaken to ensure confidentiality of the participants involved in this research project. Participants will only be identified by code numbers and the report of the research will employ the use of pseudonyms. The data analysis will be made public only after participants have been given the opportunity to comment. Field notes and data records will be secured and will be destroyed approximately five years after the completion of the project. Participants have the right to withdraw from the project at any stage if they desire, but I shall be grateful if you would give me the opportunity of discussing any concerns that you have prior to your withdrawal.

PARTICIPANT CONSENT FORM

Learners' Mental Models of Chemical Bonding

*Richard K. Coll
The University of Waikato
Hamilton, new Zealand*

Informed Consent - Student Participants

This form should be read in conjunction with the attached "Information for Prospective Participants".

I understand that participation in this research project involves the following:

- I will be involved in a study into the Learners' Mental Models of Chemical Bonding
- I will be interviewed at a place of mutual agreement
- Interviews will be audio-taped and transcribed. Transcripts will be made available to me prior to analysis to check their accuracy. I have the right to decline or approve part or all of this data
- Field notes may be taken during interviews. I have the right to decline or approve part or all of this data
- Data gathered in this project will not be made available to any third party and will be subject to the provisions of the New Zealand Privacy Act (1993)
- I will not be identified in any way other than a code number in the records of the analysis
- My participation in this project will not in any way effect my academic progress
- I may withdraw from parts of this study at any stage, and if I wish I may withdraw from the project completely.

Signed

Learners' Mental Models of Chemical Bonding

Richard K. Coll
The University of Waikato
Hamilton, new Zealand

Information for Participants

Validation of Interview Transcripts

Please find enclosed a transcript of your interview held recently. I shall be grateful if you would examine this transcript to validate it for the purpose of the study.

The purpose of this validation is so that I can be sure that I represent your views correctly and fairly. What I mean by validating the transcript is that it should be an accurate representation of how you felt about various aspects of chemical bonding that we discussed during your interview. Because this is a verbatim transcript, it will contain many apparent 'errors: e.g., in terms of correctness of grammar etc. This is not something you need to worry about, and the purpose of reviewing the transcript is not to ensure that English is correct. Rather, the transcript is an *accurate* record of the interview. But if you feel there is something reported here that is perhaps misleading, or that you upon reflection feel is not accurate please make a comment or note in the margin and initial it clearly. If there is something contained in the transcript that you wish to discuss in more depth I will be happy to do that also. To help in the interpretation of your transcript I have included a copy of the diagrams we discussed along with any drawings you made during the interview.

Please feel free to contact me if you are at all unclear about what is required. Thanks again for participating in the study.