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RESEARCH REPORT

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MENTAL MODELS IN CHEMISTRY: SENIOR CHEMISTRY STUDENTS' MENTAL MODELS OF CHEMICAL BONDING

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ABSTRACT: In this paper we describe research into learners' mental models for chemical bonding. New Zealand senior secondary students, undergraduates and postgraduates' mental models for chemical bonding were probed using an interview protocol that included the use of a variety of common substances and focus cards that depicted model use in some way. The study found that the learners' mental models were simple and realist in nature, in contrast with the sophisticated and mathematically complex models they were exposed to during instruction. The learners drew upon some concepts from other models when their models proved inadequate to explain macroscopic events. [*Chem. Educ. Res. Pract. Eur.*: 2002, *3*, 175-184]

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INTRODUCTION

Chemistry as a discipline is dominated by the use of models and modelling. Chemists like other scientists use models to explain data, to predict events and to help understand chemical reactivity (Gilbert & Rutherford, 1998a,b). These models, often highly abstract in nature, are referred to as mental models. An understanding of students' mental models is important because teachers employ increasingly complex models throughout the degree program (Johnson-Laird, 1983; Vosniadou, 1994). However, there are many reports in the literature indicating that students' understanding and use of mental models is limited in comparison with experts and desired teaching outcomes (see, e.g., Fensham & Kass, 1988; Harrison & Treagust 1996; Raghavan & Glaser, 1995; Stephens, McRobbie, & Lucas, 1999).

Chemical bonding is one of the most important topics in undergraduate chemistry and the topic involves the use of a variety of models (Fensham, 1975). Students are expected to develop an understanding of these models and to interpret a variety of representations for chemical bonds (e.g., chemical formulae, ball-and-stick models, etc.). Chemical bonding is also a topic that students' commonly find problematic and for which they develop a wide range of alternative conceptions. As such, it is notable that there have been few studies of students' mental models for chemical bonding. The few studies that have been reported are mostly confined to the secondary school level (see, however, Nicoll, 2001). What research that does exist, suggests that students hold consistent alternative conceptions (i.e., conceptions that are in disagreement with the taught models or currently accepted scientific view) across a range of ages and cultural contexts. Intermolecular bonding in particular is often problematic for students (De Posada, 1997; Peterson & Treagust, 1989) and, for example, research reveals that students' often think intermolecular bonding is stronger than intramolecular bonding (Goh, Khoo, & Chia, 1993; Peterson, Treagust, & Garnett, 1989), and invoke intramolecular bonding in inappropriate circumstances (e.g., in ionic compounds) (Butts & Smith, 1987; Taber, 1995, 1998). Other students believe that intermolecular bonding is absent in polar molecular substances such as water (Birk & Kurtz, 1999). Another highly prevalent alternative conception reported is that students think continuous covalent or ionic lattices contain molecular species (Birk & Kurtz, 1999; De Posada, 1997; Taber, 1997) and many students appear to have little appreciation of the underlying electrostatic nature of chemical bonding (Boo 1998; Peterson et al., 1989; Schmidt, 1997; Taber, 1995). Many students, likewise have a poor understanding of the bonding in metals, seeing it as weak or in some measure inferior to other forms of bonding (De Posada, 1997; Taber, 1998). Similarly, alternative conceptions have been reported for covalently bonded substances with, for example, some students believing that the number of valence electrons and number of covalent bonds are one and the same and others confusing resonance forms with molecular structures, or believing that covalent bond formation involves the transfer of electrons (Coll & Taylor, 2001a,b; Nicoll, 2001; Taber, 1997).

THEORETICAL FRAMEWORK AND METHOLOGY

The theoretical framework for this inquiry is based on Norman's (1983) typology of mental models and is that used in a prior exploratory study reported elsewhere (Coll & Treagust 2001a,b). Chemical bonding has been classified into a series of three *target systems*, namely, *metallic*, *ionic* and *covalent* bonding and as series of mental models associated with each target. The sea-of-electrons and octet rule are introduced into the New Zealand curriculum at high school Year-11 and Year-12, the band theory, valence bond approach and an introduction to molecular orbital theory in the first two years of university, and the ligand field theory and advanced molecular orbital theory in the final year of the undergraduate degree. Advanced molecular orbital theory and ligand field theory is also treated in fourth-year honours and masters level papers. Examination of curriculum material (i.e., text books, lecture notes, etc., e.g., Chang, 1998; Cotton, Wilkinson, Murillo, & Bochmann, 1999; Zumdahl & Zumdahl, 2000) shows that whilst some of these models are highly abstract (e.g., the molecular orbital theory) they are presented in a highly consistent manner, that is, there is considerable consensual agreement about how scientists view and use these models and the manner in which they are presented in the form of teaching models to students.

Data collection comprised two distinct stages as reported in the earlier study (Coll & Treagust 2001a,b). First a description of the above teaching models was produced from an examination of curriculum material; lesson plans, lecture notes, textbooks, and workbooks used by students, combined with informal interviews with the instructors involved in the inquiry. From these descriptions, criterial attributes were developed for each target model. Criterial attributes represent the essential qualities, all of which must be recognized if the model is used in a way that is acceptable to scientists. For instance, for ionic bonding, this included concepts such as ion size and shape, the formation of an ionic lattice, lattice structure, and so forth. The criterial attributes for a given target model vary depending on the level of the learner. So, for example, an undergraduate is expected to be familiar with the concept of the ionic-covalent continuum (i.e., the notion that no bond is purely ionic or purely covalent), and the polarization of covalent bonds, whereas secondary students were not expected to be familiar with these concepts.

The teaching models and criterial attributes were negotiated with six independent experts (two secondary school teachers and four tertiary level instructors). Negotiation consisted of the researchers producing a detailed description for each of the models, along with a list of the essential concepts required (e.g., ion shape, ion size, polarization, etc.). The experts then responded to the descriptions and lists, indicating, for example, concepts they thought were missing, or concepts on the original list that they thought should be omitted. Second, the students' mental models were investigated using semi-structured interviews, including the use of an *Interviews About Events* (IAE) approach. The data from this latter part of the study helped develop an understanding of students' use of their mental models and the alternative conceptions students held about their models: the results of these latter data are reported elsewhere (see, Coll, 1999, Coll & Taylor, 2001a,b). The items utilized in the interviews represented focus *activities*. Each activity (e.g., showing a participant a physical artefact like sodium chloride, or a focus card depicting model use) was accompanied by extensive probing and questioning. The interviews were of around 60 minutes duration for the younger participants and between 90 minutes and two hours for the graduates. All of the participants were provided with transcriptions of their interviews and a number of participants were re-interviewed to clarify ambiguity in descriptions and explanations.

There were a total of 30 student participants involved in two studies, one based in Australia and one in New Zealand, with 10 students from each of senior secondary school, undergraduate (second and third year of a three-year degree program) and postgraduate levels (even numbers of masters and doctoral level candidates). The secondary students were self-selected and ranged in ability (as adjudged by their teachers) and the undergraduates likewise varied in academic ability (as evidence by their academic transcripts). As might be expected the postgraduates students were high academic achievers (again based on examination of their academic transcripts) and the participants were chosen to provide a reasonably even gender balance. All of the participants described themselves as being of European ethnicity.

RESEARCH FINDINGS

The detailed description of the data presented here is a modest sampling and represents the researchers' attempt to interpret the mental models possessed by these participants. We have summarised our findings by first detailing the concepts held by most participants and then illustrating the variety of views and richness of data by providing snippets of other concepts (including alternative conceptions) held by some participants. The views were similar across all educational levels, the predominant difference being the greater detail provided by more senior students. In spite of this latter observation, the interview protocol was probing enough to uncover a large variety of conceptions across all levels (see, Coll & Taylor, 2001a,b for a detailed description of learners' alternative conceptions for chemical bonding). The richness of the data presented here, and the sheer variety of views about aspects of the bonding in a variety of substances, along with a variety of model-based explanations provided for the macroscopic events depicted on the focus cards (reported elsewhere), suggests that we have achieved a reasonably comprehensive understanding of the participants' views of the concepts under investigation.

It is worthwhile to comment on one model, the octet rule, at this point. This model is presented as a model for chemical bonding in textbooks and in the institutions involved in this study (see Chang, 1998; Zumdahl & Zumdahl, 2000). As a model for *bonding* it is very limited in explanatory power. It is useful to decide stoichiometry, to deduce molecule formation, to rationalise formation of ionic substances, and so forth. It does not, however, offer anything in the way of explanation for strength of bonds or other important aspects of bonding. Nonetheless, because it is presented as a model for bonding (we might say it is a teaching model for bonding – see, Gilbert, Boulter & Rutherford, 2000) we have chosen to treat it as model for bonding in this inquiry.

The research findings from this inquiry are summarized under three headings, learners' preferred mental models for each case of chemical bonding; metallic, ionic and covalent. The most common held view is presented and summarized first in each case. This is then followed by a description of other alternative views held by a lesser number of participants in order to give a full picture of the views held by the participants.

Students' mental models for metallic bonding

The data for secondary school students showed that most preferred the sea of electrons model (a model in which bond formation is based on the notion of an array of metal ions in a mobile or delocalised 'sea' of electrons, see, Coll & Treagust, 2001a,b), with a few students possessing no clear mental model or being highly confused. For example, June described electrons as "moving around" and "attracted by the positive centres," Nigel talked about "electrons flowing around," and Frances said, "you cannot actually see where the electrons are." Hence, most students seemed to hold the view that the valence electrons are not associated with a given ion or atom. Others tried to utilise the octet rule - invoking the formation of covalent bonds. For example, having drawn two aluminium atoms and describing the dots and crosses in his drawing as electrons, Keith stated: "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." Two students, Anne and Anita appeared not to possess a 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."

The undergraduate students shared similar views to their secondary school counterparts, with, for example, Steve, Alan, Reneé, and Jane, specifying the sea of electrons model for metallic bonding. In contrast to the secondary school students, as might be anticipated, undergraduates who chose the sea of electrons model, provided more detailed explanations as illustrated by Steve's description: "You have got a system [draws rows of Al^+ inside circles with negative signs also inside circles in other rows]. 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."

The remaining undergraduates held a variety of mental models for metallic bonding. For instance, Phil, Bob, and Mary, had no clear picture of the bonding in metals, as typified by Bob's response: "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."

The preferred mental model for postgraduates was the sea of electrons model. Although the postgraduates generally provided more complete descriptions 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: "I think I don't actually think of them as being bonded." Notwithstanding the comments about Christine and Grace, the postgraduates' descriptions of their preferred model more commonly incorporated less terminology from the sea of electrons model and made greater use of nomenclature from other models, such as 'electron cloud,' 'molecular orbital' as seen in Kevin's description:

> 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.

The secondary school students mostly failed to recognise that steel (used as a prompt during interviews) 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. More of the undergraduates than secondary school students identified steel as an alloy but they were often vague about details. For instance, Reneé and Steve both showed an appreciation of the interstitial nature of the alloy steel, Reneé indicating that carbon is "in the middle" of the metallic lattice. The postgraduate students like undergraduates, routinely identified steel as an alloy but several students 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 (and carbon).

Students' mental models for ionic bonding

The secondary school students possessed a number of mental models for ionic bonding with the preferred target model for the bonding in ionic compounds being the electrostatic model (the model in which bond formation is based on the attraction of a cation and anion, see, Coll & Treagust, 2001b). 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 better defined. He related the bonding in sodium chloride to electron transfer and the resultant electrostatic attraction between oppositely charged species.

> 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.

The undergraduate students' 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. Steve, for example, seemed to feel that he could be expected to remember the specific lattice structure for sodium chloride:

> Well once again you have got a regular repeating, a regular sort of repeating structure in an infinitely extended network of sodium plus [draws rows of Na^+ ions in a cuboid arrangement] ions, ah, sodium plus cations and chloride minus anions [draws Cl^- in centre of Na^+s]. 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.

The postgraduate students' preferred mental model for ionic bonding was the electrostatic model, their explanations being similar to those of the undergraduate and secondary school students, with James saying “It's mainly ionic, just having positive and negative sort of spheres packing together,” and “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.” But in general more detail was provided as seen in Brian’s description:

> *Brian*. Well with the sodium plus, well sodium metal itself has one electron in it's 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.

Students’ mental models for covalent bonding

The secondary school students 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 were highly variable. Most of the students said that the bonding in I_2 was covalent, but were not then able to say what the term actually meant. So, for example, Anne, said that the bonding in molecular iodine is "pure covalent" and her drawing of the bonding in I_2 simply consisted of two ‘I’ symbols with no links between the symbols.

The secondary school students' preferred mental model for the bonding in chloroform ($CHCl_3$) was much clearer, and almost all stated it was the octet rule although some initially stated that the bonding in chloroform was similar to that of iodine. Anita, to illustrate, said “they [i.e., chloroform and iodine] are similar because they are both covalent,” whereas Claire said that the carbon and chlorines “are sharing two electrons.” However, overall the students’ explanations were clearly based on the octet rule (a model in which bond formation is based on the notion of full shell stability, see Coll & Treagust, 2001b), and Neil's view is typical: “You'd have your carbon 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 who only wants one more.”

Like their secondary school counterparts, the undergraduates appeared to hold a variety of views for the bonding in I_2. However, most students expressed a preference for the octet rule. The undergraduates see the bonding in I_2 as covalent in nature, which they described as involving “the sharing of electrons,” Phil as an example, saying “the valence electrons they'd probably have an electron out on it's own looking to share with another one. So another iodine will come along and they just share electrons, quite happily share with each other.”

The undergraduates' views of the bonding in chloroform were much the same as those that they held for molecular iodine. Bob, for example, 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]. No that's Cl [writes Cl over top H]. 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.

The postgraduates' preferred mental model for the target system covalent bonding was clearly the octet rule, with all students describing covalent bonding as consisting of the sharing of electrons and going on to relate this directly to notion of full-shell stability. The postgraduates were, however, highly emphatic about the molecularity of I_2 and spontaneously introduced the concept of van der Waals forces.

> *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.

The postgraduates generated descriptions for the bonding in chloroform that were identical in nature to those they provided for molecular iodine, as seen in Jason's response.

> Jason. Ok so you have a carbon, which has four electrons 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.

SUMMARY AND CONCLUSIONS

The data gathered in this inquiry regarding students' mental models for chemical bonding supports the preliminary findings from an earlier study (Coll & Treagust, 2001b) and are briefly re-capped here. The present work suggests that students from all three academic levels prefer simple (or realist) mental models of the target systems for chemical bonding. The advanced level students typically provided more detailed explanations for their models. The extra depth of explanation for the models of bonding by undergraduates and postgraduates compared with secondary school students is probably simply a reflection of their learning experiences. As such, the findings of this study are consistent with that those of other studies involving abstract chemistry concepts like atomic structure for which students showed a preference for realist (e.g., space-filling) models of atoms and molecular species (e.g., Harrison & Treagust, 1996; Pereira & Pestana, 1991; Taber, 1998, 2001). What is of particular interest and importance is that the advanced level-students including PhD students retained clear images of simple models like the sea of electrons and octet rule that they encountered many years previously. This is rather surprising given, for example, the vast differences between the octet rule and the molecular orbital theory. But this finding does suggest that the mental models preferred by the students in this study are very stable (see, Norman, 1983).

IMPLICATIONS FOR TEACHING AND LEARNING

The present work was concerned with students' *preferred* mental models and suggests that despite competence in the description and use of sophisticated mental models for chemical bonding (as evidenced in their high achievement in examinations), these students at least, prefer simple models and relate to more abstract models only in the context of tests or examinations. This is similar to previous reports in literature for secondary school students and undergradautes (Birk & Kutz, 1999; Boo, 1998; De Posada, 1997; Harrison & Treagust, 1996; Nicoll, 2001). These students thus used the simplest models necessary to explain the bonding in a variety of chemical substances and only utilize concepts from other more sophisticated models when their simple explanations breakdown (e.g., Kleinman et al., 1987; Smith, 1992). The fact that the students clung to these models even when they broke down provides some cause for some concern in that their lecturers might well have expected their students to chose, or more quickly adopt, at least some of sophisticated mental models for chemical bonding that possess more explanatory power. The interviews did provide plenty of opportunities in which the simple models were in fact inadequate (e.g., benzene), and it is not desirable that students were so reluctant to draw on the more advanced models. As mentioned, there was some evidence that senior level students appreciated the limitations of the simple models they preferred to use – but this was rather limited.

If the students show such a strong preference for simple models, this begs the question as to the advisability of teaching sophisticated abstract mental models for the concept of chemical bonding. In fact some authors argue that instructors for general or introductory level chemistry should concentrate their efforts on descriptive chemistry and materials chemistry (e.g., Bent, 1984; Gillespie et al., 1996a,b; Tsaparlis, 1997). This might be reasonable for undergraduates who do not intend advancing in chemistry, but really only serves to place emphasis on rote learning and is hardly challenging. It is not obvious that 'dumbing down' a course will achieve very much. Lecturers use sophisticated abstract mental models of chemical bonding for much more than just describing the bonding in substances. Clearly, such models underpin much of chemistry and are used to develop other concepts such as spectroscopy and the use of reaction mechanisms or reaction schemes. Consequently, in our view, and as suggested in earlier work (Coll & Treagust, 2001b) we don't think it make sense to remove complex models from the curricula purely because students prefer to use simple models. What we recommend instead is that tertiary level instructors consider limiting the teaching of such models until the advanced levels of the undergraduate degree. This suggestion is offered, since chemistry non-majors will have little need for models in their subsequent studies.

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