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Facets of chemical bonding that enhance or encumber conceptual understanding

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The abstract multitude, concepts relevant to the study of chemical bonding

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Abstract

Chemical bonding is a vast subject, rich in abstract concepts and advanced and less-advanced explanatory models that the learner has to master. In this context, the teaching of chemical bonding at the secondary school level is extremely important, as it has the potential to increase or hinder students' further understanding of bonding.

In the absence of firm knowledge and effective mental models of chemical bonding, it almost impossible to achieve significant results in any chemical field or application. In this work, which combines the pure chemistry of bonding with didactical studies, I have used database searches, questionnaires, interviews, and textbook analyses to investigate some of the more important aspect of chemical bonding.

In the field of pure Science, bond length data have been analysed to ascertain the differences in bond strength between neutral and charged ligands in coordination compounds. While the bond strengths differ, the difference is not sufficiently large for the bonds to be classified as different types.

In the didactical field, the conceptual models of students in South Africa and Sweden and underlying causes for these mind-sets, have been investigated. The results show that the different curricula and points of emphasis foster different patterns of understanding of the topic. One finding is that 55%–60% of the students exposed to any of the curricula have a molecular view of a salt that can be traced to visual representations of single ions or formula units of a salt. Therefore, it is important to understand how, when, and which models to use, in order to help students build a more advanced understanding of chemical bonding.

Keywords: conceptual understanding, chemical bonding, secondary school, tertiary education, student surveys, coordination chemistry,

Contribution report

The contribution to the enclosed article and manuscript by the author of this thesis:

1. ***Metal-ligand bond lengths and strengths: are they correlated? A detailed CSD analysis***

   The author set up and performed the database searches. Did the data compilation and was involved in the analysis.
   The author also contributed to the writing of the article.

2. ***Teaching of chemical bonding, Success or failure?-A study of Swedish and South African students' conceptions of bonding***

   The author was a major contributor to the formulation of the research problem.
   Designed the study. Performed surveys, interviews, textbook analysis and all data compilation and the major part of the subsequent analysis.
   Major contribution in the writing of the manuscript.

Introduction

Chemical bonding is an essential part of chemistry and is the key to deciphering many chemical phenomena. A strong grasp of the topic is necessary at many levels, which range from applications in the chemical industry to different learning situations. Depending on their field of work, researchers must be able to use bonding models of various complexities to predict and interpret their results. Students who wish to progress in chemistry must first secure an understanding of the basic and central concepts before being able to gain further insights in the increasing complexity of chemical bonding. Chemistry teachers play a key role in guiding step-by-step the prospective learners.

The order and ways in which the concepts are introduced have been shown to have profound effects on the learning outcome (Dhindsa & Treagust, 2014; Nahum, Mamlok-Naaman, Hofstein, & Krajcik, 2007; Taber, 1997). All learners regardless of educational level arrive at their own interpretation of the presented concepts. This interpretation is greatly influenced by the learners' previous knowledge base and experiences, and it may result in a framework that is more or less at odds with what is scientifically accepted. Therefore, it is important for teachers to be aware not only of their own understanding of the topic, but also of the learners' conceptual worlds.

Given that chemists have their own versions of conceptual understanding, the field of chemical bonding is hotly debated. Divergent opinions cover the purely scientific questions, as well as the hybrid questions in the field of teaching. Examples of questions that provoke discussion are: What constitutes a bond? How does a specific bond work? What teaching order is best? How should bonding be introduced?

Discussions in relation to these questions can be very heated. An example is the existence of Fe-Ga and Ga-Ga triple bonds, as proposed by Robinson's group at the University of Georgia (Su, Li, Crittendon, Campana, & Robinson, 1997; Su, Li, Crittendon, & Robinson, 1997). Interpretation of the data for these bonds split the research community. As the two sides clashed, several famous exchanges were reported by Dagani (1998). F.A. Cotton stated *"that's no more a triple bond than I'm the Dalai Lama"*, to which Robinson replied that Cotton's models were *"at odds with some long-standing principles of inorganic chemistry."* Power, who collaborated with Cotton, commented on Robinson's interpretation of a bond as follows: *"The definition of what constitutes a bond has been so stretched - if you'll pardon the pun - that it no longer bears any relationship with reality. If one wants to consider any atomic interaction - no matter how weak - as a bond, that's fin*e, *but I don't think that will find widespread acceptance."*

As an upper-secondary school chemistry teacher, I have always been interested in the aspect of atomic build-up and the bonding that occurs in compounds. Therefore, I chose this topic for my application to the Licentiate Research School for Teachers at Chalmers University of Technology (Chalmers Chalmers_Lärandecentrum, 2012). This programme funded by Swedish research council aims to increase the number of research trained teachers in secondary school.

The first part of this thesis focuses on the shape and nature of the chemical bond from a scientific perspective.

Just as in the case of the Ga-Ga triple bond, the classification of network forming coordination compounds has been a matter of debate, albeit not with the same verbal vehemence. Yaghi and colleagues proposed a distinction between highly stable metal-organic frameworks with strong bonds (i.e., those with anionic ligands that form “salts”) and less stable coordination polymers with weaker bonds (i.e., those with neutral ligands) (Yaghi et al., 2003). As this categorisation has been contested by Robson (Robson, 2008), we considered it important to examine the structural evidence that might resolve this dispute.

In the article *Metal-ligand bond lengths and strengths: are they correlated? A detailed CSD analysis* (Nimmermark, Öhrstrom, & Reedijk, 2013), we analysed the bond length data from the Cambridge Structural Database (CSD), to determine if there a sufficient difference in bond strength exists between charged and uncharged ligands in a coordination compound that might merit the proposed distinction.

The second part of this thesis relates to how students can best be helped to understand the concepts of chemical bonding. The work is based on surveys and interviews conducted with students in the upper-secondary school and entry-level university students. The data from these sources, together with textbook analyses, explore the Swedish and South African students’ conceptual understanding of chemical bonding and strategies for teaching these concepts. Our manuscript titled: *Teaching of chemical bonding, Success or failure?-A study of Swedish and South African students’ conceptions of bonding.* (Nimmermark, Mårtensson, Öhrström, & Davidowitz, 2014) describes how secondary and tertiary chemistry students describe bond energetics, the shapes of molecules, and the molecularity of materials. In addition, we indicate possible causes and remedies for the observed conceptual understanding and discuss briefly the effects of the different school systems.

Together, the two papers combine the divergent viewpoints of the pure subject-oriented chemist and the chemistry teacher into a more complete picture of the essentials of chemical bonding.

We see when we correlate answers to grades, where we have these data, that two students with the same grade, can have very disparate mental models, the reason for this is probably that in the Swedish curriculum it is very much up to the teacher to choose which topics to teach, and how much time to spend on any specific topic.

Objectives

This thesis examines aspects of chemical bonding that are relevant to the understanding and teaching of the subject. The concept of chemical bonding will be discussed from both the pure Natural Science perspective and from the didactical point of view, as well as a combination of these two approaches. The overall aim of the work presented in this thesis is to develop tools for both secondary-level and tertiary-level teachers to facilitate the transition from high school-type studies to the more stringent scientific teaching at universities within the current curricula.

The following questions have been addressed in the search for these ephemeral tools:

1) Is there structural evidence that the bond between a metal and a charged ligand is fundamentally different from the bond between a metal and an uncharged ligand?
2) Are there differences in conceptual patterns between students in Sweden and South Africa, and how do they correlate to how the different curricula and textbooks address the topic of chemical bonds?
3) Are the Swedish and South African curricula successful in helping the students to understand chemical bonding, and if not, how could the curricula be improved?
4) How can further studies of chemistry and new ways of teaching chemistry help students and teachers to arrive at a more relevant picture of chemical bonding?

Background

The roles of models in Science and Science education

In Science, we never deal in absolutes, instead relying on the data from observations and experiments, which can be compiled and analysed to derive a model that explains the observed data.

In general, models can be grouped into two main categories (Haglund et al., 2013): 1) mental models, which are used to understand and conceptualise a phenomenon in the mind of the scientist, teacher or learner; and 2) external models, which are used to communicate the understanding of a concept. External models can be further categorised as scale-models, analogous models, mathematical models, and theoretical models (Black, 1962).

A good model not only provides an explanation for the data but also confers the ability to predict outcomes. When working with models it is important to keep in mind the limitations of particular models and to use a model of appropriate complexity. The choice of models can be guided by the notion of Occam's razor as adapted by scientists': "when you have two competing theories that make exactly the same predictions, the simpler one is the better"

In Science and Science education, external models are often used in the form of symbolic, verbal or visual representations. An improper representation can affect the interpretation of the concept, with the consequent risk of creating a mental model that is not aligned with current scientific knowledge, a misconception or alternative framework. This has been shown in several studies of chemical bonding, for example, in a study of lower-secondary school students' mental models of atoms and molecules (Harrison & Treagust, 1996). In that study, the researchers described the risk of the teacher creating misconceptions and alternative frameworks when using analogies, metaphors, and models without sufficient discussion or explanation. Another interesting paper is that of Bergqvist and co-workers on the use and effect of model representations in Swedish chemistry textbooks (Bergqvist, Drechsler, De Jong, & Rundgren, 2013); they proposed that the visualisations in Swedish textbooks might cause students to develop misconceptions.

That mental models can be hard-set and very resistant to change has been demonstrated by Nicoll (2001) and Coll and Treagust (2003a) in their respective cross-age studies of how secondary-, undergraduate- and graduate-level students describe bonding; they conclude that misconceptions adopted early in the education pathway can persist even at the graduate level.

The case of the triple Ga-Ga bond is an example of how the interpretation of external and individual mental models, irrespective of their validity, can be the root of very heated discussions even among scientists who are well-versed in chemical bonding.

Historical models of the chemical bond: a brief description

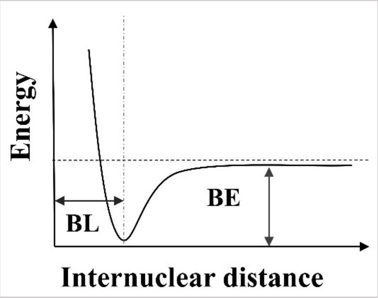

Figure 1 Morse potential energy curve for two atoms at various distances from each other. BE is the bond energy given as the potential minima, and BL is the bond length i.e. the distance between the nuclei at the potential minima.

The basic models of bonding were introduced 100 years ago in the article title *The atom and the molecule*. (Lewis, 1916) and are still in use today.

A chemical bond can be viewed essentially as an interaction between two atoms (different or identical). The bonding is due to an interplay between the electrostatic inter-actions and quantum effects. At a certain distance (Figure 1), the attractive and repulsive forces cancel each other out. At this point there will be an energy minimum, which holds the atoms at this distance, i.e., the stable bond length. The bonding phenomenon is clearly demonstrated in

Figure 1 by the graph of the potential energy as a function of the distance between two atoms.

Lewis (1916) developed a model that is mainly used to describe covalent and polar covalent bonds, as it involves the valence electrons of the atoms being joined in a bond. The bond comprises atoms sharing valence electrons to achieve a surrounding octet of electrons (also known as the noble gas configuration).

The sharing of electrons can be equal or unequal, giving rise to the polar covalent bond. Just as in the case of electrostatic interaction, traces of "shared" electrons can be detected in all bonds. Therefore, the bond types are not clear-cut, but rather represent a bond continuum with the covalent bond at one end and the ionic bond at the other end, and in between the two extremes, we find the polar covalent bonds.

Eleven years after Lewis formulated his bond model, Heitler and London (Heitler & London, 1927) used the newly developed quantum mechanics to describe Lewis's bond model for the covalent bond. They coined the term 'valence bond method'. Pauling (Pauling, 1928) modified this theory and made it, even though sophisticated computers were not yet available, more applicable. Pauling described this model in terms of localised wave functions. To account for the shapes of the molecules, Pauling introduced the term 'hybridisation' to describe the formation of the necessary σ- and π-bonds at the proper angles.

Almost parallel to the evolution of the valence bond theory (VBT), Hund (1932) and Mulliken (1928) together developed a different quantum model that described the bond not in terms of hybrid orbitals, but instead in the context of molecular orbitals (MO) formed by linear combinations of atomic orbitals. In its modern form, this is known as LCAO-MO.

MO and VBT persist as the two main models for more advanced descriptions of bonding, whereby each theory has its proponents and opponents according to the perceived merits and weaknesses of the respective models. The strength of VBT lies in its simple visual description and its direct linkage to the basic Lewis bond models, which makes it seem very intuitive. VBT is less practical for describing large molecules due to the level of complexity associated with creating the required hybrid orbitals. In contrast, MO is better at handling large molecules, owing to its lower demand for computational capacity. Both theories provide the possibility to calculate electron densities, bond lengths, and bond angles. With current visualisation techniques, MO is more visual than before, and computerised calculations have increased the use of VBT. Today, both theories are used, although 90 years after they were first proposed, the use of these tools is still debated.

Bond strength and bond length

Bond lengths can be used as a tool to assess bond strengths. The C-C bond is longer (1.54Å) than the C=C bond (1.34 Å), and this corresponds well with their measured bond energies of 348 kJ/mol and 614 kJ/mol, respectively. These data imply measurements of the bond lengths of comparable compounds can be used to estimate the bond strengths. For the ordinary covalent and ionic bonds, data on bond lengths are readily accessible, whereas data for metal-ligand bond lengths are not as easy to find.

One relatively simple way of assigning bond strength in metal complexes is through the formal bond valence theory, which states that charged ligands have a positive bond valence equal to the charge of the ligand. Since neutral ligands have no charge, they can only create bonds with a bond valence of 0 according to this theory.

Coordination chemistry

In the mid-19th century, coordination was recognized as a bond phenomenon, although a simple explanation for how the components were held together was lacking. Through elemental analyses, the constituents were determined, while the structure remained a mystery. One problem that arose was that there were more ligands bound than would be allowed by the bond valency. The compounds that did not make sense to the chemists were called ‘complexes’. Subsequently, the field was renamed to ‘coordination chemistry’ and the complexes were termed ‘coordination compounds’, since the metal appeared to coordinate the ligands at certain geometric positions. Today, the structures of coordination compounds can easily be deduced with the help of X-ray diffraction techniques.

The scientist who initiated the understanding of the field is Nobel Prize laureate Alfred Werner, who studied the bonding between metal ions and uncharged ligands, such as ammonia, during the start of the 20th century; these coordination compounds are commonly known as Werner compounds.

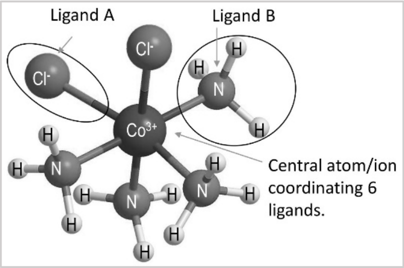

Figure 2 Tetramminedichlorocobalt-(III) ion, showing the constituents of a coordination compound. This compound has two types of ligands 4 ammonia and 2 chloride ions. The coordination number is thus six.

In essence, the bonding can be described either as a directional dative bond between the central metal atom or ion and the surrounding molecule or ion (ligand) (Figure 2) or as a non-specific electrostatic interaction. The dative bond is formed in an acid-base type of process. The ligand acts as a Lewis base, and it can be either charged or uncharged. It donates one electron pair to an empty orbital on the metal or metal ion, which acts as a Lewis acid in accepting the electron pair. The electron pair sharing results in a metal–ligand bond. Bond strengths depend among other things atomic size and on the basicity of the ligands.

Coordination compounds

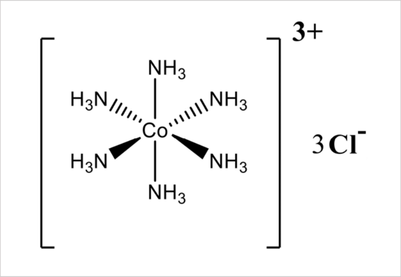

Figure 3 Hexaamminecobalt(III)chloride a classic Werner compound

An example of a Werner compound is shown in Figure 3. A Werner compound involves the coordination of an uncharged ligand to a positive metal ion. Since the ligand is uncharged, the coordination in itself forms an ion. Depending of the energetics and type of anion, a salt precipitate may form, although it is often the case that the complex ion remains dissolved in the solvent. A characteristic of Werner compounds is that they are exchange-inert, i.e., the ammonia shown in Figure 3 is linked so tightly to the metal that it cannot easily be replaced by another ligand and it will not dissociate to allow for protonation of the ammonia. Compounds of this type are generally brightly coloured owing to the electrons in the metallic d-orbitals; the hexaamminecobalt(III) ion solutions and salts are yellow.

Ligands

While ligands can be of various types, they are commonly nitrogen- and oxygen-containing compounds and ions. Alcohols/alkoxides are systems that coordinate through the lone pair of electrons on the oxygen, while the same is true for the carboxylic acids and the carboxylate ions. The difference between the alcohol systems and the carboxylic acids is that in the case of the acids, two different coordinative modes are possible: M-OH-O-R coordination and coordination through the more basic keto carbon in the acid. In

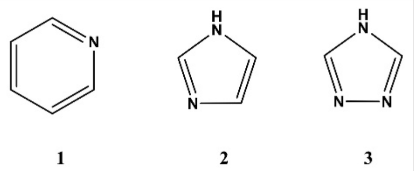

Figure 4 Representative N - heterocycles, 1 = pyridine, 2 = imidazole and 3 = triazole

the case of carboxylate ions, no coordination ambiguity is possible, except for carboxylates that bridge two metal centres.

Heterocyclic compounds (Figure 4) are very common ligands in coordination chemistry. These are ring-shaped compounds that contain at least two species of non-hydrogen atoms. Nitrogen is a very common heteroatom in many heterocyclic compounds. The compounds can be organic (carbon-based) or inorganic. The structure of the ligand is stabilised when the p-orbitals overlap to form alternating π-bonds. If all the atoms in these rings have p-orbitals the electrons can be delocalised over all the atoms in the ring, i.e., rings that obey the Hückel rule and contain alternating double bonds and/or free lone pairs are stable and very common.

One of the electron pairs not forming the π-bonds on nitrogen can be donated to a metal atom or a cation (metal ion), thereby forming a dative bond. This capability of nitrogen to bond metal atoms and cations is what makes N-heterocycles so useful as ligands in coordination chemistry. Pyridine, which is one of the simplest N-containing heterocycles, is analogous to benzene, containing five carbons and one nitrogen atom. It coordinates through the nitrogen, and as the nitrogen does not bind any hydrogen or other substituent, it is always a neutral ligand. Imidazoles (Figure 5) can coordinate two metal ions if both of the N positions are used. Since it loses the hydrogen attached to the nitrogen, it acts as an anionic (negatively charged) ligand.

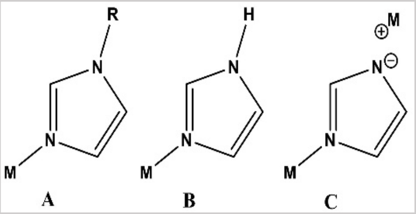

Figure 5 Coordinative modes of Imidazole and Imidazolate systems, A and B corresponds to the uncharged imidazole species and C is the charged imidazolates.

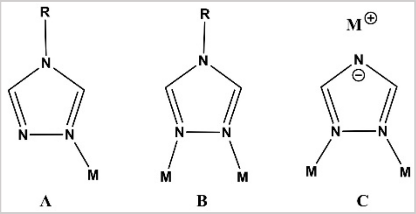

Figure 6 Coordinative modes of Triazole and triazolate systems, A is unequivocally neutral, B can be ambiguous with regards to charge and C is charged -1.

However, if it coordinates only through the nitrogen that has a double bond to one of the carbons it behaves as a neutral ligand, similar to pyridine. The manner of imidazole coordination is depicted in Figure 5. Further increasing the number of nitrogens in the five-membered ring generates the triazole systems, which have possibility to coordinate up to three metal atoms. The triazole that coordinates in the same way as pyridine is a neutral ligand. The two co-ordinating triazoles can be neutral or anionic depending on the substituent on nitrogen number 4. All triazoles that bind to three metal atoms or cations are anionic. The different coordinative modes of triazoles are shown in Figure 6.

Ligand effects

The number of ligands bound to the metal ion is called its coordination number (CN). Based on the number of ligands, certain geometries of the complexes can be expected. For example, six ligands usually coordinate in an octahedral geometry, four in a tetrahedral shape, and three ligands will have a trigonal planar geometry. These are the optimal geometries for maximising the bonding interactions and minimising the potential energies of the systems (complexes). A more detailed description of the origin of coordination geometry is given below.

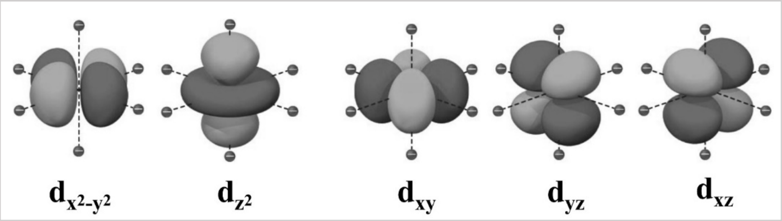

Figure 7 The different geometries of the atomic d-orbitals.

One way of explaining the observed geometries of the coordination compounds is with the help of crystal field theory, which uses the electrostatic interactions between the electrons in the d-orbitals on the central atom and an imaginary negative point charge in the place of the ligand. This causes repulsion between the charge and the central atom's d-orbitals. To depict this repulsion, the d-orbitals are envisioned as being filled and the ligands are replaced with negative point charges. Since the five d-orbitals (Figure 7) of the metal have different symmetries and thus, either point towards a charge or in between the charges, the electrons in the different d-orbitals will experience different repulsive forces. The charge densities described by the d-orbitals that are aligned towards the ligand will have a large electrostatic interaction. This interaction increases the repulsion between the electrons, which means that the energy of the orbitals pointing in that direction increases. The non-interacting orbitals do not experience as much repulsion and remain relatively unaffected in terms of energy. Due to these symmetry effects, the d-orbitals will always split when a non-spherical ligand sphere approaches. The magnitude of the splitting, i.e., how much the d-orbitals will be raised in energy, depends on the CN, the oxidation number of the metal, and the type of ligand. (see Figure 8)

Another and more complex way of describing the effects of ligands on the atomic orbitals of the metal is using the more modern ligand field theory. In the ligand field theory, molecular orbitals and symmetry elements are used instead of the negative point charges, providing a more accurate description of the ligand effects.

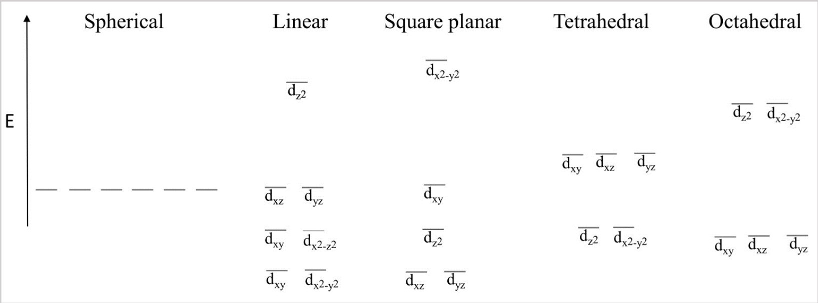

Figure 8 Crystal field splitting for ligands of various geometry. In this figure the ligands are seen as negative point charge, no account is taken for ligands being π-acids or π-bases

A common consequence of symmetry and electronic degeneracy in a ligand field is the Jahn-Teller distortion.

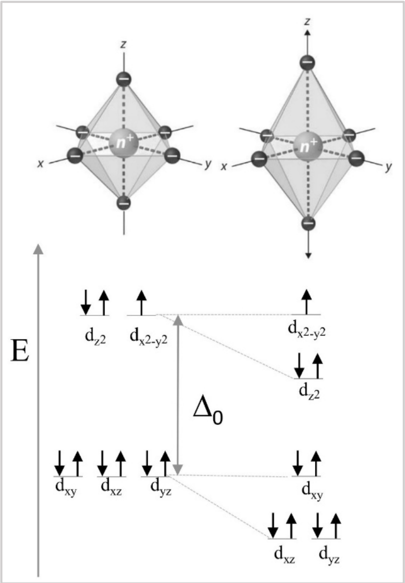

Figure 9 **Top**: Jahn-Teller elongation in a Cu(II) complex. **Bottom**: The d-orbitals with a z component are stabilized and will be lowered in energy if the z- axis bonds are elongated. This also removes the degeneracy of the ground state $d_{x^2-y^2}$ and d_{z^2}

This is a phenomenon that occurs in octahedral complexes that have an uneven number of electrons in the e_g orbitals (d_{z^2} and $d_{x^2-y^2}$ orbitals). In these complexes, the bonds along the *z*-axis are either elongated or shortened (see Figure 9, top). The most common examples of the Jahn-Teller effect are octahedral Cu(II) compounds, one of which will be used as an example to explain why certain complexes become distorted. A Cu(II) ion has nine d-electrons, so there will be three electrons in the high-energy upper d_{z^2} and $d_{x^2-y^2}$ orbitals (see Figure 9, bottom). This results in a degenerate ground state (there are partially filled orbitals of the same energy). While this is an energetically unfavourable state, it can be avoided if the bonds along the *z*-axis elongate, thereby lowering the repulsive force, as in crystal field theory, between the charges of the *z*-aligned ligands and the *z*-aligned electron densities represented by d-orbitals. This results in a splitting of the d-orbitals aligned in the *z*-direction, which will have reduced energy compared to the two d-orbitals (d_{xy} and $d_{x^2-y^2}$) that lack a *z*-component and thus remain unaffected. When this splitting occurs the degeneracy is removed and thus, the energy of the complex as a whole is reduced, creating a more stable geometry.

Metal-organic frameworks

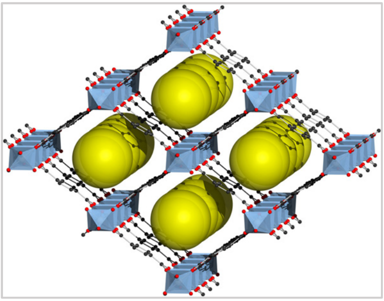

Figure 10 Representation of the 3-dimensionality of MOF-5. The blue dots signifies copper, red oxygen and black carbon. The yellow spheres indicates the different pores in the structure. The shaded octahedral visualise the geometry of coordination.

A metal-organic framework (MOF) represents a group of coordination compounds that are formed by linking organic molecules or ions (ligand) to metal ions (central atom) in a 2- or 3-dimensional network (Batten et al., 2012). A MOF is generally a rather open structure that consists of large channels and pores (see Figure 10). The size, properties, and shapes of these cavities can be designed through the use of ligands with specific structures or properties.

Typical ligands consist of a Lewis base (molecules that contain atoms with free electron pairs, such as oxygen or nitrogen), which is capable of donating an electron pair to the metal, which acts as a Lewis acid in accepting the electron pair and thereby forming the dative coordination bond. To create the 2- and 3-dimensional networks characteristic of a MOF, the ligand must be capable of connecting to two metal ions. The type of ligand will have a strong impact on the resulting network. For instance, the use of a chiral ligand results in a chiral network, whereas employing a large ligand generally generates larger pores and channels. A MOF is typically synthesised by adding a metal salt to a molecular compound and heating or grinding them together, sometimes in the presence of an organic solvent and a base. With the appropriate proportions and conditions, the MOF will crystallise out of the mixture.

A major goal in MOF research has been to find ways of predicting the structure of the network. One difficulty with this is that the bond angles between the ligand and the metal ion often vary significantly, making it difficult to predict and control the shape of the network. One way to avoid this uncertainty is to first chelate the metal ion to various multi-dentate carboxylic acids, thereby ensuring that the bond angles are fixed and producing a rigid entity that is known as the secondary building unit (SBU). Depending on the choice of organic acid, these SBUs will only be extendable at certain positions, thus making it possible to predict and design the shape when the MOF is assembled by joining the SBUs with organic linkers (Tranchemontagne, Mendoza-Cortes, O'Keeffe, & Yaghi, 2009).

MOFs are of interest for many application due to their versatility. Among other things, they can be used for gas storage, as chemical sensors, and as effective and durable catalysts either by themselves or through the incorporation of the actual catalyst inside a pore.

One example of an application is that the Mercedes-Benz F125 concept car employs MOFs as a means to store the hydrogen for its fuel cells. (Clarke, 2014)

Teaching and learning the concepts of chemical bonding

Figure 11 The Nürnberg funnel as a way of teaching. In a comic from the 19th century people are waiting to be filled with knowledge.

Teaching, learning and understanding chemical bonding can be challenging, since the level of abstraction is high and the acceptance of new, refined models can be hampered by students using unfortunate heuristics (Talanquer, 2006) and having a limited understanding of previously encountered models (Coll & Treagust, 2003a). Central and complex concepts or phenomena are defined early in the education pathway, although often in such restricted terms that a single concept or phenomena needs several distinct definitions to be covered fully. As shown above, the use of different models in different situations comes more or less naturally to the teacher/scientist. However, for students, the reasons for model juggling, moving back and forth between simple and complex models, can be a complete mystery. This is probably why we find students presenting concepts in a somewhat fuzzy and naive way. In short, there is a need for the teachers of any subject to "make sense" to the student. The ability to understand a field and make it available to students, through sequencing, explanations, visualisations, and activities, is called the teachers pedagogical content knowledge (PCK) (Shulman, 1986). For hundreds of years, the dogma in relation to teaching has been empiristic, in which students are described as vessels to be filled with knowledge (Figure 11). In the last 100 years, this view of learning has lost credibility. The work of Piaget and Vygotskij, with a foot in cognitive science, paved the way for a more modern view of learning. In the constructivist framework, knowledge is something that is constructed based on the prior knowledge and experiences of the learner, and learning can occur both on an individual basis and in a socio-cultural context. This viewpoint places the teacher in the role of setting up learning activities that encourage the students' curiosity and motivation to learn.

Conceptual change is one such constructivist approach, which tries to come to terms with the construction of mental models so as to facilitate the learning of a specific concept. Every student creates their own individual interpretations of the scientific explanations to which they have been exposed in different learning situations. These interpretations make up the students' framework theories, which together constitute their conceptual ecology (Hewson, 1992). The framework theories may be very entrenched and take priority over the scientifically correct ones. An actual conceptual change may be very difficult to achieve due to the high status of the current framework theory (Vosniadou, 1994). Unless the high status of the alternative framework is lowered, no meaningful learning will occur.

One way to achieve this can be found in the four conditions listed by Posner, Strike, Hewson and Gertzog (1982) in relation to conceptual change. First, all the student have to become dissatisfied with the old framework. Second, the new concept needs to be presented in a way that seems intelligent to the learner. Third, the new concept must also be perceived as initially plausible, and fourth, it must be capable of providing fruitful solutions for the present problems.

Aside from fulfilling the conditions listed by Posner and colleagues, the teacher must create a learning environment of trust, situations that stimulate the asking of questions, and activities that challenge the students' beliefs, indicate limitations to their existing framework theories, and encourage them to step outside their regular thought patterns. Creating situations that include all the specific conditions in the list of Posner et al. and the general learning situations described above is what lies at the heart of being a teacher. No meaningful learning and no actual conceptual change will occur if the teacher fails to incorporate these conditions into the learning situation or fails to take into account that students and teachers often enter into a dialogue with different interpretive frames (Driver & Easley, 1978).

Aside from the cognitive aspects of the conceptual change theory, a slightly different cognitive perspective can be used to argue that the understanding and subsequent creation of a conceptual framework for a chemistry topic can be influenced by what Talanquer calls *Common sense chemistry* (Talanquer, 2006). Common sense chemistry attributes the mainly involuntary empirical and heuristical thought processes to the origin of alternative conceptions. Two examples of heuristic reasoning and empirical assumptions that lead to the wrong conclusions are given below.

> *"Copper is red, thus the Cu atom is also red"*
>
> *"At equilibrium, the forward reaction is completed before the reverse reaction commences"*

Without knowledge of the conditions to be met and the empirical assumptions and reasoning heuristics employed by the students, it is impossible to construct effective learning activities. These are activities that help the students to challenge their conceptual ecology in a way that encourage conceptual change.

Methodology

Cambridge structural database-CSD

The CSD was founded in 1965 at Cambridge University as part of the organic crystallography group and was designed to serve as a database for numerical results derived from x-ray and neutron diffraction studies. The CSD collects and curates data on small-molecule crystal structures (up to 500 non-H atoms). Currently, the CSD contains more than 500,000 individual crystal structures. Both single crystal and powder diffraction data are included.

The main search method for the CSD is to draw the Lewis-type structure (complete or partly) that is being sought; see Figure 12 for the structures searched for in our study.

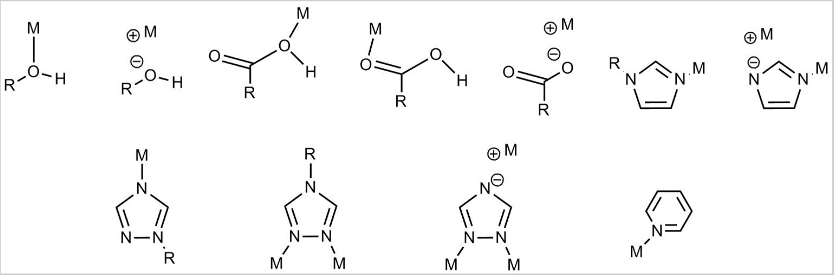

Figure 12 Systems searched in the Cambridge Structural Database (CSD). M=Co, Ni, Cu, Zn. For comparison we have also searched pyridine systems although in this case there is no appropriate anion to compare with. Note that formal charges are emphasized in this figure, the actual searching was performed with a formal bond between M^+ and L^-. (R=H or organic fragment). Only the most frequently occurring structures of the triazole complexes were considered.

The CNs and connectivities can be specified in this mode, as can the bond lengths and angles etc. to be included in the search results. It is also possible to filter the results for various items, such as disorder and type of diffraction. Table 1 summarises the data available in the database.

Table 1 Summary of information content of the Cambridge Structural Database. (Allen, 2002)

Bibliographic and chemical text	**Chemical class (e.g. alkaloid, steroid etc.)**	**Crystal structure data**	**Derived information**
Compound name(s), systematic and trivial	Text comment concerning disorder, errors located during validation and special structural features	Cell dimensions and s.u.'s (standard uncertainties)	Bit-encoded screen records
Amino acid sequence for peptides	Chemical connection table	Space group and symmetry operators	Reduced cell parameters
Chemical formula	Formal two-dimensional chemical structure diagram in terms of atom and bond properties	Atomic coordinates and s.u.'s for the crystal chemical unit	Z^0, the number of chemical entities per asymmetric unit
Text indicating special experimental conditions or results (e.g. neutron study, powder study, non-ambient temperature or pressure, absolute configuration determined etc.)	Bond types used in CSD connection tables are: single, double, triple, quadruple (metal-metal), aromatic, delocalized double and π-bonds		Matching of 2-dimensional and 3-dimen-sional connectivity representations
Authors' names			Calculated density
Journal name and literature citation			

Surveys, interviews, curricula and textbooks

In carrying out educational research, one often has to rely on surveys and interviews to gain insights into the thinking processes of the learners. These studies are often performed to evaluate the efficiency of a certain programme, teaching model or curriculum change.

Constructing and performing surveys

In the case of the study presented in this work, a questionnaire that covers some basic aspects of bonding was prepared and used.
The questionnaire comprised three types of questions: multiple choice; two-tiered multiple choice; and open-ended.

Each question type has its own strengths and weaknesses. Multiple choice questions can give a quick overview of the topic and are easy to compile and analyse with the help of computers and advanced statistical methods. It is possible, albeit laborious, to produce a multiple choice question that probes more than superficial knowledge. One of the more difficult tasks in the composition of multiple choice questions is to generate response statements that check for deeper knowledge, without relying on the use of small semantic differences in the text. In the case of responses with a long and complex text, the risk always exists that what is tested is not knowledge of the subject but rather the respondents' language skills. Another drawback is that there is a risk that the respondent just randomly ticks off the responses; this risk increases as the response text becomes more complex and longer. To avoid some of the limitations of an ordinary multiple choice question, the two-tiered multiple choice question was invented.

A two-tiered question involves an initial statement for which the answer is true or false. This question is followed by a second multiple choice where the respondents are asked to pick one statement as a rationale for their initial response of true or false. A question that is phrased in this way is more valuable in probing the thought patterns of the respondent, since it not only provides information on knowledge of the concept, but also reveals how it is interpreted in the context of the mental model of the student.

An example of how a questionnaire can be constructed using two-tiered multiple choice questions is presented by Peterson, Treagust and Garnett (1989).

Since open-ended questions allow respondents the freedom to express themselves in their own words, they are efficient at probing deeper knowledge. The drawback is that the respondent may consider open-ended questions as requiring too much effort to answer fully. It is not uncommon for respondents to avoid answering this type of question. This was certainly the case in our study of chemical bonding, where the response rates for the open-ended questions were much lower than those for the multiple choice questions. Another issue is that the answers to open-ended questions need to be categorised in some way before they can be analysed. The simplest way to achieve this is to read all the answers and then group them according to common points, which will then constitute the different categories. A more advanced and structured strategy is to use a rubric, i.e., a usually pre-set matrix of criteria that is used to evaluate the answers.

We used both methods to compile the responses obtained for the following open-ended questions: *"Describe in detail how the carbon atom and the hydrogen atoms are held together in the methane molecule!"*; and *"Describe in detail in which region you would find the different electrons in the methane molecule!"* To create general categories, we used the read-through method, where another experienced teacher validated the categorisation. To discover which specific concepts, e.g., quantum mechanics, stability etc., were present we used a rubric. Table 2 lists the resulting categories and the matrix used to compile the first of the two open-ended questions described above.

To create a survey that collects relevant data with the help of the question types described above, a test or trial survey is usually performed in advance of the full data collection. The test version gives insights into how the respondent perceives the questions and checks understanding and the ordering of questions and whether statements or questions that should be included are missing.
The chemical bonding survey reported in this thesis used two trial groups, one with subjects who were still attending upper-secondary school, and one with subjects who were starting tertiary education at Chalmers University of Technology.

Apart from the manner in which the questions are posed, another important factor when implementing surveys is the manner of distribution. Online web services, such as Webbenkäter[1], are powerful tools for creating and distributing surveys. Web links to survey sites are particularly efficient if the respondents have a wide geographical distribution. If it is feasible, it is beneficial to set aside some time for the answering of the survey, since this will radically increase the response rate. In the present work, we used both paper forms and web links to collect data, which then were analysed using the Excel 2013 software.

Table 2 Example of main categories derived from read through and the specific concepts rubrics.

Main category	**Specific concepts**
1 Simple explanations, without conceptual explanations or descriptions	**A** Explanation of full shell
2 Explanations are more complex, including some concepts and states electron sharing or sigma bonds	**B** Electro-negativity
3 Advanced explanations including concepts i.e. octet rule, orbital reasoning etc.	**C** Uses energetics for reasoning
4 Describes the bond as being intermolecular,	**D** Stability reasons
5 Describes the bond as some kind of ionic interaction	**E** Some kind of orbital/quantum explanation
6 General explanations or descriptions	**F** Electrostatic interaction
7 No response	

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[1] https://www.webbenkater.com/

Preparing and performing interviews

Interviews can be of three main types: open; structured; and semi-structured.

The open interview format is best described as a conversation on a general topic, involving a dynamic exchange of ideas and questions. It has no or few pre-set questions or subtopics to be covered, and the direction of the interview will evolve as the result of the interactions between the interviewer and the interviewee.

In contrast, the structured interview has a very strictly set list of questions and a specific focus that the interviewer enforces during the interview. It has a very low level of freedom, which has the benefit of making it easy to compare one interview to another. However, the strict format carries the risk of losing openings that might provide insights into areas close to the topic at hand.

In the semi-structured interview, the interviewer has prepared in advance a checklist of topics and questions to be covered. This framework will steer the interview in the intended direction, although since it is loosely enforced, it gives more room for discussions of related topics without losing the focus on the overall goal.

The six interviews discussed in this thesis were all of the semi-structured type, using the framework listed in Appendix 1 and having the overall goal of exploring the levels of knowledge of atomic theory, the *aufbau* principle, and chemical bonding.

Curricula and textbook contents.

We were interested to know how and to what extent the different national curricula and textbooks describe facets of bonding, bond energetics, and molecular geometry. The use and choices of representational tools, the teaching order, and the starting point for the explanations were also relevant to our study. These aspects, as well as the three general foci of our study, were used to create a matrix that set a structure for the text analyses of the books and curricula. An example of this type of matrix is presented in Table 3. The most commonly used textbooks[2] in each of the curricula were chosen; in total, four Swedish and five South African textbooks were selected.

Table 3 Textbook analysis matrix. Example of specific topics that were included in the textbook analysis

Number of space filling models	Number of ball and stick models	Total number of represent-tational models (BS + SF)	Shell/Bohr model as main explanatory tool	Quantum models /atomic orbitals as main explanatory tool	Energy level diagrams describing bond breaking and formation
Describes and uses molecular orbitals to some extent when describing bonding	Uses the potential bond curve as a fundament for chemical bonding	Order of introducing bond types	Describes and uses the VSEPR model	Main descriptive model for ionic bonding	

Sample groups

The sample groups described in detail paper 2 were chosen to represent students who were still in upper-secondary school and first-year university students, from two different cultures and school systems, Sweden and South Africa.

The groups SWE, CH13, UCT, and CH14 have the following compositions:

SWE: Swedish students enrolled in the upper-secondary school Natural Science or Technology programme; the criterion for inclusion is that they have completed the chemical bonding topic taught in the upper-secondary school.

CH13: Swedish students who are starting tertiary-level education at Chalmers University of Technology. The survey was performed

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[2] The titles of the textbooks are listed in Paper 2 of this thesis.

prior to the initial studies of chemical bonding at the tertiary level. These students have a background similar to that of the SWE group, but are expected to be more interested in chemistry, due to their choice of tertiary education.

UCT: South African students who have starting tertiary level education at the University of Cape Town. The survey was performed prior to commencement of studies of chemical bonding at the tertiary level.

CH14: Swedish students from the CH13 cohort who participated in the survey only after completion of the tertiary entry-level topic of chemical bonding.

Results

The data listed below contain a description of the findings in relation to bond lengths and bond strengths, the students understanding of chemical bonding, and the analyses of textbooks.

Bond length data from CSD

This section contains results presented in the article *Metal-ligand bond lengths and strengths: Are they correlated? A detailed CSD analysis (Nimmermark et al., 2013)* The complete record and discussion are to be found in the attached article. (Paper 1)

Metal alcohol and alkoxide systems

As expected for compounds that contain Cu(II), we found that the alcohol ligands had two different bond lengths, due to Jahn-Teller elongation. In contrast, the alkoxide systems did not show any elongation. The alkoxides were found to coordinate either in the equatorial plane of an octahedral complex or in square planar geometries. The effective difference in bond

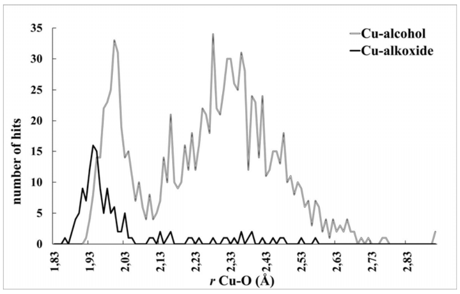


Figure 13 CSD search results for copper-alcohol and copper-alkoxide structures, with all the CNs used and more than 98% of the compounds containing Cu(II). The peak at around 2.33Å represents the Jahn-Teller elongated axial bonds.

strength between the alcohol and alkoxide ligands to Cu(II), measured as the bond length (Figure 13), was 2.5%. (1.94 vs. 1.99 Å)

Metal carboxylic acid and carboxylate systems

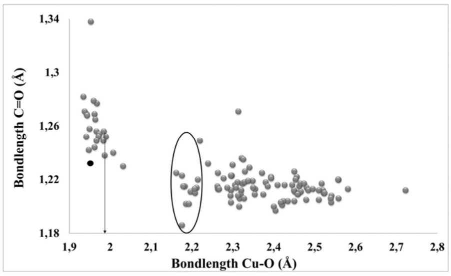


Figure 14 Cu-O distances (x-axis) for keto-coordinating copper(II) neutral carboxylic acid complexes versus C=O bond lengths (y-axis). “Normal” C=O and C-O distances are 1.20 and 1.43 Å respectively and the most frequent Cu-O bond length in carboxylate complexes is 1.95 Å (red/black dot). The arrow indicates BL for carboxylic acid complexes. The circled complexes are 4 coordinated paddle-wheels.

These systems, even though they are more ambiguous in terms of protonation state and coordinative modes, show the same patterns as the Cu-alcohol and Cu-alkoxide systems. The difference in bond length between keto-coordinated copper and the few copper ions that coordinate to the carboxylic acid is 0.04 Å (1.95 Å and 1.99 Å, respectively). The longer bond lengths (2.3–2.6 Å) shown in Figure 14 represent mainly Jahn-Teller elongated Cu(II) complexes.

Metal imidazole and imidazolate systems

For systems that contain a five-membered heterocyclic ring with two nitrogen atoms, coordination of the uncharged imidazoles (A and B in Figure 5) occurs *via* the lone pair of electrons on the nitrogen at position 3. We found no significant difference in bond length (2.01 Å for both species) between imidazole and imidazole substituted with a carbon (dashed grey and grey curves, respectively, in Figure 15). The charged imidazolate systems, which bridge two metals, have a slightly but significantly shorter average bond length (1.99 Å).

The reduction is approx.imately 0.02Å but as there are 2 Zn-H bonds in these structures, this bond length decrease is of the same magnitude as for the systems described above.

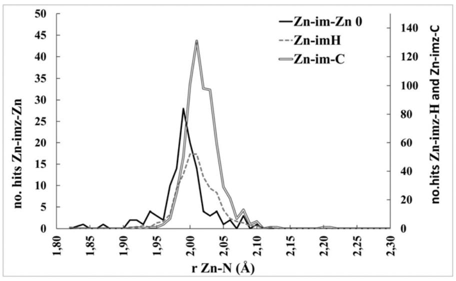


Figure 15 Zn--N distances for four-coordinated zinc imidazole (left *y*-axis) and imidazolates (right *y*-axis). For the imidazolates that bridge two metals, there are two (in some cases it is slightly different) Zn-N distances for each structure, although these have the same profile and have been summed (number of hits plotted on the left *y*-axis).

Triazole systems

The triazoles, which contain three nitrogens, can coordinate one, two or three metal ions (see Figure 6). Copper-co-ordinating triazole systems were commonly noted in our retrieved dataset, and the bond lengths for these systems are shown in Figure 16. These data are more difficult to interpret due to ambiguity with regard to the charge of the bridging 1,2-Cu-triazoles and the fact that for the triazole systems, numerous Cu(I) compounds are present.

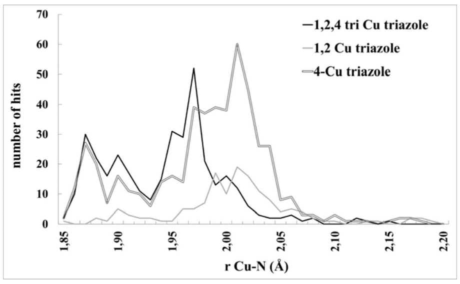


Figure 16 Cu—N distances of copper triazole compounds for mono, di and tri coordinated triazole. The peaks at 1.87 Å correspond to three-coordinating Cu(I) (and a few three coordinated Cu(II)) and here there is no difference between charged and uncharged ligands. Cu(II) and higher coordination numbers are found at longer distances 1.97 (charged) -2.01 Å (uncharged)

From the extraction of a sample of structures with bond lengths of around 1.87 Å, it is clear that the origin of this peak is Cu(I) complexes that coordinate three ligands rather than Jahn-Teller distorted Cu(II) complexes with some shorter bond lengths. In the dataset, we also find that for Cu(II) with higher CNs, there is a bond length difference of 0.04 Å between the charged (1.97 Å) and uncharged ligands (2.01 Å), as also noted in the previously investigated systems.

Comparison to pyridine systems

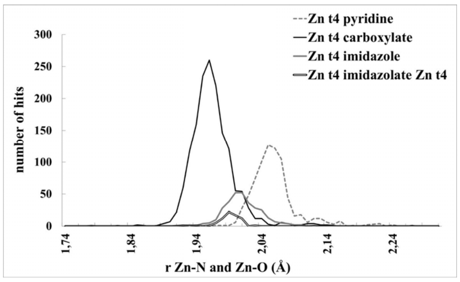


Figure 17 Zn—N and Zn—O distances for four-coordinate Zn-imidazole, Zn-pyridine and Zn-carboxylate compounds from the CSD

As the pyridines (Figure 4) have no suitable anion for comparative purposes, we instead looked at the influences of two different neutral aromatic ligands that bind to nitrogen: pyridine and neutral imidazole, and we also compared these to the imidazolates and carboxylates. Figure 17 reveals the Zn-N and Zn-O distances for four-coordinated Zn(II) bound to pyridine and imidazole or bound to imidazolates and carboxylates. Comparing neutral pyridine to neutral imidazole (2.05 Å and 2.01 Å, respectively) we note that the difference in bond length is of the same magnitude as that between anionic ligands and neutral ligands. That the pyridine group is slightly more sterically demanding may be the simplest explanation for this difference.

The large difference in bond length (0.09 Å) between the carboxylate and pyridine systems may also reflect a steric effect caused by the bulky pyridine ligand.

Studies of conceptual understanding

This section contains data from the studies on conceptual understanding of chemical bonding that were performed at Chalmers University of Technology, the University of Cape Town, and in various Swedish upper-secondary schools during the period 2012–2014. The work is detailed in the attached manuscript titled *Teaching of chemical bonding, Success or failure?-A study of Swedish and South African students' conceptions of bonding.* (Paper 2)

Students' conceptions of bond energetics

We asked the students to choose one option from among the three or four statements listed below, to allow us to probe their thinking about the energetics of breakage and formation of single bonds.

What is true about bond energetics?

A	*It takes energy to create a chemical bond from single atoms!*
B	*When a chemical bond is formed, energy is liberated!*
C	*It always takes energy/work to break a chemical bond!?*
D	*Sometimes energy is released and sometimes it takes energy to form a chemical bond! (CH14 only)*

Several studies have previously been conducted in this field. The paper *Students' understandings of chemical bonds and the energetics of chemical reactions* published by Boo (1998) gives good examples of the type of misconceptions that can be present in an ordinary group of students.

Figure 18 reveals that bond energetics remains a problematic field, in that the Swedish and South African students clearly have misconceptions regarding the energetics related to the formation and breakage of a single bond.

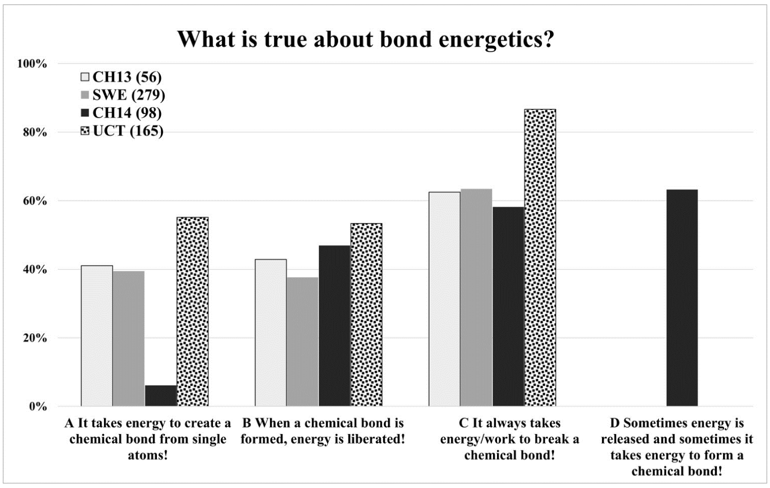


Figure 18 Survey of student responses regarding bond energetics. All the student groups were presented with three statements. Statements B and C are true. Frequencies calculated as % of number of respondents. The fourth alternative was only included for the CH14 group.

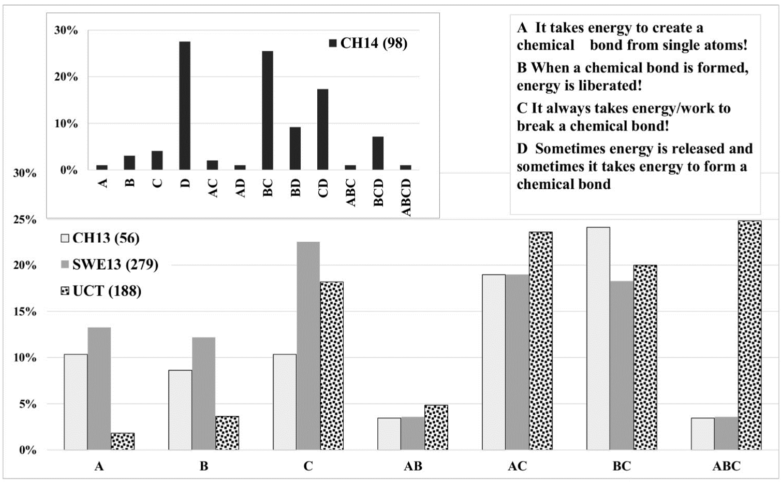


Figure 19 Single or combinations of statement choices for the question "What is true about bond energetics?" Answers containing statement D were only collected in the CH14 follow up after 2/3 of a year of tertiary chemistry (insert). Correct combination is statements B+C.

In the data derived from combining choices of statements (Figure 19), we find that the proportion of students who chose the correct combination of B and C for any of the groups is 18%–26%, indicating that few students have a clear grasp of bond energetics. Overall, the students are more familiar with the fact that energy is required for breaking a bond than with the fact that formation of a bond always releases energy. More than 60% of the CH14 group chose alternative D (Figure 19) as one of their statements.

Teaching aspects of bond energetics

There is a marked difference in the ways in which basic bond types and the explanations for bonding are presented in the Swedish textbooks compared to the textbooks from South Africa. A diagram showing the change in potential energy (Morse potential) during bond formation (Figure 1) is used as the basis for describing bonding at several points in the South African curriculum and in the South African textbooks, whereas it is neither mentioned nor used in the Swedish curriculum or textbooks. The South African curriculum specifically states that teachers should emphasize that the main reason for bonding is the increased stability due to a potential energy minimum at a given internuclear distance. No such guidance regarding stability and potential energy is given in the Swedish syllabus or textbooks. Swedish chemistry teachers usually do not use this type of diagram when they introduce chemical bonding.

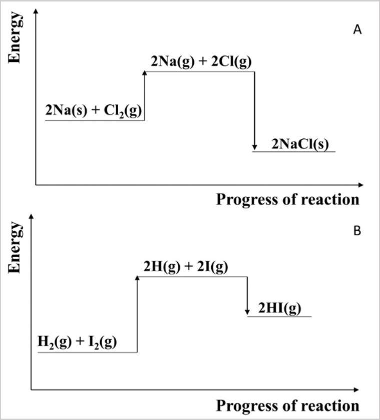
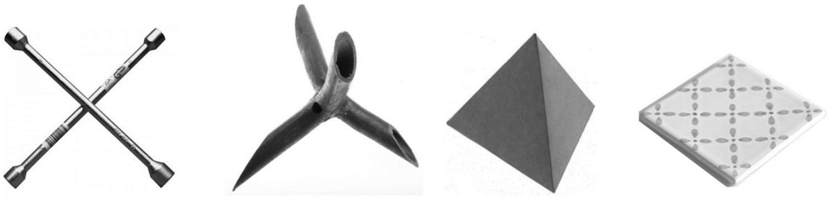


Figure 20 Examples of Energy diagram used for visualising energetics of breaking and forming of bonds.

The typical way in the Swedish teaching tradition for connecting chemical bonds to energetics is through the use of Born-Haber-type diagrams, which depict atomisation of reactants and the subsequent energy release as the new bonds form (Figure 20). Several of the Swedish textbooks use these diagrams to illustrate bond energetics. These diagrams are generally missing from the South African books. Instead, the South African curriculum and textbooks emphasise that energy is released when an individual bond forms, and that energy is absorbed when an individual bond is broken. These written definitions are usually less obvious in the Swedish textbooks, and the students are often left to figure it out for themselves from the diagrams supplied.

In terms of definitions of bond energy and bond length, only one of the Swedish books states a definition of bond energy and/or bond length, while the South African curriculum and textbooks for the most part (see Appendix T 1) utilise the Morse potential curve (Figure 1) to define both bond energy and bond length.

Students' geometrical representations of CH_4



Wheel spanner **Caltrop** **Tetrahedron** **Ceramic tile**

Figure 21 Real life objects used to probe the students awareness of geometry in methane

The following question was posed to probe students' understanding of the shape of a molecule, namely methane.

If you were to photograph a methane molecule, which of the representations above *would be the closest to the actual shape?* (Figure 21).

Figure 22 shows that most of the students demonstrated a firm grip of the 3-dimensionality of molecules, i.e., they choose either the caltrop or the tetrahedron.

We note that some groups showed a clear preference, as evidenced by the sharp points in the graphs. The CH13 group favoured the caltrop, while the CH14 group preferred the tetrahedron. The students from the upper-secondary school in the SWE group showed no specific preference for any representation. The UCT group was similar to the CH14 group in terms of their choice of representations.

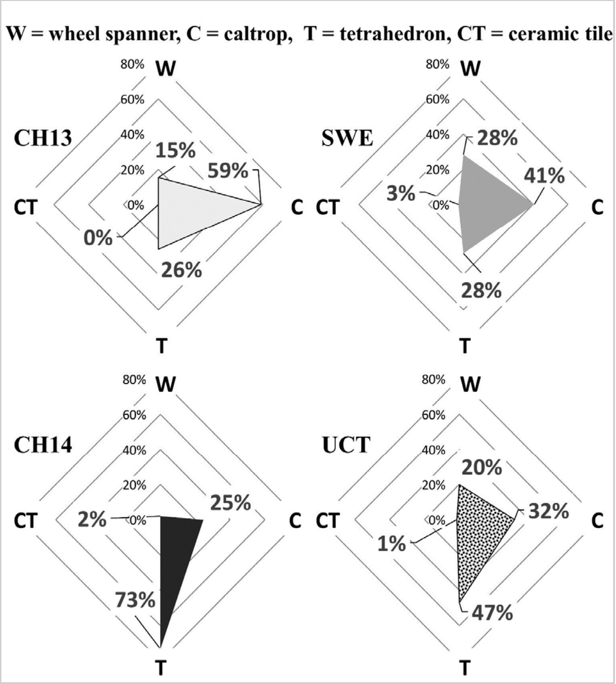


Figure 22 Graphical view of student responses to the question: If you were to photograph a methane molecule, which of the representations above would be the closest to the actual shape? *The sharpest point in the figure indicates the most preferred representation, a blunter shape indicate less preference for any given representation.*

The use of visual representations, i.e., ball and stick or space-filling models, differed greatly between the Swedish and South African textbooks (See Appendix T 2).

The South African textbooks are much more limited with respect to the use of illustrations, using less than half the number of visualisations displayed in the Swedish textbooks. In the Swedish textbooks, we also noted a shift from the mainly ball and stick models in the old curriculum Chemistry A (Andersson, Sonesson, Stålhandske, & Tullberg, 2000) towards more space-filling models in the textbooks for the new curriculum Chemistry 1 (Andersson, Sonesson, Svahn, & Tullberg, 2012; Pilström et al., 2011). In the South African textbooks, apart from the Everything Science by Siyavula, the dominant model representation is the ball and stick-type.

With respect to the overall use of illustrations in the textbooks, the difference is even greater. The Swedish textbooks have at least one illustration on each page, with the illustrations being anything from pictures, visual models to drawings of molecules and atoms in anthropomorphic (Bergqvist et al., 2013 p.594) or animistic settings. The exception to the highly restricted use of illustrations in the South African textbooks is the Oxford Successful series. This book is similar to the Swedish textbooks in terms of the number of illustrations that it contains, although is still much more restrictive in the representational modes employed.

The Swedish books frequently use anthropomorphic or animistic representations, whereas the South African textbooks refrain from using these types of visualisation.

All the textbooks to some extent introduce and try to visualise the three-dimensionality of chemical compounds. This is mainly achieved through ball and stick and space-filling models, which are sometimes inscribed in geometrical shapes, e.g., a tetrahedron for methane. The foundation for these representations is the Valence

Shell Electron Pair Repulsion (VSEPR) theory, but it is only in the South African textbooks that this theory is both introduced and explained. The theoretical background is missing in the Swedish textbooks, where only the result is displayed and used with no further explanation.

The use of ball and stick models predominates in the actual teaching situations in Sweden, due to the fact that most chemistry model kits are of this type. One of the respondents in the interviews described the learning situation as follows: *"We mostly worked with ball and sticks, when we had things to test by ourselves"*. The use of models in schools is more limited in South Africa than in Sweden, due to the cost of prefabricated model kits. According to an experienced South African teacher and researcher, only about 500 upper-secondary schools out of approximately 6500 have any kind of model kit available to the teachers for use in the classroom. To compensate, it is recommended in the curriculum to make use of play dough and toothpicks or similar materials to construct 3D models of molecules and compounds. Even if the approaches and the types of models used differ, both the Swedish and the South African groups are highly familiar with the three-dimensional nature of chemical geometry.

Student's descriptions of the methane molecule

In these open-ended questions, the students were asked to answer in a comprehensive manner the following two questions:

> *Describe in detail how the carbon atom and the hydrogen atoms are held together in the methane molecule!*
>
> *Describe in detail in which region you would find the different electrons in the methane molecule.*

From an initial analysis of the responses obtained to the first question (Figure 23), it is clear that the covalent framework is firmly set in the minds of all the students, with few students seeing the bonding as being ionic or intermolecular. The way in which the covalent framework is described reveals a large difference between the Swedish and the South African students. Most Swedish students (50%–65%) (CH14 excluded) used the general bond description or the simple covalent model, with answers such as: "*They are covalently bonded by the means of single bonds*". While the UCT students usually included some conceptualisation, such as: "*By sharing of electrons via covalent bonding*", their answers were often a lot more advanced (Category 2 or 3). In terms of specific concepts (Figure 24), it can be noted that the Swedish groups mostly based their discussions on the use of full shells, while the South African students used more specialised concepts, such as electrostatic interactions and orbital theory. When the results for CH13 and CH14 are compared, it becomes evident that a large shift in conceptual advancement occurs during the first term of higher-level chemistry education. In the initial survey, no student in the

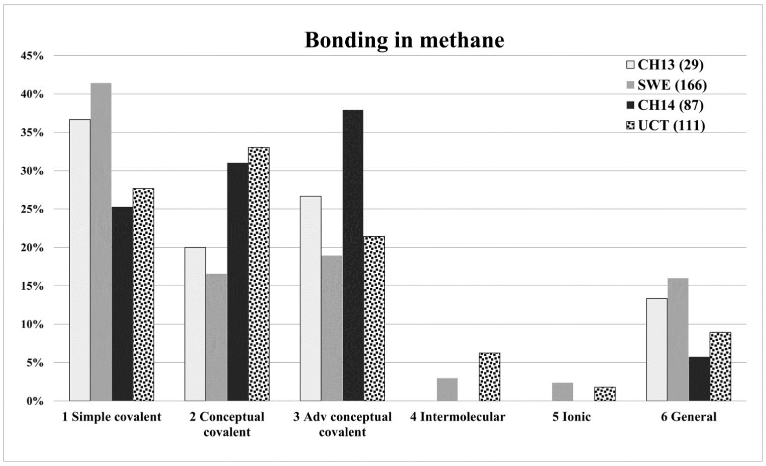


Figure 23 Categorized open ended answers used by the students to explain the bonding in methane

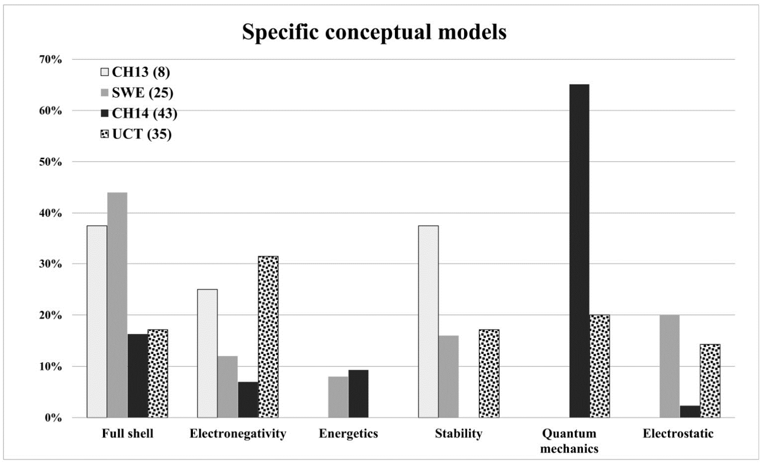


Figure 24 Students' use of more advanced conceptual models when explaining the bonding in methane. The number of respondents in the CH13 group is small and these data must be considered carefully.

CH13 group used orbital or quantum concepts (Figure 24), whereas in the CH14 group, already after one term of tertiary chemistry these types of explanations had increased to almost 70% of the answers using specific concepts.

In the second question (Figure 25), students were asked to describe the whereabouts of the electrons in the methane bond. All groups clearly favoured the localised bond model, i.e., saw the electrons as being held between the atoms. Just as in the first question, the answers were sorted based on specific concepttualisations. For this question, the three categories of probabilities, electro-negativity, and orbitals emerged from the students' answers (Figure 26). A few students discussed how the two electrons completely surround the two atoms, describing some kind of molecular orbital. These students also stated that the electrons most probably are found in between the atoms. More of the South African students used more advanced conceptualisation than the students in the Swedish groups. Among the three groups (CH13 was excluded) in which the number of respondents made it possible to analyse trends, electronegativity was the most used conceptualisation in the SWE and UCT groups.

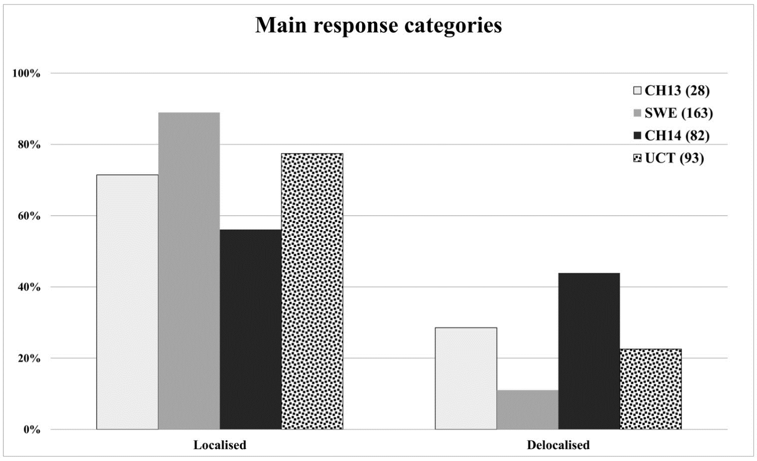


Figure 25 Main category answers used in the explanation of electron localisation in methane. Answers stating electrons as being held in the bond / the area in between the atoms or in atomic orbitals were categorized as localised.

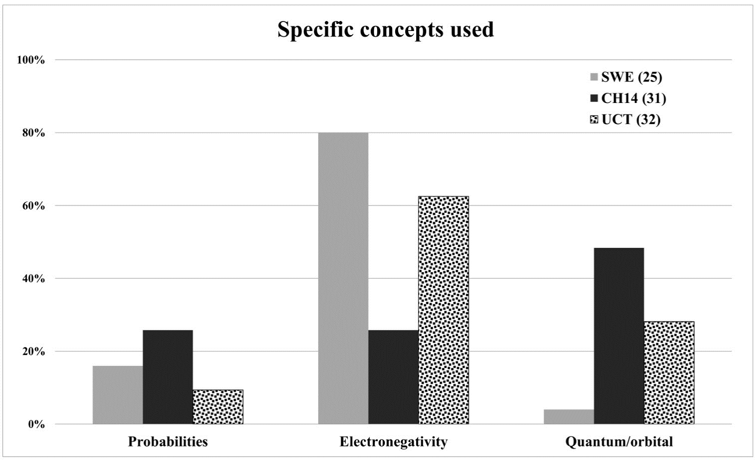


Figure 26 The three recurring specific concepts used to explain the localisation of the electrons in methane. Calculated as percentage of answers of these types. CH13, from which only four students responded, is omitted.

In the Swedish curriculum for Chemistry A, the following sentence is the complete description of the learning outcomes of the chemical bonding section in upper-secondary school chemistry: *"Be able to describe how models of different types of chemical bonding are based on the atom's electronic structure and be able to relate the properties of elements to type of bonding and its strength, as well as to the structure of the element"* (Swedish National Agency for Education, 2000, p 56). The current Swedish curriculum uses the same brief descriptions for the bonding content of the course: *"Models and theories of the structure and classification of matter. Chemical bonding and its impact on e.g., the occurrence, properties and application areas of organic and inorganic substances*" (Swedish National Agency for Education 2010). The South African NCS curriculum (Department of Education, 2006) is much more detailed in defining the learning outcomes for the covalent bond but omits the metallic and ionic bonds. The exclusion of these bonds from the NCS curriculum is also evident in some of the textbooks, where "Physical Sciences Explained" omits metallic bonding and the "Spot On" series excludes both ionic and metallic bonding. All other analysed South African books include all basic bond types, regardless of coverage in the NCS.

In Appendix T 1, it can be seen that the Swedish Chemistry books commonly start with the ionic bond, followed by the covalent bond, and lastly the metallic bond. The South African books start with either the covalent or the metallic bond. It can also be seen in the same table that all the South African books introduce the dative bond, which is omitted from the Swedish books.

How the chemical bonds are introduced and modelled varies between the textbooks (Appendix T 1). The South African NCS curriculum emphasizes that bonding should be explained in the following way: "*A chemical bond as the net electrostatic force two* *atoms sharing electrons exert on each other*" (Department of Education, 2006). Shared valence electrons and the octet rule constitute the main explanation for covalent bonding in all the textbooks. Three of the Swedish textbooks mention that the electrons reside in a shared electron cloud surrounding the molecule. Siyavula Everything Science (2012) takes the explanation further and uses the concept of overlapping orbitals that form molecular orbitals responsible for bonding instead of the shared electron clouds. In the Study and Master series, even more detail is given, as it uses hybridisation of atomic orbitals to explain bonding and geometry.

In a few Swedish textbooks, there is a short extra-curricular section in which atomic orbitals are introduced, although most of the books omit even this brief introduction. If the topic is covered at all, the level of detail is much less than that presented in the South African curriculum. The focus in the South African textbooks when describing the ionic bonding is on the octet rule and the subsequent transfer of electrons as the atoms acquire a full octet for their ions. Two of the Swedish books (Henriksson, 2011; Pilström et al., 2011) clearly describe an electrostatic model to explain ionic bonding. These two books also clearly separate ionic bonding from the formation of ions. The two books by Andersson et al. (2000; 2012) indicate that ionic bonding is connected to the transfer of electrons to complete the octet rule.

South African textbooks that mention the ionic bond generally employ Lewis dot diagrams, electron transfer, and the subsequent charge attraction as the foundations for the ionic bond. The discussion of ionic bonding invariably takes its start-point from the perspective of single atoms or ions, followed by an introduction to the crystal lattice. None of the textbooks from either curriculum explains how to interpret the depicted lattice model in terms of bond interactions, and only one book emphasises that the bonding is non-directional. The common representational choice in all books is to depict the crystal lattice with ball and stick models.

That the different ways of describing and explaining ionic bonding might yield very different results is my observation from teaching situations. Students who have been taught ionic bonding through the octet framework and electron transfer struggle to understand why silver chloride precipitates when sodium chloride and silver nitrate solutions are mixed together. This confusion is visible in the following discussion about precipitation, documented during a practical activity:

Student A: "*What makes them stick together?.... I mean they both already have full octets!"*
Student B: *"No idea!... No electrons are transferred! Is it a salt?..... Silver is +1 and chloride is -1, I know opposites attract but why these two and not the others?"*

Students' views of ionic bonding and lattices

The two-tiered question below was used to probe student understanding of ionic structures and bonds.

Potassium chloride exists in the form of molecules! True or False!

A The potassium atom shares a pair of electrons with the chlorine atom to form a simple molecule!
B After donating its valence electron to the chlorine atom, the potassium ion forms a molecule with the chloride ion!
C Potassium chloride exists as a lattice consisting of potassium ions and chloride ions!
D Potassium chloride exists as a lattice of covalently bonded potassium and chlorine atoms!

Figure 27 (inset) shows that most students have the view that potassium chloride is molecular in its build-up. Among the students who believe in molecular KCl, alternatives A and B are common explanations. The upper-secondary school group SWE prefers statement A, indicating adherence to the covalent bond model. The mental models of the CH13 and UCT groups are slightly more advanced and recognize the constituents of KCl as being ions, although they still adhere to the covalent bond model and probably associate electron donation with a pairing of ions. The paired ions are then seen as a molecule. The number of students in the CH14 group who believe in the molecular framework is not significantly lower than it was prior to their bonding studies, although there is a large shift towards explanation C. This indicates that the molecular framework is difficult to influence, and that it is retained in the sense of molecular paired ions/atoms even if the students accept the fact that crystals of KCl form an ionic lattice.

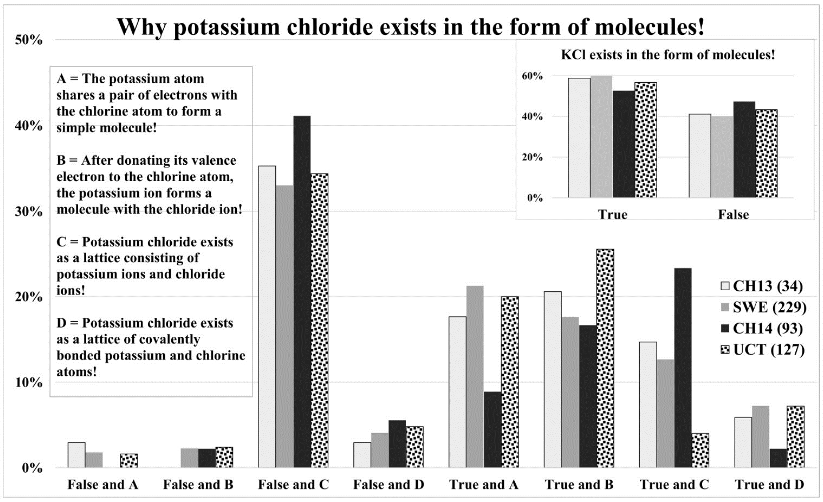


Figure 27 Answer combinations for molecularity of salt, calculated in relation to number of respondents. The phrasing of the alternatives is shown in the picture. Numbers in parentheses in the diagram relate to total number of respondents. CH13 and CH14 are the same student group separated in time.

That the students to a large extent confuse the molecular and ionic models became readily apparent during the interviews with six students from the CH13 group. To help them visualise the build-up of sodium chloride, they were shown a ball and stick picture of the ionic lattice. All of the students had trouble identifying and describing the bonding inside the crystal lattice. Table 4 summarises the outcomes of the discussions. All the students struggled to some extent with describing the bond that holds the lattice together. Most of the students used the term ionic bonding, although only half of the students described the bonding in terms of charge attraction and repulsion between the ions. One student described the bonding as a "*magnetic attraction between the ions.*"

Two students used a mixed or purely covalent model, i.e., mentioned shared electrons.

Table 4 Summary of interview results for the ionic bonding section

Student	States bonding in NaCl described as being:	Explanation for the bonding in NaCl	Bonding is seen as unidirectional	Confuses formula unit with a molecule (indicates covalent bond)
A	Ionic	Charge attraction	Yes	Yes
B	Ionic	Mixed shared electrons and charge attraction	Unclear	Yes
C	Unspecified	Shared electron pair	No	Yes
D	Ionic	Magnetic attraction between the ions	Yes	Yes
E	Ionic	Charge attraction	Yes	Yes
F	Ionic	Charge attraction	Yes	Yes

The non-directionality of the ionic bond is not clear to the students, as evidenced by the response of student C:

***I*-** *What is it that keeps a single chloride ion together with these six sodium ions?*
S- *No idea!.. According to the picture the sodium has given away three or four looking at the side of the crystal!*
***I*-** *If you look at this central chloride instead, does it clarify things?*
S- *No idea, nothing of what I have said makes sense!*

The model in the picture was itself regarded as confusing, and the students interviewed displayed the same bewilderment about schematic representations in figures of a lattice, such as the one previously reported by Coll and Treagust (2003a).

When asked: "*What do the lines in the picture mean?*" Student C revealed her uncertainty by replying: *"Aren't those the bonds? In between the atoms!"*

Finally, it is clear that all the interviewed students had misconceptions that made them associate a formula unit with a molecule. Examples of these misconceptions can be seen in the short excerpts from the interviews below. Additional excerpts are provided in Appendix T 3.

Student B

I- *What type of bonding is there in the formula unit?*

S- *Ion-ion*

I- *Would you call it a molecule?*

S- *Yes*

I- *Why?*

S- *because... want to find an explanation without any loop holes.. but yes 2... A molecule is 2 or more atoms that interacts, that binds each other.*

Student E

I- *What is the smallest unit in the crystal?*

S- *NaCl*

I- *What would you call this smallest unit?*

S- *a formula unit*

I - *Would you call it a molecule?*

S- *Yes, in the upper-secondary school I actually would, we didn't differentiate between molecules and ionic compounds, this is something I picked up in my new chemistry book in the "preliminary chapter" a formula unit, we had a lesson with so to speak a support teacher here at the university , where I asked what a formula unit was. He had to look it up, he was that unsure about it... So.. In the upper-secondary school I would absolutely have called it a molecule!*

Discussion

Model understanding in science and education

It is interesting to note that the models that are currently used to describe chemical bonding are the theories presented by Lewis, Pauling, Hund and Mulliken almost a century ago. That these models, after revision and refinement, are still the best tools available is testament to their explanatory powers. With the help of computers, the modelling capacities of the molecular orbital theory and, perhaps especially, that of the VBT have been greatly increased. Currently, scientists use computer-generated electron density simulations to predict and depict bonding and reactions in compounds of interest. Nevertheless, decisions as to which variables to use are decided by the human intellect. Therefore, now more than evener, it is crucial to have a firm understanding of the fundamental principles of chemical bonding. In this thesis, we show that each individual creates their own mental model of how a concept, such as chemical bonding, is understood.

While exploring the mental models of chemists is not the primary goal of the present work, it is possible to extrapolate from studies in the literature and the work done on students' mental models that in general, research chemists do not share a singular set of mental models. Although the general bond models are probably relatively congruent from chemist to chemist, they entail various modes of internal conceptualisation that are sometimes at odds with the current scientific model. This is not always negative, since this capability of the human mind to use previous experiences and prior knowledge to build a coherent mental model is what drives scientific endeavour forward. Without these different individual mental models there would be no critical questioning of the current theories and paradigms.

Interpretations – ways to model systems

It is shown in this thesis and has been shown elsewhere (Coll & Treagust, 2003b; Vosniadou, 1994) that incorrect mental models can be very difficult to change once they become established. Thus, it is crucial to give students as correct an understanding as possible. To accomplish this, the teacher must be aware of the current mental models held by the students. Furthermore, the teacher must have knowledge of the mechanisms underlying the creation of a mental model. Only if these two conditions are fulfilled is it possible for the teacher to help the student to build a correct framework. A correct framework is in this context defined as a framework that is aligned with current scientific knowledge, which can serve as a firm foundation for a continuous learning process. The mental models of scientists are have spurred intense debates and contesting theories. We have investigated and tried to resolve one such debate, in which the main issue relates to the description of the coordinative bond, by examining bond length data from the CSD.

Ligand systems- do they differ in bond strength?

Our findings based on model systems (Figure 12) indicate that there are no significant differences in bond strengths, measured as bond lengths, between metals that coordinate anionic ligands and metals that bind neutral ligands.

In investigating these systems, many different aspects, apart from ligand charge, influence the measured bond lengths. The CNs of compared species need to be considered, since a lower CN has been shown to correlate with shorter bond lengths. Another factor is secondary coordination by Lewis acids, such as H^+. One way to quantify these effects on bond strength is to calculate the valence of the metal-ligand bond.

In all the investigated systems, we found the bond length to be 0.02–0.05 Å or (1.0%–2.5%) shorter when the ligand became charged. The included data were chosen to be as free of ambiguity as possible.

In terms of the calculated bond valence (Equation 1) for the imidazole systems, the smaller difference in bond length corresponds to a bond valence difference of 0.029. We can compare this to formal bond valence theory in which the Zn-Im-Zn should have a bond valence of 0.5.

$$v = e^{\frac{R-d}{b}}$$

Equation 1 A general and broadly accepted equation for calculating bond valences from bond lengths, where R is the experimental single bond length and b is the Brown Altermatt constant b = 0.37 Å. A bond length of >3.5 Å corresponds to a valence of close to zero.

The difference in formal bond valence between a charged and an uncharged ligand is much larger than the difference calculated from actual bond length data. This large discrepancy between the calculated and formal bond valences indicates that ligand charge alone cannot be used as a tool for determining bond strengths. The bond strength may also be influenced by back bonding between the metal and the ligand. Brown has argued that even though the calculated Ru-S bond in dimethylsulfoxide)pentaammine-ruthenium(II)hexafluoridophosphate (DMSARU) has a weak bond valence (v=0.22), the bond is rather strong due to back-bonding effects between the ruthenium and sulfur atoms (Brown, 2002).

Another factor of importance when comparing bond strength is the shape and structure of the ligand. We have shown that a sterically hindered ligand can produce bond length differences comparable to the differences in bond length observed between charged and uncharged ligands (see Figure 17).

In the present study, we do not see definitive support for the strict categorisation of network forming coordination compounds into less stable coordination polymers and stable metal-organic frameworks. Undoubtedly, there is a difference. However, the bonding is not so dissimilar that it should be considered to be of two types. Instead, the charge effect can be regarded in the same way as in the case of charge-assisted hydrogen bonding (Braga & Grepioni, 2000; Son, Reingold, Carpenter, Czech, & Sweigart, 2006).

Visualization –effects of the model systems

The disputes based on different scientists' mental models are external conflicts that can be possibly resolved by objective research. Addressing the problem is more difficult when different models clash in the mind of the individual.

To understand more fully the confusion that can arise from these internal mental models, we have to go back to how models are introduced and used in the school curricula.

Today, the electrostatic bond model and Lewis 100-year-old bond model are the most commonly used descriptors at the secondary school level.

In some instances, the models described above are augmented with atomic orbitals to explain the rule of two or eight. Less commonly, simplified versions of valence bond theory VBT or molecular orbital theory are used to explain bonding at the secondary school level.

At the tertiary education level, students are introduced to molecular orbital theory as part of the discussion on diatomic molecules and hybridisation (VBT) in the context of bonding in hydrocarbons.

The students have a very limited understanding of atomic build-up and chemical bonding when they arrive in the upper-secondary school. The *aufbau* principle and the introduction of the chemical bond are greatly simplified in the Swedish lower-secondary school (grades 7–9), and the situation is only marginally better in the upper-secondary school. The foundation for teaching about bonding in grades 7–9 mainly entails over-emphasis of the Bohr model adapted to multi-electron atoms and the octet rule. In some instances, a further adaptation of the shell model is used, one that is inconsistent with the main energy levels (principal quantum number). The original Bohr model is based on the principal quantum numbers and is thus true in this aspect. In the case of the incorrect model, the students are taught that the shells can hold the following numbers of electrons: 2:8:8:18. The adaptation is designed to be consistent with the octet rule and the first four rows of the periodic table of the elements. It neatly avoids having to explain that the higher shells are interlaced. This model does not make sense from any perspective apart from the octet rule and the 4 periods, and it fails to serve as an explanation for atomic properties, such as those of the transition metals.

Throughout the upper-secondary school, the Bohr model is the preferred framework in Swedish textbooks, with all textbooks including a short discussion of shells not being shells, but rather that they should be seen as electron clouds, within which the electron is randomly localised. This is the only concession made towards a more advanced atomic model.

Another difference between Sweden and South Africa is that there is very little discussion in the Swedish curriculum on what a model is and on the use of models and their limitations. The Swedish textbooks often present models in a way that can be interpreted by the students as being true, rather than as the currently best way of describing a very complex situation whereas the South African are more consistent in describing them as tools to envision the concept.

It has been shown that students need to be aware of what a model is in order to be able to understand and use it (Harrison & Treagust, 1996). Introducing a model without explaining its origin and its limitations carries the risk of creating misconceptions. Some of these misconceptions, which are due to failures to understand the limitations of models or stem from conflicting models, will be discussed below.

Molecular geometry

The preferred models for visualisation of a methane molecule by the sample groups are shown in Figure 22. The Swedish groups, apart from CH14, favoured the caltrop, while the South African UCT group showed a preference for the tetrahedron.

This is a good example of how the models used in teaching situations influence the creation of a mental model. If the students are subjected primarily to one type of visual model, this model becomes ingrained in the mind of the student, where it is manifested in the mental model of that individual.

In the Swedish upper-secondary school curriculum, the main model used for visualising molecules is the ball and stick model. It is widely used in practical learning situations and in the textbooks for the Swedish and South African curricula. (see Appendix T 2) The use of space-filling models in practical learning activities is a lot less common, so in essence, the Swedish students only use ball and stick models.

In contrast, in South Africa, prefabricated model kits are uncommon and the textbooks contain fewer visualisations, only employing them when they are necessary to highlight or clarify a topic. The Swedish textbooks on the other hand have an overzealous belief in the proverb *"a picture is worth a thousand words"*, in the sense that there exists a multitude of visualisations. The feeling that is conveyed is that illustrations are added to make the book look more appealing, i.e., visualisations are added without any reflection regarding the effect of the representation.

The lack of ready-to-use models and the scarcity of representations in the South African curriculum and textbooks may have a positive side, since it allows the teacher to place more emphasis on the space-filling aspects of atoms and molecules in the learning activities. It is probably also beneficial that the South African students are required to construct their own real-life "mental models" of atoms from play dough etc., as this may help the students to understand better the roles of models in chemistry.

Another difference between the South African and the Swedish curricula is the emphasis on the VSEPR theory in the former and the lack thereof in the latter. The UCT students who have been subjected to the VSEPR theory during their upper-secondary school education show a much higher preference for the tetrahedron than the Swedish students whose secondary chemistry education had fewer examples of the VSEPR theory. This finding is supported by the preference for the tetrahedron demonstrated by the CH14 students, who during their first semester at the University were given a rich introduction to Lewis dot formulas, VSEPR theory, and the geometrical shapes that follow from this.

From the data, it can be argued that the curriculum for Chemistry (Swedish National Agency for Education2000, 2010) taught in the Swedish upper-secondary school promotes of the notion that molecules and compounds resemble in shape the ball and stick models (e.g., CH13 in Figure 22).

Bond energetics

Confusion about models is probably one of the reasons that students have problems are uncertain as to whether energy is taken up or released when a bond is formed. All the groups displayed misconceptions (Figure 19) about the energetics coupled to the breakage and formation of bonds. Most of the students (all groups) marked as true statement C: "*It always takes energy/work to break a chemical bond!*" This means that the majority of students correctly understand that bond breaking is associated with an uptake of energy, whereas fewer students realise that bond formation releases energy. The uptake of energy associated with bond breakage is intuitive and can be visualised in macroscopic everyday life, in that energy is required to tear up something. The energy release of bond formation is harder to visualise. In the media today there is a lot of discussion of high-energy compounds, such as sugars. The naïve logic of this is that you need to pump energy in to a compound to make it "energy-rich".

The formula for the biological origin of sugars in photosynthesis is probably one of the few formulas that students recognise:

$$\mathbf{6CO_2 + 6H_2O + energy\ (h\nu) \rightarrow C_6H_{12}O_6 + 6O_2}$$

A student who reads this formula easily deduces that to make the bonds in the sugar you need an input of energy. This everyday biological framework for "energy-rich" molecules obviously clashes with the scientifically correct framework of bond formation releasing energy.

The teaching of chemistry in Sweden relies heavily on Born-Haber type energy diagrams (Figure 20) to visualise bond energetics. These diagrams distinguish between the creation of the high-energy reactive atomic or ionic species (by breakage of old bonds) and the formation of the new bonds and the subsequent release of energy as the new bond is formed. In the South African system, these diagrams are less usual, at least in the context of bond formation; instead, these books employ the Morse potential bond energy curve (Figure 1) to explain the foundation of a chemical bond.

It would seem that the use of the Born-Haber-type diagrams helps the students to resolve the confusing models of the chemical and biological frameworks. The fact that Swedish schools employ to a greater extent these visualisations probably explains why so many more UCT students chose alternative A: "*It takes energy to create a chemical bond from single atoms!*"

The very high preference rate for alternative D *"Sometimes energy is liberated and sometimes energy is needed when a chemical bond is formed"* in the CH14 group (Figure 19, insert) and the choice of the combination ABC by the UCT group reveal that both groups see the release of energy when a bond forms situation-dependent. The origin of this belief lies, in my opinion, in the confusion that surrounds the issues of how energy can be released or taken up in an overall reaction and the fate of a single bond. Clearly, the students cannot separate what always happens when a bond forms from the fact that in the case of an endothermic reaction, energy is taken up and the opposite occurs in an exothermic reaction.

From the data it is evident that only about one in five students in any entry-level university chemistry class in Sweden or South Africa has a correct understanding of bond energetics.

It is my opinion, based on 10 years of empirical classroom observations, that a failure to separate the endothermic and exothermic properties from the discussion of bond formations, together with an unclear explanation as to why some compounds are said to be high in energy are the most important contributory factors to the students' failure to understand properly bond energetics.

Salt or molecule-models of potassium chloride

Another aspect of confusion about models becomes evident when students are asked to describe ionic bonding in potassium chloride. A majority of the students (55%–60%) from all educational levels and curricula had a molecular perspective on the build-up of a salt, i.e., answered 'true' to the initial statement: *"Potassium chloride exists in the form of molecules!"* This question was taken from the *"Chemical bonding diagnostic instrument"* (Tan & Treagust, 1999) and it is noteworthy that the results presented in this thesis in Figure 27 are slightly better than the results obtained in the original study, where close to 80% of the students in an upper-secondary school in Singapore believed in a molecular salt. In the 15 years that separates the two studies, one would be forgiven for hoping that more would have been done in relation to the teaching of ionic bonding in the Swedish and South African curricula to avoid the formation of this alternative framework.The perceived molecular build-up of a salt is closely related to the sequence in which the different bonds and their specific concepts are introduced.

Several studies have explored this issue. Taber (1997) proposed that bonding should be taught with an emphasis on the electrostatic framework starting with metallic bonding, through ionic bonding, so as to end with covalent bonding. Nahum et al. (2010) also proposed the electrostatic framework as the basis for teaching chemical bonding, using the bond continuum as the foundation stone for describing the different bond types. However, Dhindsa (2014) proposed, based on a cognitive approach, that the best sequence for teaching bonding was to follow the order of: covalent; polar covalent; and ionic bonding.

Not just the sequence of the topics, but also the manner in which they are introduced can strongly affect the learning outcome.
The molecular framework can be traced to visual representations of single ions or formula units of a salt. Most textbooks do not emphasise what the formula unit represents, with the consequence that the students come to see them as analogous to molecules, since they appear to resemble simple molecules, such as HCl, CO_2 etc.

In textbooks and when introducing ionic bonding, the starting point is often a single alkali atom that donates its electrons to a halogen. The ions formed are then paired and seen to be representative of the ionic bond. The use of this type of example carries the risk of creating the molecular framework through the association described above. That this is the case for at least some Swedish students is evident from the transcripts of the interviews, as all the interviewed students (Table 4) when asked about the formula unit equated it with a molecule.

We teachers and scientists are unfortunately also major contributors to the creation of the molecular framework, since we often tend to be sloppy when we discuss salts and ions. In lectures, classes, and discussions, I have overheard lecturers, teachers, and students use statements such as: *"This sodium chloride molecule then reacts…*" and other similar examples. Accumulatively, these statements promote the view of ionic compounds as being built up from molecular parts.

That the molecular framework is viewed as being built up from paired ions is evident from the high number of students who gave the answer combinations True and B or True and C. These students are aware that a salt contains ions but do not understand the ionic bond; to them, the only way to make sense of the apparently discrepant information is to pair the ions into "molecules". It is probably inherent to this model that the students fail to see ionic bonding as being non-directional. Instead, it is strictly seen as a bond between the two ions. In the textbooks analysed in the present study, I have found that ionic bonding is not always presented clearly and with the emphasis on the charge attraction and its non-directionality. Instead, many textbooks mix their explanations with the formation of ions and the pairing of ions in the formula unit. These aspects, together with the less than stringent use of phrasing and illustrations shown in the learning situation probably lead to the formation of the "ionic molecular" framework described above.

Students not having the molecular framework tend to also know how a salt lattice is held together, as evidenced by the vast majority making the choice of alternative C. From these answers, it is clear that if the students through learning activities come to know how ionic compounds are held together and learn to differentiate between a formula unit and a molecule, this also helps them to visualise the ionic lattice in the correct way.

It is also important to note that the molecular framework persists even after tertiary-level teaching on bonding (see CH14 in Figure 8). This indicates that the molecular framework is probably established early on and is enhanced through the improper or less-stringent use of schematic models of reactions, oral or written explanations, and visualisations of ionic and molecular compounds in different learning situations. Taken together, these aspects make the alternate framework theory highly resistant to change, which is evident from a comparison of the results for the CH13 and CH14 groups.

The first chemistry course at university level at Chalmers University of Technology clearly fails to decrease the prevalence of aspects of the molecular framework, as there is no significant difference between the CH13 and CH14 groups in terms of their responses to the initial statement. I can only speculate that the situation at the University of Cape Town is similar, based on the high degree of retention of the alternate framework theory revealed in the present study.

In one sense, tertiary-level education seems to be at least partly successful, i.e., in fostering a proper view of the build-up of a lattice. The rate of preference for alternative C increased by 20% during the semester at Chalmers. This trend has also been shown previously by Coll (2003a).

The results for the UCT group are not dissimilar to those for the Swedish groups, which is intriguing because the ionic bond is excluded from the NCS curriculum. It is clear from the results that most South African chemistry teachers employed their pedagogical content knowledge and introduced and talked about ionic bonding in their classes, even if this topic was at the time excluded from the curriculum. It is important to note that the omission of ionic and metallic bonding from the NCS curriculum has been remedied in the new CAPS syllabus (Department of Basic Education, 2012).

In the interviews, all of the students struggled to a certain extent with explaining the bonding that occurs in NaCl, with some stating that it is an ionic bond but explaining it with a covalent bond model of shared electrons. One aspect of this failure to understand how the crystal lattice is held together probably stems from students having the ionic molecular framework described above. Students who employ this framework will also have trouble understanding that the ionic bond due to its mainly electrostatic nature is non-directional and thus, every ion in the salt crystal has several closest neighbours that share the attractive and repulsive forces. Most of the students interviewed displayed just this type of bewilderment.

Another part of the misunderstanding of the ionic bond probably originates from the fact that the representations of lattices used in books and learning activities at the secondary level are seldom thoroughly explained. In most visualisations, ball and stick models are used, and from these it is easy for the student to deduce that each stick is a bond in terms of a shared electron pair, since this is the common description used for the sticks when these models are used in organic chemistry.

Bonding in methane

In the sections above, we underlined the importance of helping students to understand and use a concept. However, what happens when we try to do this but choose inadequate models as the starting point?

The two open-ended questions on bonding probed the ability of students to describe bonding in the methane molecule (Figure 23–26).

In the results, there is a clear indication that the South African students use more advanced concepts to a greater extent than their Swedish counterparts.

It can be argued that the richer foundation given to the South African students in terms of knowledge of the potential bond curve, atomic orbitals, Hund’s rule, Pauli’s exclusion principle, and to some extent molecular orbitals or hybridisation facilitates a larger explanatory toolbox. The UCT group also employs more extensively stability, electrostatic or quantum explanations in explaining the bonding that occurs in methane, as compared with the SWE or CH13 groups. The lack of even the most basic quantum models in the Swedish textbooks and teaching situations clearly puts at a disadvantage those students who are trying to understand the concept of bonding and especially, the covalent bond.

How the students visualise the locations of the electrons in a bond is another interesting aspect that gives us insight into the formation of mental models of bonding. We explored the extent to which a student is familiar with probability clouds or molecular orbitals and how understanding of these concepts affects the description of the whereabouts of the electrons in a bond or molecule.

In Figure 25, we show that most students described the electrons as being localised between the atoms, which is in agreement with the fact that the Lewis covalent model is the favoured model of the upper-secondary school, i.e., the model to which most students are exposed. Three recurring specific concepts were found in the answers, with electronegativity being the favoured explanation for all the groups, except CH14. This is a strong indication that in the minds of the students, electronegativity is firmly associated with the localisation of electrons in a bond. Teachers invariably use electronegativity when discussing polar covalent bonds, which correctly attributes electron localisation to this concept. The question that arises is how much effort is spent in discussing the outcomes of the cases in which the electronegativity is comparable for the two atomic species. In the present survey, many of the students who discussed localisation based on electronegativity did so without knowing that carbon and hydrogen have the same electronegativity, which means that the bond will be non-polar. Orbital discussions were the alternative choice of the UCT group, whereby most of the South African students categorised in the quantum/orbital group discussed electrons as being held in the atomic orbitals. This is consistent with the fact that these students are all introduced to atomic orbitals. The group that showed the highest preference rate for the quantum/orbital model was, unsurprisingly, the CH14 group, with many of the students in this group discussing molecular orbitals, sigma bonds, hybridisations etc.

Admittedly, the number of students who used specific concepts overall was low, and there can be several reasons for the simpler answers given by the Swedish group. One such reason, as argued by Jennifer Trusted (1987) and used by some to explain the drop in Swedish PISA results, is that it takes more effort to produce a good explanation than to give a short answer. She discusses how rewards must compensate this higher effort if good answers are to be expected, and this might be a factor that influences especially the open-ended questions in the present study. However, since this theory should also apply to the South African students to some degree, it cannot be used as the sole explanation for the observed differences.

It is my opinion that there is a real difference in conceptual understanding of covalent bonding between the students in the two countries. The origin of the difference can be attributed to students getting different sets of explanatory tools from the prioritisations in their respective curricula, textbooks and learning situations.

This observation is strengthened by the CH14 students who studied chemical bonding at the tertiary level and thus had been subjected to quantum models etc. The students in this group showed a high level of adaptation to advanced conceptual explanations that contained quantum or molecular orbital concepts, as compared with the other Swedish groups. It has also been argued by Dhindsa and Treagust (Dhindsa & Treagust, 2014) that there is a lot to be gained in terms of understanding chemical bonding by introducing basic orbital reasoning at the secondary level.

Comment on response frequencies

In the data-set the CH13 group consequently have a lower response frequency than the CH14 even though they are the same cohort only separated in time. The main reason for this difference lies in my opinion in the way the surveys were presented to the students.

The CH13 group had a short briefing in a lecture and were then asked to complete the survey through a web link at their convenience. The CH14 group on the other hand were given paper surveys to complete during class, in this group almost all students handed in the survey.

The SWE group probably have about the same response frequency as the CH13 since the manner of distribution was similar. The UCT group is like ways similar to CH14 due to distribution mode.

Implications for teaching

In terms of model use, there is a need to improve the explanations as to why and how we use models. Swedish textbooks have a strong tendency to use a multitude of different visualisations. Visualisations in textbooks should be considered critically, and most of the anthropomorphic and animistic figures should be omitted from the books to avoid creating misconceptions.

To increase students' understanding of the geometry of a molecule, more emphasis should be placed on the space-filling model rather than excessive use of the ball and stick models. Students at the upper-secondary level should also be allowed to learn the ideas behind basic VSEPR theory.

By introducing atomic orbitals, discussing the *aufbau* model, and showing how orbitals can interact, students will gain a better understanding of the bond concept.

Confusion regarding models is likely to arise when ionic bonding is introduced from the perspective of single atoms forming ion pairs, in the absence of a discussion of the difference between a formula unit and a molecule. When introducing ionic bonding it is important to separate the formation of ions from the concept of ionic bonding and to attribute ionic bonding to mainly electrostatic attraction between the ions. The Morse potential bond energy curve can be employed to illustrate this concept.

A specific area that also needs consideration is the three-dimensionality and build-up of crystal lattices.

It is recommended to introduce ionic bonding using a precipitation reaction from the mixing of two ionic solutions, to show that there is no need for electron transfer during the formation of an ionic bond.

Bond energetics is another area in which there are many misconceptions and few clear mental models. Care should be taken not to discuss bond energetics of a single bond in terms of it being exothermic or endothermic, as these concepts relate to an overall process.

It is important to explain and discuss what it means when a molecule is said to be energy-rich in the everyday perspective; the well-known photosynthesis reaction could be used for this purpose. The use of a Born-Haber-type reaction diagram can help to show the release of energy from the separated atoms as the new bond forms.

We see when we correlate answers to grades, where we have these data, indications that two students with the same grade, can have very disparate mental models, the reason for this is probably that in the Swedish curriculum it is very much up to the teacher to choose which topics to teach, and how much time to spend on any specific topic.

Why and how teachers should be involved in research?

It is necessary to point out that in the following section I discuss involvement in research in the sense of Science teachers becoming PhD students.

I propose that the field of research should be a hybrid of pure scientific research and educational research in the teacher's main subject, to optimise the gains for the involved parties.

I will try to discuss the benefits of the hybrid programme in which I have been involved from four different perspectives.

Performing laboratory work, analysing and discussing scientific results, and taking advanced courses certainly deepen knowledge of the subject. If in addition one foot is kept in the field of educational research, the subject knowledge is more easily integrated into the teacher's mental model of the learning of the subject.

A teacher who has forgotten what it is to learn is severely limited in his interactions with students. Through the research programme, the teacher rediscovers the role of the student. Being put in the position of a student gives the teacher a better understanding of the student, which will increase the chance of successful dialogues (Driver & Easley, 1978).

If the teaching is well aligned with results from current educational research the subject will be perceived as more logical, and the risk of scaring off future students will probably diminish. Therefore, it can be said that a teacher versed in educational research will give the student a greater chance of succeeding.

A more knowledgeable teacher with a personal view of a research field has the potential to elaborate more and to open avenues of discussion previously not accessible to the students, thereby stimulating students' interest in a given topic.Teachers with greater pedagogical content knowledge will also be beneficial to the school as a driving force for pedagogical discussions and didactical development, not only in the subject but also across subjects. A second benefit for the employing school lies in the network of contacts at the university that is created through the teacher.

The time spent in the research programme will allow the teacher to revise and rework the learning of the subject.

From the points of view of the individual students and the school at which the teacher works, much is to be gained from the mixing of research fields. But what do the departments at the university gain from this? Apart from the obvious subject of the research performed, insights might be gained into the conceptual frameworks of the students enrolled at the tertiary level. The teacher as a researcher will probably inspire discussions on the topics of teaching and learning and can give clues and direction as to how one can better align the teaching to the learning outcomes and mind-sets of the students.

Conclusion

The modelling of chemical bonding and what it is that actually constitutes a bond is and will probably always be topics that attract divergent opinions. In the case of coordination chemistry, our contribution regarding ligand charge and bond strength indicates that there is no fundamental difference between the bonding of a charged ligand and an uncharged ligand to a central metal atom. We show that the difference in bond length is approximately 2.5% shorter for the charged system than for the uncharged system. This type of bond length elongation can probably be caused by steric effects. In the dataset, there is no significant reason to subdivide network forming coordination compounds into stable metal-organic frameworks and the less-stable coordination polymers.

It is my conclusion that there is a real difference in the conceptual understanding of bonding between the students from Sweden and South Africa in the present study. The origin of the difference can be attributed to the students being exposed to different sets of explanatory tools from the prioritisations in the curricula, textbooks, and learning situations.

The Swedish curriculum has limited success in terms of conveying the foundations of chemical bonding to the students.

As a way of remedying this, I have suggested how to adjust the teaching and visualisations of chemical bonding in the Swedish secondary school curricula and textbooks.

In the present study, there is an indication that the understanding and depth of knowledge displayed by two Swedish students taught by different teachers can be very dissimilar, even if they receive the same grade. It is my opinion that a curriculum similar to the current South African CAPS (Department of Basic Education, 2012) that clearly states which concepts to be covered would probably be a good way to avoid this unequal grading and enhance the overall knowledge of chemistry. It is probably also a good idea to employ a mandatory national test in chemistry, to further limit the variation in grading.

Teachers and lecturers at the tertiary level must be aware that the students they come in contact with often have faulty or incomplete mental models of chemical bonding. The students' understanding and ability to express knowledge of chemical bonding are hampered by the sometimes inadequate explanatory tools available to them. The data indicate that in particular bond energetics, the geometry of molecules, and the build-up of a salt are problematic topics for students.

During my studies in the Licentiate programme for teachers, I have gained insight into research on chemical bonding as pure Science (Nimmermark et al., 2013) and from an educational perspective (Nimmermark et al., 2014). I have vastly increased both my general chemical knowledge and my pedagogical content knowledge and I have had time to reconstruct completely my way of thinking about teaching and learning.

It is my suggestion that if this licentiate programme in the future is offered to new groups of teachers, there should be emphasis on educational research in addition to only basic scientific research.

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Appendix- ***interviews, text analysis and figure rights***

Appendix 1 Questions used in the semi structured interviews with the CH13 students

1. Draw and describe the build-up of a potassium atom.
    1. *What does the circles represent?*
    2. *Is/Are that/those the only place/places you will find electrons?*
    3. *What is the difference between two shells?*
    4. *Why doesn't the M shell fill completely before electrons are placed in the N shell?*
    5. *Are there any other systems for relating information about the electrons surrounding the atom?*

2. What types of chemical bonding do you know of? Explain the differences
    1. *Are there large differences between them?*
    2. *Give an example each of compounds with different bond types*

3. What types of atoms forms covalent bonds?
    1. Explain how the chemical bond arises between the atoms?
    2. *What happens if the shell is full?*
    3. *How does the electronegativity affect the bonding?*
    4. *Where do you find the electrons?*

4. Are there compounds that are pure ionics or pure covalent?

5. Draw a picture of a NaCl crystal and explain how it is composed (show a picture)
    1. *Which are the parts in the crystals?*
    2. *Are there differences in the bonds you've drawn or can see in the picture?*

6. The substances in the middle of the periodic table, what are they called?
    1. *What is so special with them?*
    2. *These compounds can have several ionic charges, why and how?*

Appendix T 1 Text book analysis. Results after reading and correlating textbooks according to the matrix presented in Table 3

Book	Describes and uses molecular orbitals to some extent when describing bonding	Uses the potential bond curve as a fundament for chemical bonding	Order of introducing bond types; I ionic, C covalent, PC polar covalent, DC dative covalent M metallic bond	Describes and uses the VSEPR model	Main descriptive model for ionic bonding	Energy level diagrams describing bond breaking and formation
Swedish curricula and textbooks						
Chemistry A Syllabi	No	No	Not stated	Not stated	Not stated	Not stated
Chemistry 1 Syllabi	no	No	Not stated	Not stated	Not stated	Not stated
Syntes kemi 1	e-clouds mentioned M-bonds explained as common e-cloud	No	I,C,PC,M no DC	not mentioned but the idea is present, mainly in terms of lone pair repulsion	Charge attraction as main model. Both formula unit and lattice depicted and explained.	the energetics part not mentioned together with bonding
Gymnasiekemi 1	e-clouds mentioned M-bonds explained as common e-cloud	No	M,I,C,PC no DC	not mentioned but the idea is present	Electron transfer due to the octet rule as main model. Both formula unit and lattice depicted and explained	2 step energy level diagram
Modell och verklighet	e-clouds	no, but explained in a way that makes it possible to construct the curve	I,C,PC,M no DC	not mentioned but the idea is present	Charge attraction, points out that bonding is directionless, lattice and formula unit depicted.	2 step energy level diagram
Gymnasiekemi A	shared e clouds constitutes the bond	No	I,C,PC,M no DC	not mentioned but the idea is present	Electron transfer due to the octet rule as main model. Both formula unit and lattice depicted and explained	no connection made

South African curricula and textbooks						
NCS Syllabi	no	Yes	only C, PC and DC included M and I missing	yes	none	none
Siyavula gr 10 11 NCS	AO overlap	Yes	C,PC, DC,I,M	yes	electron transfer due to high electronegativity then charge attraction, lattice and formula unit	yes in text no diagram
Physical sciences explained	no	no, but explained in a way that makes it possible to construct the curve	C,I,CP,DC included M missing	yes	electron transfer due to high electronegativity, then charge attraction, lattice and formula unit	yes
Spot on- physical Sciences	no	Yes	C,PC,DC (PC very short one sentence) I,M missing,	yes	excluded IB	yes
Study and master Physical Sciences	yes hybrid orbitals and s and p bonding	Yes	M,C,I	yes	Electron transfer. Both formula unit and lattice depicted and explained	yes Born Haber cycle
Oxford Successful Physical Sciences	No	No	M,C,PC,I	yes	very weak explanation, octet rule based, electrostatic attraction	No

Appendix T 2 Textbook analysis continued. Following the matrix for analysis Table 3

Book	Number of space filling models	% of all model represen-tations	Number of ball and stick models	% of all model represen-tations	Total number of represen-tational models	Shell/Bohr model as main explanatory tool	Qantum models /atomic orbitals as main explanatory tool
Swedish curriculum							
Syntes 1	16	36%	29	64%	45	Yes	1/2 page extra curricular
Gy kemi 1	27	56%	21	44%	48	yes	no
Mod o verk	33	56%	26	44%	59	yes	1 page extra curricular
Gy kem A	16	41%	23	59%	39	yes	No
South African curriculum							
NCS Syllabi						yes	no
CAPS syllabi						yes	yes
Siyavula gr 10 gr11 CAPS	16	64%	9	36%	25	no	6,5 pages
Siyavula gr 10 11 NCS	11	73%	4	27%	15	no	yes 5 pages aufbau, pauli
Physical sciences explained gr10,gr11	4	44%	5	56%	9	yes	no
Spot on- Physical Sciences	2	33%	4	67%	6	no	3 pages
Study and master Physical Sciences	4	44%	5	56%	9	no	7,5 pages +2,5 pages on hybridisation
Oxford succesful Physical Sciences grade 10 and 11	4	36%	7	64%	11	yes short	No only in terms of quantisation of energy

Appendix T 3 Excerpts from the interviews: Students responses to selected questions investigating a molecular view of a salt. **I** =interviewer, S= Student

Student B:

I -If the smallest unit in the crystal is NaCl, how would you describe it and what would you call it?

S -NaCl is a salt two ions, one +1 and one -1

I -What type of bonding is there in the formula unit?

S -Ion-ion

I -Would you call it a molecule?

S -Yes

I -Why?

S -because… want to find an explanation without any loop holes.. but yes 2… A molecule is 2 or more atoms that interacts, that binds each other.

Student C:

I -What is it that keeps the sodium chloride crystal together

S -(long silence) The fact that de have bonded in several directions… three or four different, that it is not just the chloride and the sodium ion, the two of them but that they sit together in a large portion.

I -What does the lines in the picture mean?

S -aren't those the bonds? In between the atoms.

I -Where are the valence electrons in the crystal?

S -Everywhere or are those the bonds?

I -What is it that keeps a single chloride ion together with these six sodium ions?

S -No idea according to the picture the sodium have given away three or four looking at the side of the crystal.

I -If you look at this central chloride instead, does it clearify things?

S -No idea, nothing of what I have said makes sense with this!

I -A single NaCl unit how would they stick together?

S -Since the chloride ion is negatively charged and the sodium ion is positive, they will cancel each other out, so then all there is is sodium chloride

I -And how do they stick together?

S - Well they probably share this single electron that sodium had, so they stick together in the way that they form an electron pair, where there before were a single electron on the chlorine.

Student D:

I -What is the smallest unit in the crystal which still is NaCl?

S -Ok then I must…. Yes if we look at the picture then this must…. If you want this specific structure, then you must have at least….. but I assume it is enough with one molecule, just one Na and one Cl that creates a chemical bond, then there will be others that adds and adds to it, because technically this is a lot of…. It is one sodium and one chlorine that bonds six other chlorides and sodiums so I guess that the smallest unit would be a NaCl.

I -What would you call this smallest unit?

S -A molecule.

Student E:

I -What is the smallest unit in the crystal?

S -NaCl

I -What would you call this smallest unit?

S -a formula unit

I -Would you call it a molecule?

S -Yes in the upper secondary school I actually would, we didn't differentiate between molecules and ionic compounds, this is something I picked up in my new chemistry book in the "preliminary chapter" a formula unit, we had a lesson with so to speak a support teacher here at the university , where I asked what a formula unit was. He had to look it up, he was that unsure about it… So.. In the Upper secondary school I would absolutely have called it a molecule!

I - So the crystal is made up from molecules?

S - Well no it is more so that the whole crystal is one large molecule in the sense that in it the bond is repeated. I mean each .. in each of… I never at all went this deep into it in my previous school there I would if I given it some thought absolutely thought that every chloride ion binds to a sodium ion which binds another sodium ion in all eternity assuming we have a homogeneous crystal, therefore I would have called it a molecule.

Appendix T 4 Figure rights

Figure 7 The different geometries of the atomic d-orbitals.	Adapted from http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Crystal_Field_Theory/Crystal_Field_Theory	under http://creativecommons.org/licenses/by-nc-sa/3.0/us/legalcode
Figure 9 Jahn-Teller distortion	Adapted from http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Coordination_Chemistry/Coordination_Numbers/Jahn-Teller_Distortions	under http://creativecommons.org/licenses/by-nc-sa/3.0/us/legalcode
Figure 10 IRMOF	„MIL-53ht“ von Tony Boehle - Tony Boehle. http://commons.wikimedia.org/wiki/File:MIL-53ht.png#mediaviewer/File:MIL-53ht.png	Lizenziert unter Public domain über Wikimedia Commons -
Figure 11	„Der Nürnberger Trichter“ von Unbekannt - MDZ München. http://commons.wikimedia.org/wiki/File:Der_N%C3%BCrnberger_Trichter.jpg#mediaviewer/File:Der_N%C3%BCrnberger_Trichter.jpg	Lizenziert unter Public domain über Wikimedia Commons -