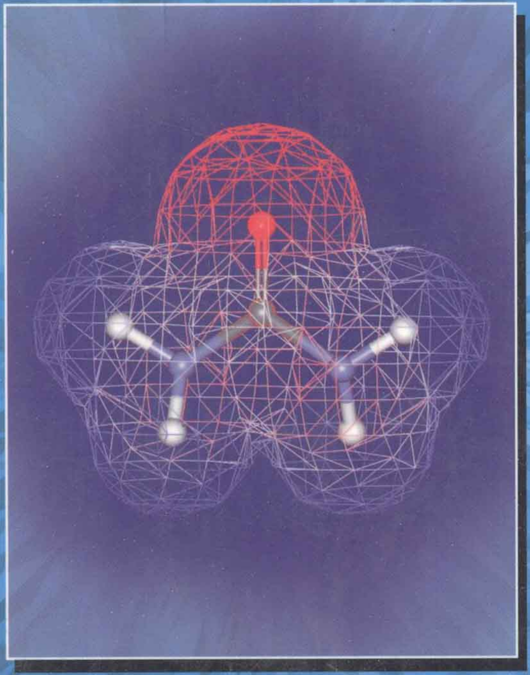
The Molecular World



Molecular Modelling and Bonding

edited by Elaine Moore

The Open University

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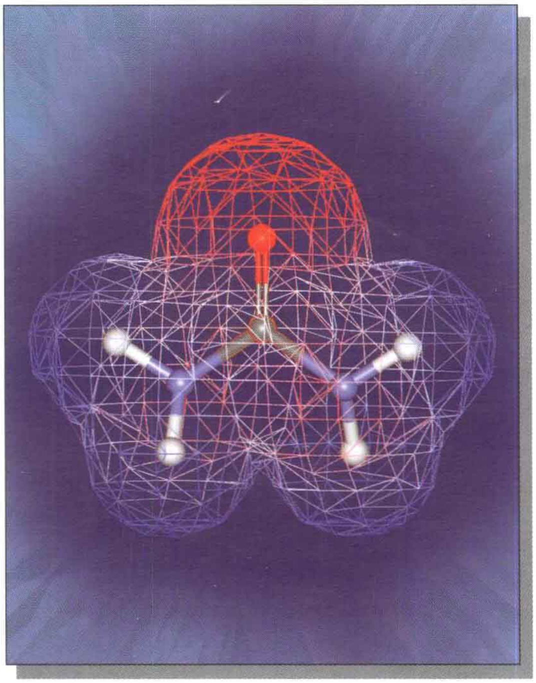

Molecular Modelling and Bonding

edited by Elaine Moore

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Elaine Moore

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1

INTRODUCTION

There is no substitute for practical laboratory experience, but computer modelling methods play an important role both as an aid in interpreting experimental results and as a means of explaining these results. Molecular modelling is now used not just in chemistry but in a wide range of subjects such as pharmacology and mineralogy. Figure 1.1, for example, shows a computer model of the protein haemoglobin.

One example of the computer modelling approach is to provide a reasonably accurate first guess at a structure which can then be used in methods such as X-ray diffraction of powders which, unlike the X-ray diffraction of single crystals, do not provide enough information to determine the total structure from scratch.

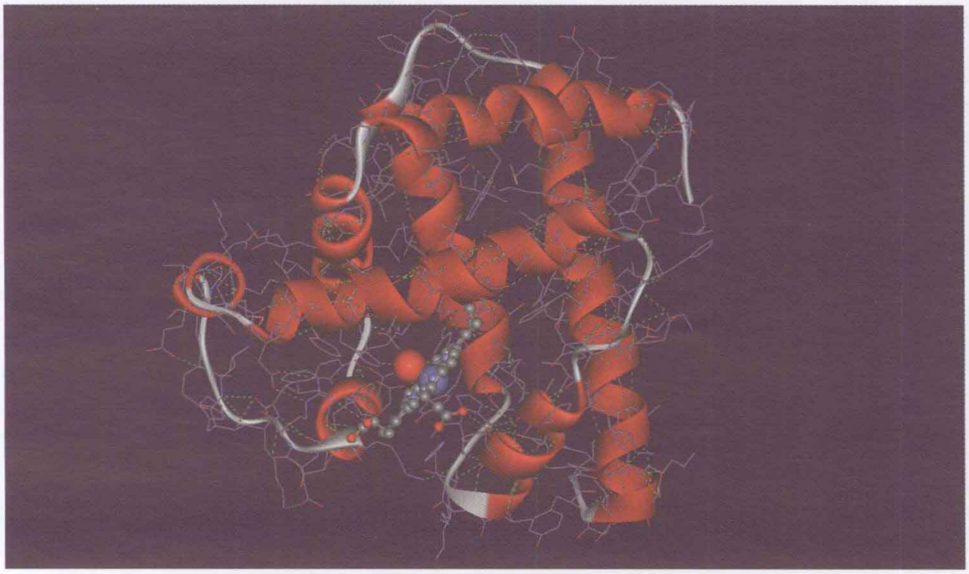

Figure 1.1
Computer model of haemoglobin, a protein. 🖳 *

In the field of drug design, computer methods have been used to screen for potentially active compounds or suggest modifications of known compounds that would be more active. Testing of inactive compounds can be avoided.

Zeolites and other structures with cages or channels will accommodate some molecules at the expense of others. Modelling of these structures has enabled planned synthesis of required molecules by predicting the cavity needed to produce the molecule.

There are areas of chemistry where it is difficult or impossible to obtain experimental results. A good example of this is the determination of the nature of reaction intermediates in chemical kinetics. In favourable cases, reaction intermediates can be studied spectroscopically using specialized techniques that allow observations on a very short time-scale of the order 10^{-9}–10^{-15} seconds.

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* This symbol, 🖳, indicates that this Figure can be viewed using WebLab ViewerLite™ or Orbital Viewer from the CD-ROM associated with this Book.

However, in the majority of cases, the path of a reaction is inferred from the stereochemistry or distribution of products and the effect of changing reaction conditions such as the polarity of the solvent. Modern computational techniques allow us to follow a reaction path. In solids very simple techniques can be used to find the most favourable path for diffusion of ions. At the other extreme, very sophisticated and accurate molecular orbital techniques can calculate the energy along the entire reaction path from reactant(s) to product(s) for gas phase reactions of small molecules. More often modelling is used to calculate the relative stabilities of proposed intermediates.

It is possible to model molecules or structures that only exist at high temperatures and/or high pressures or are too dangerous to handle. Theoretical methods have been used, for example, to predict that at the temperatures and pressures in the interior of the planet Jupiter (Figure 1.2), hydrogen can exist as a liquid metal. Conditions under which such a form of hydrogen would occur were not achieved experimentally on Earth until 1996.

You are going to look in this Book at some of the methods used to model molecules and at the principles behind them. On the CD-ROM, you will study some examples.

We start by looking at a simple, but surprisingly effective, model that is based on a picture of molecules as charged spheres linked by springs.

Figure 1.2
Jupiter as viewed by the Voyager spacecraft.

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2

MOLECULAR MECHANICS

Molecular mechanics has proved particularly useful for studying large molecules and crystalline solids where more accurate methods are very demanding of computer resources.

We shall look at the principles behind this method by considering some examples. First we consider a simple ionic solid, then move to an example where some allowance for covalency is required. Finally we consider the modelling of organic molecules.

2.1 Ionic solids

The starting point for the application of molecular mechanics to ionic solids is similar to the starting point for lattice energy calculations.* Indeed the method can be used to calculate lattice energies, but it is also used to study the effect of defects, the nature of crystal surfaces and properties of crystals.

As for lattice energies, we start by placing the ions of the crystal on their lattice sites.

● What is the force holding ions together in a crystal?

● Electrostatic attraction between the positively- and negatively-charged ions.

The ions are assumed to be on their lattice sites with their formal charges, so that in NaCl, for example, we have an array of Na^+ and Cl^- ions. The net interaction can be obtained by summing the interactions over all the pairs of ions, including not only the attraction between Na^+ and Cl^- but also the repulsion between ions of the same sign. The net interaction decreases with distance but slowly so that it is difficult to obtain an accurate value.

To calculate lattice energies, this summation can be achieved for simple lattice structures by introducing the Madelung constant. However, for layer structures with low symmetry this approach is not feasible, as a single Madelung constant will not suffice. Since the computer programs in use are set up to be of general application, they employ methods that give a good approximation to the sum over an infinite lattice for any unit cell.

However, electrostatic interaction is not all that has to be considered. We know, for example, that ions are not just point charges but have a size; the shell of electrons around each nucleus prevents too close an approach by other ions. We therefore include a term to allow for the interaction between shells on the different ions. It would be possible to give each ion a fixed size and insist that the ions cannot be closer than their combined radii. However, most programs use a different approach by including terms representing intermolecular forces.

---

* The determination of lattice energies is discussed in more detail in *Metals and Chemical Change*.[1] See the references in Further Reading (p. 123) for details of other titles in *The Molecular World* series that are relevant.

The intermolecular forces act between cations, and between cations and anions, as well as between anions. For oxides in particular, however, the cation–cation term is often ignored.

Salts such as magnesium oxide can be thought of as close-packed* arrays of anions with cations occupying the octahedral holes.

Do the cations come into contact with each other in such a structure?

No, not if the anions have the larger ionic radius.

Because the cations are held apart by the anions, the cation–cation interaction is unimportant.

The final thing we need to take into account is the polarizability of the ions. This is a measure of how easily the ions are deformed from their normal spherical shape. In a perfect crystal, the ions are in very symmetrical environments and can be thought of as spherical. If one ion moves to an interstitial site, leaving its original position vacant, then the environment may not be so symmetrical and it may be deformed by the surrounding ions. A very simple way to model this is to divide the ionic charge between a core that stays fixed at the position of the ion and a surrounding shell that can move off-centre. The distribution of the charge is obtained by adjustment to fit the properties of a crystal containing that ion. The model is illustrated in Figure 2.1. The shell behaves as though it were attached to the core by springs. Take a chloride ion, for example. If the surrounding ions move so that there is a greater positive charge in one direction, then the shell will move so that the total charge on the ion is distributed over two centres producing a dipole. Opposing this will be the pull of the springs that attach it to the core.

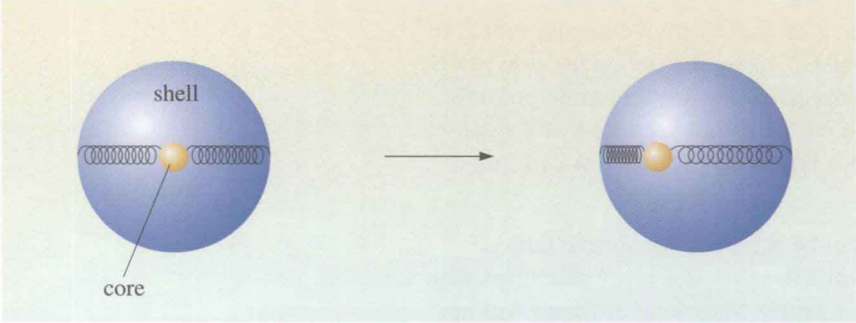


Figure 2.1
Shell model for a polarizable ion.

For ionic solids, the most important term for lattice energies is the electrostatic term; for sodium chloride, for example, the total lattice energy in a typical calculation is $-762.073\,\mathrm{kJ\,mol^{-1}}$, of which $-861.135\,\mathrm{kJ\,mol^{-1}}$ is due to the electrostatic interaction while the intermolecular force and shell terms contribute $+99.062\,\mathrm{kJ\,mol^{-1}}$. Thus the contributions of the intermolecular force and shell terms are about 10% of the electrostatic interactions. These other terms may have a greater relevance in the study of defects.

2.1.1 Crystal defects in silver chloride

Silver halides are used in photography to capture light and form an image. The action of light on the halide produces silver which forms the black areas of the negative (Figure 2.2). The formation of silver depends on the presence of Frenkel defects in the crystal.

---

* Close packed arrays are discussed in *The Third Dimension*.[2]

Figure 2.2
A black and white photograph and its negative.

- The two most common point defects in crystals are Frenkel defects and Schottky defects. What are these?

- In Schottky defects, equal numbers of cations and anions are missing (for 1 : 1 structures such as AgCl). In Frenkel defects, an ion is displaced from its lattice site to an interstitial site; for example, a small cation in a crystal with the NaCl structure can move to a tetrahedral hole from the octahedral hole normally occupied.

We can use molecular mechanics to estimate the energies of these defects in silver halides.

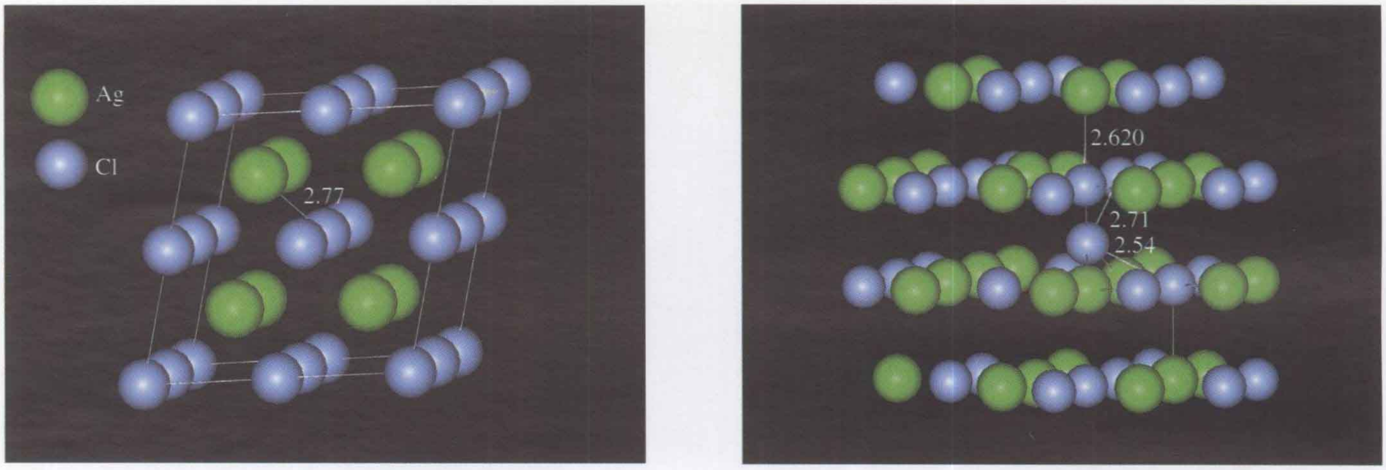
The dominant defect in silver halides is a Frenkel defect, in which a silver ion moves to an interstitial site. To calculate the energy required to form this defect we simply remove a silver ion from one position, put it in its new position and compare the energy of the crystal lattice with that of the perfect lattice.

- In a Frenkel defect, there is a vacancy where an ion should be and an ion in a more crowded interstitial position. Would you expect the ions in the vicinity of the defect to stay on their lattice positions?

- It would be reasonable to suppose that the ions would adjust their positions to allow the interstitial atom more room, and to take up the space left by the vacancy.

When calculating the energy of formation of the defect the nearest atoms are allowed to adjust their position to obtain the lowest energy for the crystal including the defect. Figure 2.3 (overleaf) shows how the chloride ions move when a Frenkel defect forms in AgCl; in the perfect crystal (Figure 2.3a) there is just one Ag—Cl bond length, whereas in the defect crystal (Figure 2.3b) the Ag—Cl bond lengths are shortened and variable.

For an estimate of the actual numbers of defects we need to know the Gibbs energy of formation, but the major contribution comes from the internal energy. Calculated values for the energy of formation of cation Frenkel defects in NaCl and AgCl are 308 kJ mol^{-1} and 154 kJ mol^{-1}, respectively.



(a)

(b)

Figure 2.3 (a) Perfect AgCl. (b) A Frenkel defect in AgCl.

Will NaCl or AgCl be expected to contain more Frenkel defects at room temperature?

AgCl. The defect energy is much lower.

The energy for Schottky defects in which there are cation and anion vacancies is 222 kJ mol^{-1} for NaCl.

Will NaCl have more Schottky or more Frenkel defects?

Schottky. These are of lower energy.

QUESTION 2.1

List the types of force that would be employed in a typical molecular mechanics calculation of Schottky defects in caesium fluoride.

QUESTION 2.2

The energies of Schottky defects in KF, KCl, KBr and KI have been calculated as 244, 241, 219 and 210 kJ mol^{-1}, respectively. Which halide will have the most defects at room temperature?

STUDY NOTE

A set of interactive self-assessment questions is provided on the *Molecular Modelling and Bonding* CD-ROM. The questions are scored, and you can come back to the questions as many or as few times as you wish in order to improve your score on some or all of them, and this is a good way of reinforcing the knowledge you have gained while studying this Book.

2.1.2 Zeolites

Zeolites* have frameworks of silicon, aluminium and oxygen atoms which form channels and cages, e.g. Figure 2.4. They form a wide variety of structures but all are based on silicon tetrahedrally bound to oxygen. Differing numbers of silicon

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* Zeolites are discussed in some detail in the Case Study in *Chemical Kinetics and Mechanism*.[3]

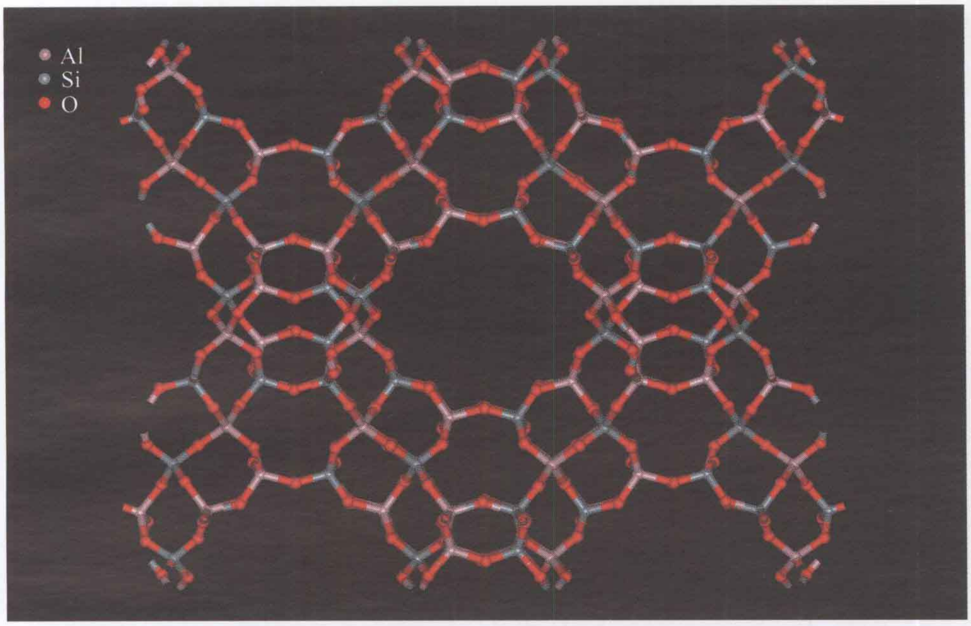


Figure 2.4
A zeolite, faujasite. Note the large channel in the centre of the structure, and the smaller ones surrounding it. Some or all of these channels can be occupied by balancing cations and by molecules. Occupation of these channels by molecules leads to the use of zeolites as catalysts.

atoms are replaced by aluminium. Other cations, notably those of Groups I, II and the lanthanides, are present in the structures to balance the charge.

Surprisingly such structures can be very successfully modelled by considering them as a collection of ions and using the methods discussed in the previous Section.

- Why is this surprising?
- Silicon is not normally thought of as forming Si^{4+} ions; indeed silica, SiO_2, and silicates do contain silicon covalently bonded to oxygen.

We do have to make some allowance for the covalency of the Si—O bonds. The most successful way of doing this is to add a term that represents the resistance of $\angle$OSiO and $\angle$OAlO bond angles to deviation from the tetrahedral angle. The covalency of zeolites and related compounds is also reflected in the relative size of the electrostatic and other terms. For one form of silica, SiO_2, for example, a calculated lattice energy of $-12\,416.977\ \text{kJ mol}^{-1}$ had contributions of $-16\,029.976\ \text{kJ mol}^{-1}$ from electrostatic interactions, $+3\,553.796\ \text{kJ mol}^{-1}$ from intermolecular force terms and the core–shell spring term, and $1.913\ \text{kJ mol}^{-1}$ from those $\angle$OSiO bond angles that were not tetrahedral. Here the intermolecular force terms are about 20% of the electrostatic interaction. The energy due to the term keeping the angles tetrahedral is small, but without this term the zeolite structure is lost.

With this addition, the structures of a wide variety of zeolites, both naturally occurring minerals and synthetic zeolites tailored to act as catalysts, can be modelled and then used to answer questions such as which position will the non-framework ions and molecules occupy and how do ions travel through the structure?

One example of the use of molecular mechanics is in investigating the mechanism of oxygen diffusion in albite, $NaAlSi_3O_8$, a mineral related to zeolites. Experiments indicate that diffusion of oxygen in albite is faster in the presence of water. Molecular mechanics calculations show that the activation energy for OH^- diffusing through the solid is lower than that for diffusion for O^{2-}.

2.2 Modelling organic molecules

Molecular mechanics modelling of organic molecules is well-developed and widely used in the pharmaceutical industry, where it is employed to model drugs and their interactions with receptors.

The power of this method for organic molecules lies in the adoption of a relatively small set of parameters that can be transferred to any molecule you want.

But what sort of parameters might be needed? Can we simply use electrostatic and intermolecular forces? How do we allow for bonds and different conformations?

Let us start by looking at a very simple molecule — ethane. Ethane is $H_3C{-}CH_3$. As for solids, we do need to include an electrostatic interaction, but what charge are we going to give carbon and hydrogen atoms? Obviously +4 or –4 on C and +1 or –1 on H are unrealistic and would not even give a neutral molecule. Think for a moment about the process of bond formation. When two atoms form a covalent bond, they share electrons. If the atoms are unalike then one atom has a larger share than the other, resulting in a positive charge on one atom and a negative charge on the other. But the charge transferred is less than one electron. For diatomic molecules, the charge on each atom can be obtained experimentally. In the molecule HCl, for example, the hydrogen atom has a charge of +0.18 and the chlorine atom a charge of –0.18. The fractional charges are known as **partial charges**. A convenient way of setting up a set of transferable partial charges is to give each atom a contribution to the partial charge from each type of bond that it is involved in. For example, in chloroethane, CH_3CH_2Cl, we need to consider contributions for the carbon atoms for carbon bound to carbon, carbon bound to hydrogen and carbon bound to chlorine. Carbon bound to carbon is given a value of zero. For elements such as oxygen, which can be singly or doubly bonded (C—O or C=O), we need different partial charge contributions for each type of bond.

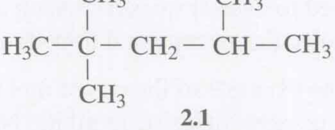
In one available computer program carbon bonded to hydrogen gives a contribution of +0.053.

- What is the partial charge on carbon in methane using this value?
- The carbon in methane is attached to four hydrogens so its partial charge is 4×0.053, or 0.212.

- What is the partial charge on the hydrogen atoms?
- Since methane is a neutral molecule, the hydrogens must each have a partial charge of –0.053.

QUESTION 2.3

Calculate the partial charges on all carbons in 2,2,4-trimethylpentane, **2.1**, using the value +0.053 for carbon bound to hydrogen.



$$\begin{array}{ccccccccc} & & \mathrm{CH_3} & & & & \mathrm{CH_3} & & \\ & & | & & & & | & & \\ \mathrm{H_3C} & - & \mathrm{C} & - & \mathrm{CH_2} & - & \mathrm{CH} & - & \mathrm{CH_3} \\ & & | & & & & & & \\ & & \mathrm{CH_3} & & & & & & \end{array}$$

2.1

As well as the electrostatic interaction arising from the partial charges, we also need intermolecular forces. These can be important for large atoms such as bromine or iodine.

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