Chapter 1
Learning at the Sub-micro Level: Structural Representations

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Abstract This chapter examines the importance of visualisation and language, both verbal and pictorial, on the understanding of the sub-microscopic level of chemistry. We begin by examining what is meant by the term ‘sub-microscopic level’ and how it is different from the macroscopic level. Here we stress the need for the careful use of language to distinguish the two levels and we provide some examples of how the imprecise use of language can blur this distinction. The challenges associated with the description and depictions of the arrangement of electrons in atoms, ions and molecules are then addressed. For a good understanding of chemistry it is critical that students visualise chemical reactions as multiple particle processes and examples are provided where misconceptions arise from a single particle perspective. The need for students to learn, and instructors/textbooks to explain, the conventions and styles of molecular representations is then highlighted. Without a good understanding of the meaning of these forms of molecular representations, students cannot visualise spatial/structural features of a molecule or consider implications of these features on reactivity. Finally we return to the need for a clear distinction between the sub-microscopic ‘reality’ and their representations.

What Is the Sub-microscopic Level?

Bent (1984) had a very sharp appreciation of the distinction, and of the interdependent relationship, between the macroscopic and sub-microscopic levels of operation of chemists. He says

> Evidently there’s more to seeing than meets the eye. To see what a chemist sees one needs to know what a chemist knows.
>
> One of my favorite examples of the connection between chemical thought and chemical behaviour is the classic demonstration of the properties of molten sulfur seen through the spectacles of a chemical model.

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Bent discusses how the sulphur melts to form a fluid liquid, which then becomes quite viscous before being poured into cold water; we imagine the breaking of S_8 rings, polymerisation of small chains and then 'quenching' of the polymeric chains without re-formation of S_8 rings for some time.

> 'Seeing as a chemist sees is a fact-supported, theory-laden exercise of a lively imagination. The entire covalent chemistry of the non-metals .... is revealed to the mind's eye in the sulfur-in-a-test-tube-heated-in-air-and-water-quenched demonstration when viewed through the thought-focusing fields of molecular models. To see in that way is to understand. And when we understand in that way, we say 'I see.'

To elucidate the distinction between the sub-microscopic and macroscopic worlds, Table 1.1 lists some observable chemical phenomena (the macroscopic level) along with the corresponding explanatory models that we use at the sub-microscropic level.

The chemists' sub-microscopic level concerns the world of atoms and their derivatives; ions and molecules. This is an unobservable world, accessible only by imagination. Imagination is such a key component of advances in chemistry at the research level, as well as of rich student understandings that its significance cannot be underestimated, and we would do well to raise our students' consciousness of it in order that they might try to develop their visualisation abilities.

Our very first recommendation concerns careful use of language to distinguish between these two levels. Scientists, instructors and textbook writers are all guilty of loose use of language on occasions – with the result that the distinction between the macroscopic and sub-microscopic levels is blurred, rather than sharpened. To be precise, benzene does not have a plane of symmetry (although its molecules do), water is not composed of the elements (as substances) hydrogen and oxygen, C_8H_{18} is not octane (although octane's composition can be represented as C_8H_{18}), nylon is not a long molecule (although its molecules are long), polyethylene is not an

Table 1.1 Examples of macroscopic and corresponding sub-microscopic levels of chemical operation

Macroscopic behaviour	Sub-microscopic explanation
Pressure of a gas	Collisions of rapidly moving particles on vessel walls
Melting	Temperature is high enough that the particles have enough energy to overcome some intermolecular forces
Sodium chloride dissolves in water	Ion-dipole forces of attraction between water molecules and ions are sufficient to overcome the forces between oppositely charged ions in the solid lattice.
Reactions proceed more quickly at higher temperature	A higher fraction of collisions have total energy of colliding particles greater than the activation energy required for reaction.
A substance displays optical activity	Molecules of the substance are asymmetrical. Interactions between the molecules and electromagnetic radiation is such that the plane of polarisation of the radiation is always rotated in the same direction

enormous alkane, liquid limonene is not chiral (although it is optically active), a reaction energy profile diagram does not plot the energies of the reactants and products during reaction (although it may plot the combined energies of a small group of atoms before, during and after a single fruitful collisional event between reactant molecules, ions or atoms), and the substance concentrated sulphuric acid is a powerful oxidising agent (not the S atom in the +6 oxidation state). That members of the chemistry community know precisely what they mean by such loose statements does not mitigate the lack of awareness of students about the distinction between chemistry's levels. Should we take the trouble to be more careful and precise, even if to do so means being more wordy?

Any discussion of the problematic issues of chemical education will include concerns about how to model for students (and for ourselves!) this 'reality' of atoms, ions and molecules. We should firstly appreciate that there is a tension between the pragmatism of accepting this 'reality', which we try to model, and the truth that this 'reality' is itself a grand model. Perhaps, then, our task is to develop useful students' models of the chemists' models.

We all accept that matter is particulate, and indeed very young pupils are told, and expected to accept, that matter consists of atoms. This is no mean feat: after all many of the best brains in the world, from the times of the ancient Greeks up till the second half of the nineteenth century, debated heatedly whether matter was continuous or particulate. For half a century after Dalton's laws based on an atomic view of matter, this debate raged. Legend has it that Boltzmann's suicide in a fit of depression was brought on by the perception that opponents of the atomic model were winning the day. Regardless of the veracity of this claim, we should perhaps question how facile it is for students to accept the atomic view when the shared understanding of scientists, armed with all of the empirical evidence of the times, took so long to evolve.

One college-level textbook Silberberg (2006) reports:

> 'Atoms? Humbug! Rarely does a major new concept receive unanimous acceptance. Despite the atomic theory's impact, several major scientists denied the existence of atoms for another century. In 1877, Adolf Kolbe, an eminent organic chemist, said "[Dalton's atoms are] . . . no more than stupid hallucinations . . .mere table-tapping and supernatural explanations." The influential physicist Ernst Mach believed that scientists should look at facts, not hypothetical entities such as atoms. It was not until 1908 that the famous chemist and outspoken opponent of atomism Wilhelm Ostwald wrote, "I am now convinced [by recent] experimental evidence of the discrete or grained nature of matter, which the atomic hypothesis sought in vain for hundreds and thousands of years."(p.45)

He was referring to the discovery of the electron.

Why do we accept that matter is particulate? Posed to students, this question can be seen to have two possible levels of intent:

(i) Why do you (the student) believe that all matter comprise particles?
(ii) Why is it the shared understanding of the community of chemists that all matter comprise particles? What is the evidence on which this belief is based?

It is our experience that to the first question, the most common student response is something akin to ‘Because my teacher told me so’. One is tempted to say that it is a pity that the scientific belief of so many students is sourced from an authority, rather than from empirical evidence – except that when chemists are asked question (ii), they find it not at all easy to answer. There is, after all, no single defining experiment that conclusively proves the claim, even though it was the phenomenon of Brownian motion that finally seems to have clinched the day for the atomists 150 or so years ago. Of course, from atomic forced microscopy (AFM), we ‘see’ pictures of gold atoms being manipulated one by one – but the output from AFM is itself the result of application of interpretive models.

Despite all of the above questioning of our sub-microscopic reality, the weight of circumstantial evidence is overwhelming. The ability to use high-precision mass spectrometers to determine not only the molar mass, but the elemental composition of compounds, based on deflection of charged particles in a magnetic field, is convincing. So too are the design and NMR validation of the complex structures synthesised in the supramolecular chemistry research laboratory, and the synthesis of drugs designed specifically to ‘trick’ pathogen molecules by matching regions of molecular shape, perhaps including recognition of chirality.

Let us accept a particulate sub-microscopic world. One of the challenges of chemistry education is to deal with a tension that most macroscopic properties are continuously varying, at least so far as our measurements allow, while our modelling at the sub-microscopic level to explain these macroscopic phenomena is based on a discontinuous picture of matter. Mass, volume, shape, electrical conductivity, solution concentration, the change of reaction rate over time, the dependence of reaction rate on temperature, phase changes, optical activity and the dependence of the equilibrium vapour pressure of solutions on solute concentration are all apparently continuously variable. Reconciliation of the continuous nature of these phenomena with the discrete nature of the explanatory model requires some appreciation of the miniscule size of the particles in our sub-microscopic world. Every teacher knows the difficulty of achieving this unambiguously when we are forced to use descriptors such as ‘particle’ or ‘grain’, to which students have already assigned everyday macro-level meanings.

Accepting atoms as our reality for pragmatic reasons does not address the question of what they are, or what they are like. Many textbooks avoid the awkward question of what they are, preferring instead to simply discuss Dalton’s propositions concerning their existence, and how his model can make sense of the Law of Multiple Proportions, for example. This approach at least emphasises the modelling aspect of their existence. At the first introduction of the concept of atoms to students, attempts to link elements and atoms may include statements such as ‘All of the atoms of an element are the same’. This, of course, has a degree of truth insofar as atomic number and electronic configuration are concerned, but is not correct in relation to the possible existence of isotopes. And yet most would agree that it is not possible to introduce the concept of isotope before a discussion of atoms. What a dilemma!

At least this mode of presentation does not introduce the hazards underlying statements such as ‘An atom is the smallest unit of subdivision of an element that still retains the characteristics of that element'. One can't help but wonder if the findings of early 'misconceptions' research has heightened our sensitivities to the dangers of even tangential suggestion that the properties of particles are those of the macroscopic substance. More than two decades ago, Brook, Briggs, and Driver (1984) diagnosed that some students imagined that the particles melt when substances reach their melting points. Similarly, Ben-Zvi, Eylon, and Silberstein (1986) reported students' conceptions of malleable copper atoms and green chlorine molecules. According to Griffiths and Preston (1992) and Lee, Eichinger, Anderson, Berkheimer, and Blakeslee (1993), there is a common belief that as the temperature of a substance is raised, the particles get hotter. These findings point to the challenges of sub-microscopic representation of phenomena that depend (according to chemists' models) on cooperative interactions amongst particles rather than on the characteristics of the particles themselves.

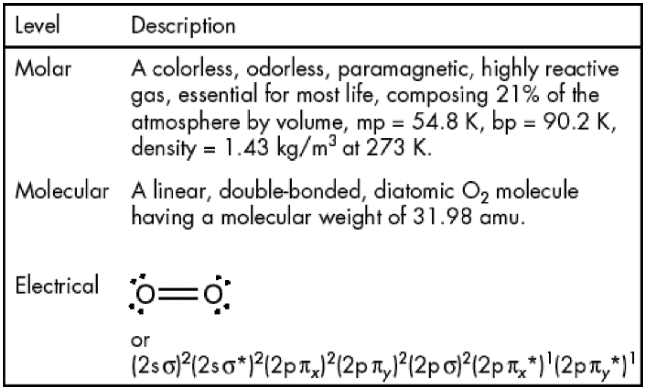
Problems arise from both the limitations of two-dimensional (2D) representations and carelessness in textbook diagrams, and although Hill (1988) referred to such issues long ago, misleading diagrams are still to be seen. Andersson (1990) has brought our attention to a remarkable representation of liquid water showing only 12 water molecules in a beaker of water. That is bad enough, but the same diagram shows these water molecules below a horizontal line representing a liquid surface, suggesting that the water molecules are within a medium, rather than that they actually comprise the medium. An inability to portray a sense of the enormous number of molecules in a beaker of water and of the dynamic nature of even a solid substance is an inherent problem of representation on the printed page. Computers have now opened up new ways of sub-microscopic representation, especially in relation to the dynamic nature of our models.

Fine Resolution: Molecular and Intramolecular Levels

Jensen (1998a) proposes two sub-levels of the imagined sub-microscopic world of atoms: molecules and ions. The *molecular* level concerns structural elements of molecules such as connectivity, bond angles and bond lengths; characteristics that might be 'seen' from nearby molecules. On the other hand, he recognises an *electrical* level, perhaps preferably called the *intramolecular* level, which refers to distribution of electrons within an atom, molecule or ion. In a later paper, Jensen (1998b) makes the distinction between these sub-levels with simple examples in relation to dioxygen gas (Table 1.2).

Visualisation at the intramolecular sub-microscopic level has its challenges. How can we reconcile wave models of electrons in atoms with diagrams that purport to represent probability of position? How difficult to appreciate is the difference between the plot of ψ^2 vs. distance (indicating the probability of finding the electron at a given distance from the nucleus along direction), and the plot of $4\pi r^2\psi^2$ vs. distance (indicating the probability of finding the electron on the surface of a sphere at a given distance from the nucleus)? What is meant by charge density? What challenges are presented in understanding the concept of iso-density contour

Table 1.2 *Aspects of dioxygen gas at the molar, molecular and electrical (intramolecular) levels of discourse*. Taken from Jensen (1998b). (Jensen's use of the term *molar* level corresponds with the more common *macroscopic* level.)



Level	Description
Molar	A colorless, odorless, paramagnetic, highly reactive gas, essential for most life, composing 21% of the atmosphere by volume, mp = 54.8 K, bp = 90.2 K, density = 1.43 kg/m^3 at 273 K.
Molecular	A linear, double-bonded, diatomic O_2 molecule having a molecular weight of 31.98 amu.
Electrical	or $(2s\sigma)^2(2s\sigma^*)^2(2p\pi_x)^2(2p\pi_y)^2(2p\sigma)^2(2p\pi_x^*)^1(2p\pi_y^*)^1$

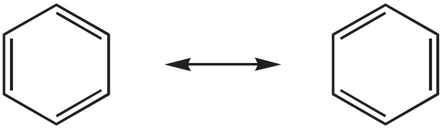
surfaces, of which there are an infinite number? What does it mean that electrons in the 3p orbital of an atom can interpenetrate the distributions of those electrons in the 1s, 2s and 2p orbitals? This latter question begs the further question (theoretically invalid, we believe) of whether electrons in atoms retain their identity. How can one electron in a p orbital have real probabilities of being in either 'lobe', and yet zero probability at a point between the lobes? What is an electron cloud? What does an atom look like?

Keogh (1991) asked high performing first year university students what components they would need to hypothetically construct a lithium atom. One replied that they would need a nucleus, three electrons and an electron cloud. On further investigation, it turned out that this student perceived a need for the electron cloud as a place for the electrons to be put. Despite a 'remedial' discussion, this student demonstrated the same conception several months later.

Representations showing electrons in molecules seem to suggest localisation of the valence electrons, but there are problematic issues in this regard. For example, we might ask if dioxygen has a double bond and two lone pairs on each O atom (as in Table 1.1) – a structure that does not reconcile with the paramagnetic nature of the substance – or a single bond and an odd number of electrons localised on each atom, as shown here:

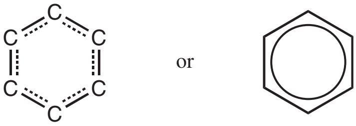
There is not a universally accepted representation of dioxygen's intramolecular electron distribution.

A related issue is that of resonance structures, the classical case of which is benzene. In order to deal with the experimental evidence that all of the C-C bond lengths are equal, it is common to represent the structure of benzene molecules in the following way:



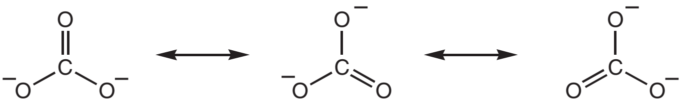
The double-headed arrow is intended to imply the existence of a 'resonance hybrid': a structure with an electronic distribution intermediate between the two shown. Every instructor knows the hazards of this portrayal. Firstly, the double-headed arrow is misinterpreted by some students to mean either (i) that there is an equilibrium condition involving the two different species, or (ii) that 'flipping' occurs between the two species. A second problem is demonstrated by those students who ask 'Are these not the same? If we rotate one of the molecules by 60°, we see that they are identical'. We can hypothesise that the latter problem may be exacerbated by the tendency of textbooks (and probably teachers) to talk about these two different resonance structures as though we are referring to two different molecules – when, in fact, we are talking about different electron distributions in just one molecule. It seems so important for instructors to refer to just one set of six carbon atoms joined by σ bonds, and then to discuss alternative distributions of the six π electrons within that system.

Representations less prone to misinterpretation, and perhaps closer to 'reality' are the following:



These representations are intended to mean that each C–C bond comprises three electrons. This in itself seems not such a difficult concept, but since students are usually 'indoctrinated' to the idea that a covalent bond is two shared electrons, the notion of $1^1/_2$ bonds between each pair of C atoms may be bewildering for some.

If this is not difficult enough an idea, have sympathy for students who are told that the carbonate ion, for example, can be represented by the following resonance structures:



One can only wonder what sense some students make of the instruction that the 'reality' involves eight electrons distributed over the three C-O bonds: that is, $2^2/_3$ electrons per bond, or each bond equivalent to $1^1/_3$ 'classical two-electron bonds'!

Professional chemists have a view of a rather fluid, easily distorted, electron cloud in molecules, able to be pushed and pulled by whichever species (or part of a species) is close by. This is an important component of understanding reaction mechanisms, the origin of dispersion forces between non-polar substances, and polarisability of the electron clouds of anions by highly charged cations as explanations of variance of ionic/covalent bond character and acid/base character of metal oxides. While it is common to see textbook discussions of a fluid 'sea of electrons' in metals, there remain challenges for developing, and representing, the idea of fluidity of electron clouds in molecules. In a discussion of the hazards of using curved arrows to denote motions of electrons in representations of reaction mechanisms, Laszlo (2002) makes the following scathing comment about using Lewis formulas in mechanistic representations:

> This limitation was already painfully obvious to the organic chemists in the 1880s: these are static structures, whereas of course any molecule at any temperature is a jelly-like pulsating, librating and vibrating entity. Only a terribly simplistic eye would see a molecule frozen into this Platonic archetype of the structural formula.

Many of the properties of substances are rationalised on the grounds of different electronegativities of bonded atoms, giving rise to polar molecules (unless the symmetry of the molecules causes cancellation of bond dipole moments). The notion that a region of a molecule can have 'partial negative charge' if the amount of electron matter around a nucleus exceeds the charge on the nucleus is a subtle one. Partial charges are usually denoted by δ+ or δ−, no matter on which atoms, in different molecules or within the same molecule. Can we blame students for presuming that the magnitude of charge on the oxygen atom in a water molecule (expressed as δ−) is the same as that on each of the hydrogen atoms (written as δ+)?

An increasingly popular, and very useful, explanatory model of polarity is the electrostatic potential map, an example of which is shown in Fig. 1.1.

In qualitative terms, the more intense the red coloration the greater is the excess of electron charge over nuclear charge, and the intensity of blue coloration indicates the extent to which nuclear charge dominates electron charge in particular regions of the molecule.

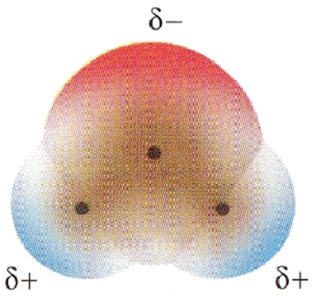


Fig. 1.1 An electrostatic potential map of a water molecule [Scanned from Silberberg (2006, 4th edition)]

While electrostatic potential maps are useful as indicators of likely orientation of molecules to each other, and of points of reactivity to nucleophiles or electrophiles, their precise meaning is not easily accessible to science novices. These maps are achieved by calculation of the potentials of a point unit positive charge at all points on an iso-density surface of the electron cloud, the strength of attraction of the positive charge at some regions being correlated with intensity of red colour, and strength of repulsion at other regions correlated with depth of blue colour.

Students need to be aware that the colours in electrostatic potential maps bear no relationship to portrayal of molecules with differently coloured atoms – such as a red sphere to represent the oxygen atom in a water molecule and white spheres to represent the hydrogen atoms. Of course, while the use of differently coloured spheres to portray different types of atom has some usefulness, it is important that students appreciate the artificiality of the use of these colours. Indeed mature chemical understanding leads to the recognition that atoms do not even retain their identity in molecules. For example, a water molecule does not consist of an oxygen atom and two hydrogen atoms, each of which has 'its own' electrons; a more sophisticated view is that it consists of an oxygen nucleus and two hydrogen nuclei surrounded by 10 mutually shared electrons.

Before leaving the subject of distribution of electrons within molecules, and its attribution to the origin of molecular polarity, with consequent effect on intermolecular forces (with further consequent effects on solubilities and melting points), it is pertinent to remind ourselves of two significant challenges faced by chemistry instructors: (i) to graphically represent forces of attraction between molecules and (ii) to develop the imagery that in the liquid state, orientation of molecules toward each other because of polarities is transitory, even if more probable, as they move past each other.

Fine Resolution: Single-Particle and Many-Particle Images

Further resolution of the sub-microscopic world at Jensen's molecular level can be useful. Bucat (2004) has stressed the importance of recognition that sometimes we use single-particle images, and sometimes it is necessary to use many-particle images. For example, we generally use representations of single molecules to understand (i) connectivity and bond angles, (ii) stereochemistry, (iii) *cis–trans* isomerism and (iv) molecular polarity. On the other hand, it is not possible to rationalise boiling, or dissolving, with a portrayal of just one molecule of a substance – even though a visualisation of a polar molecule, for example, might help us to understand different boiling points or solubilities. Similarly, rationalisation of chemical equilibrium, the states of matter (or changes between them), diffusion, optical activity, or brittleness of ionic solids demand visual images with many particles to make sense.

Does it matter? The following, some taken from research and some from experience, provide justification for employing this fine resolution to analysis of pedagogical issues in chemistry teaching. Ben-Zvi, Eylon, and Silberstein (1987) have shown that some school students in Israel have responded to a question asking whether it is possible for N_2O_5 to be formed by reaction between N_2 and O_2 by saying 'No. Where from did we get three additional oxygen atoms?' Obviously these students did not appreciate that they needed to consider a many-particle picture in this situation. Ben-Zvi et al. speculate that this may be because textbooks usually present single-particle images to portray chemical reactions.

Ladhams Zieba (2004) has found that university students can be confused when a single-particle representation of S_N1 substitution leads to a racemic mixture of products (Fig. 1.2).

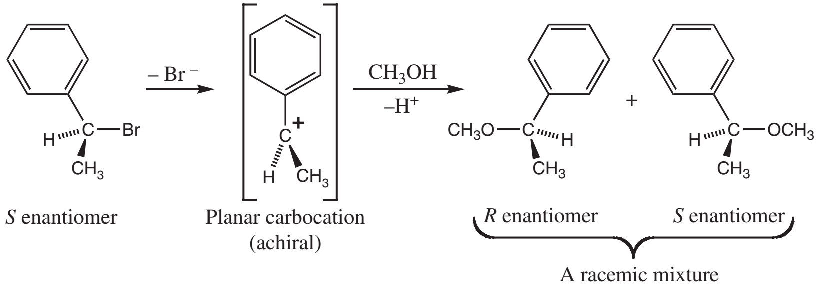


Fig. 1.2 A single particle representation of racemate production

How can we get two molecules of product from only one molecule of starting compound? Perhaps, at least until students are more experienced, this diagram needs to be supplemented by a diagram or animation showing many reactant particles, half of which form one enantiomer and half the other enantiomer.

The accepted mechanism of S_N2 substitution reactions is based on the experimental evidence that their reaction rates are directly proportional to the concentrations of both the substrate and the nucleophile. However, in discussion of this type of reaction, textbooks usually present a single-particle representation of the process (Fig. 1.3).

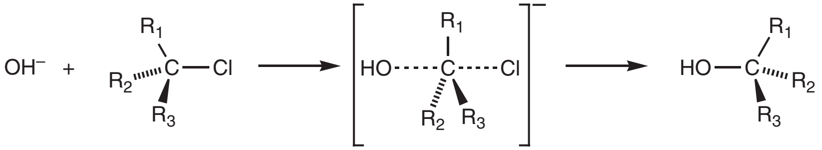


Fig. 1.3 A single-particle representation of an S_N2 substitution reaction

It is common experience that, when given this diagram, many university students say that what is meant by 'the rate of the substitution reaction' is how quickly the single event portrayed in the diagram happens. However, there is no sense to be made from the notion that the speed of this single event depends on the concentrations of both reactants. Of course, the real meaning of ‘rate of reaction’ concerns how many such reaction events occur per unit time, and this meaning can only be developed with a multi-particle image of the reaction mixture.

Visualisation of a chemical reaction as a single event is sometimes unconsciously encouraged by the language that we use. For example, this extract placed alongside a mechanistic representation of an S_N2 substitution reaction from a popular textbook is similar to that in many others:

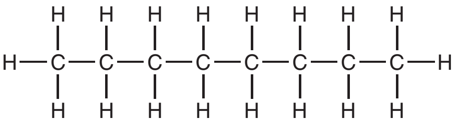
> The nucleophile OH^- uses its lone pair electrons to attack the alkyl halide carbon 180° away from the departing halogen. This leads to a transition state with a partially formed C-O bond and a partially broken C-X bond. The stereochemistry is inverted as the C-O bond fully forms, and the halide ion departs with the electron pair from the former C-X bond.

Only one nucleophile particle and only one alkyl halide molecule? One bond broken and one bond formed? Leaving aside the implication of intent on the part of the nucleophile (rather than a probabilistic view of the event), this extract would be acceptable if it were explicitly stated that it focussed on just one of the very many reaction events that occurred at various points in time in the reaction mixture.

A less obvious example that needs careful consideration to understand is our usual explanation of the dependence of reaction rates on temperature. Two diagrams are usually used in conjunction: (i) the so-called reaction energy profile diagram indicating an activation energy barrier and (ii) a Boltzmann distribution of kinetic energies of the reactant particles. We need to be aware that the former concerns the combined energies of particles in a single-particle (of each reactant species) event, while the latter relates to statistical distribution of energies of the very many particles in the reaction mixture. It is by no means certain that students comfortably and successfully reconcile the vastly different contexts of these two diagrams.

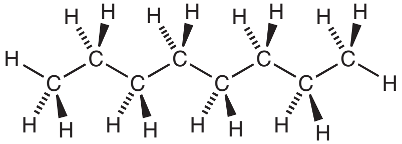
Portrayal of Structures of Molecules

Portrayal of molecules is done in a large variety of ways, each having particular advantages and disadvantages. It has been common for textbooks to present a molecule of octane, for example, in the following form:



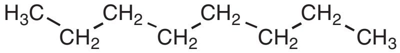
$$\begin{array}{ccccccccccccccccccc} & & H & & H & & H & & H & & H & & H & & H & & H & & \\ & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \\ H & - & C & - & C & - & C & - & C & - & C & - & C & - & C & - & C & - & H \\ & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \mid & & \\ & & H & & H & & H & & H & & H & & H & & H & & H & & \end{array}$$

This type of representation, probably used because of limitations in typesetting technology in the past, indicates connectivity correctly, but gives a very poor image of the bond angles and the flexibility of the carbon chain due to the rotation about single C-C bonds. A much more powerful image is the following, which at least portrays the tetrahedral arrangement of bonds around each carbon atom.



To ‘read’ this structural representation, one needs to understand the inherent conventions concerning ‘wedge’ and dashed lines. But even this portrayal is static, able to show neither the vibrations of the atoms nor rotation about the single bonds – giving rise to the apparent twisting of the chain into more probable orientations. Furthermore, it is limited in its ability to show the most stable staggered conformer, and does not make obvious the steric hindrances that may arise because of the size of atoms or functional groups (as a space-filling model can). Very powerful computer simulations that seem to have great potential as visualisation aids are now available.

Abbreviated forms of the octane molecular representations include the following:



These last two portrayals demand knowledge of how to ‘read’ them and the last (so-called ‘line structure’) can be tricky for students to interpret, especially in the case of more complex molecules and cyclic structures.

Bodner and Domin (2000) demonstrated the inability of many university students to interpret abbreviated structural portrayals with some atoms implied, rather than shown. The students were asked to predict the major products of the reaction of bromine with methylcyclopentane portrayed as in Fig. 1.2, and to estimate the ratio of the products if bromine radicals were just as likely to attack one hydrogen atom as another. Most of the 200 students predicted three products, with a relative abundance 3:2:2 (Fig. 1.4).

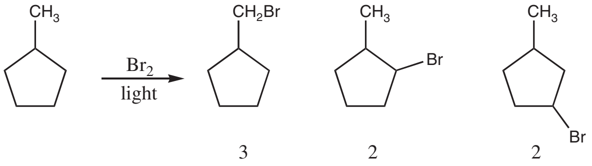


Fig. 1.4 Products, and relative abundances, predicted by most students in the research of Bodner and Domin

A minority of students correctly predicted four products in the ratio 3:4:4:1 (Fig. 1.5).

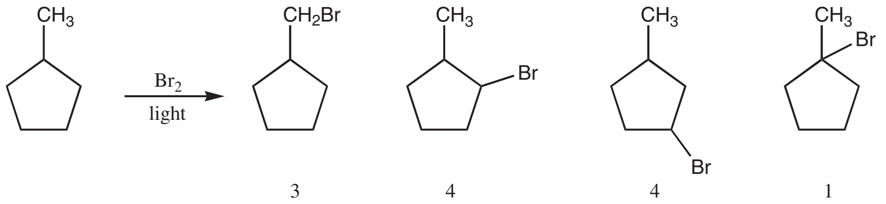


Fig. 1.5 The correct prediction required students to realise that there is a hydrogen atom at the carbon with methyl substituent, and two hydrogens at each other ring carbon

The remarkable finding from this research was that every student who answered correctly firstly re-drew the starting material as shown in Fig. 1.6, and none of those who answered incorrectly did so. The recognition of implied atoms is something that we do automatically as we become more experienced in chemistry.

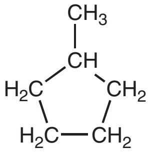


Fig. 1.6 The re-drawn structure of methylcyclopentane, showing all hydrogen atoms, that was the key to students answering correctly the task given by Bodner and Domin (2000)

Chemists do not make things easy for the novice: molecules of a substance can be represented in a variety of ways to illustrate particular features, and to the novice these can seem to be different structures. Hoffman (1995) and Hoffman and Laszlo (1991) illustrate this point well through various representations of a molecule of camphor (Fig. 1.7).

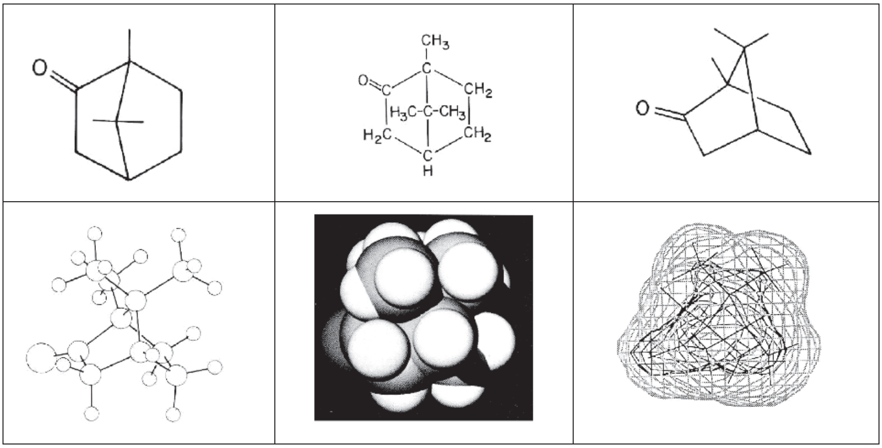


Fig. 1.7 Different-looking representations of a camphor molecule (From Hoffmann and Laszlo, 1991)

Spatial Visualisation: Demands and Abilities

Operation at the sub-microscopic level of chemistry requires a degree of imagination and visualisation ability that differs from person to person. Valuable essays on the importance of these visualisation abilities have been published by Francoeur (1997), Habraken (1996, 2004), Hoffmann (1995), Hoffmann and Laszlo (1991), Briggs and Bodner (2007) and Kozma and Russell (2007).

For example, chemists are required to interpret diagrams of a molecule of cyclohexane, or of substituted cyclohexanes, when it is represented as a flat-looking hexagonal projection, or as a side-on view to show the 'chair' form, or as a Newman projection (Fig. 1.8).

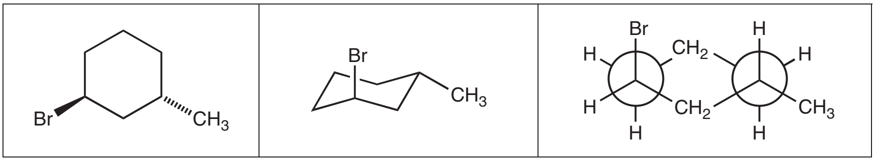


Fig. 1.8 Different representations of 2-bromomethylcyclohexane

Even using the same style, chemists can represent a simple methyl group in different ways, as demonstrated in the example of methylcyclohexane (Fig. 1.9). A chemist will interpret these diagrams, usually subconsciously, as all being equivalent in that they all represent the same molecule, methylcyclohexane.

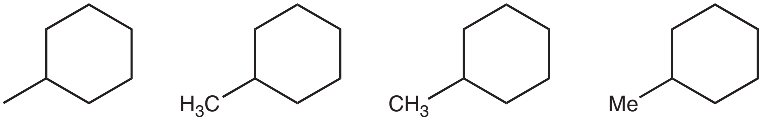


Fig. 1.9 Different representations of a methyl group in methylcyclohexane (From Hoffmann and Laszlo, 1991)

Bodner and Domin (2000) provide research evidence that even some university students do not find it easy to visualise these structures. Students were asked to give the systematic names of the compounds whose molecules were represented as in Fig. 1.10.

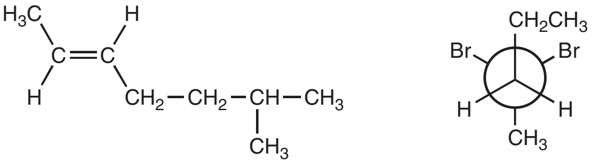


Fig. 1.10 Representations given in the naming exercise given by Bodner and Domin (2000)

Although most students were successful with the structure on the left, many could not name the one on the right, even in two later exams during the same course. The students complained that this question was ‘not fair’, apparently because they had trouble in visualising a side view of the molecule. This finding is consistent with earlier work that demonstrated the difficulty that many students find with tasks that involve (i) interpreting a 2D representation into a 3D image, (ii) performing a mental operation, such as rotation or reflection, on the 3D image and (iii) re-representation of the newly visualised 3D image as a 2D diagram (Seddon, Tariq, & Dos Santos Viega, 1982, Seddon & Shubbar, 1984, Tuckey, Selvaratnam, & Bradley, 1991). Head, Bucat, Mocerino, and Treagust (2005) report similar findings with respect to changing one’s mind’s-eye perspective from one style of representation of a molecule of a substituted cyclohexane to another style of representation. Both Ferk, Blejec, and Gril (2003) and Kuo, Jones, Pulos, and Hyslop (2004) have demonstrated better student understanding with physical models than with schematic representations.

In the case of representation of chiral molecules, the demands of spatial visualisation ability on understanding become critical. Head and Bucat (2002) have reported the outcomes from interviews with students and lecturers in relation to tasks such as that shown in Fig. 1.11.

Alanine: Are these mirror images or superimposable?

Fig. 1.11 A task used by Head and Bucat (2002) to probe visualisation abilities

They report wide differences of visualisation abilities (of both students and lecturers) and that each person consistently employed idiosyncratic decision-making strategies from task to task. Most students employ a strategy of rotation to align a corresponding bond in each structure, thus reducing the problem to a 2D consideration of the clockwise/anticlockwise orientation of the other three function groups. The students found mental rotation about the vertical bond easier than about the other bonds. This is consistent with the findings of Kuo et al. (2004) who investigated student’s strategies of assigning R or S configurations to structures of chiral molecules. Students found the task easier when the lowest-priority group was oriented towards the back or the side of the molecular representation, rather than towards the top or to the front.

Distinguishing Between Representations and the Reality Represented

Common teaching experience suggests that sometimes students’ sense-making operates on representations, rather than on the sub-microscopic ‘reality’ that they represent. How powerful it would be if, on seeing a formula, a molecular structure, a diagram of molecular interaction, or a chemical equation, students visualised the substance or the reaction mixture, rather than the symbolism on the page or computer screen. There is research evidence that this is, at least sometimes, not the case.

Kleinman, Griffin, and Kerner (1987) refer to a student who was shown a diagram of bromobenzene (Fig. 1.12) and asked if the molecule has a plane of symmetry.

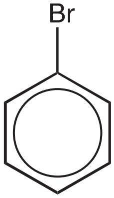


Fig. 1.12 A diagram of a bromobenzene molecule, similar to that used by Kleinman et al. (1987)

The student decided that the molecule does not have a plane of symmetry because, referring to the bromine atom, B ≠ r.

Ladhams-Zieba (2004) has demonstrated that university students working on reaction mechanisms in organic chemistry also operate on the drawings on the page, rather than on what they represent. She asked 18 second year university students to predict and draw the product species most likely to be produced from the substitution reaction of hydroxide ion into 2 bromobutane, represented as in Fig. 1.13(a). Ten of them drew the inverted substitution product that you might expect from 'backside attack' in an S_N2 reaction (Fig. 1.13(b)).

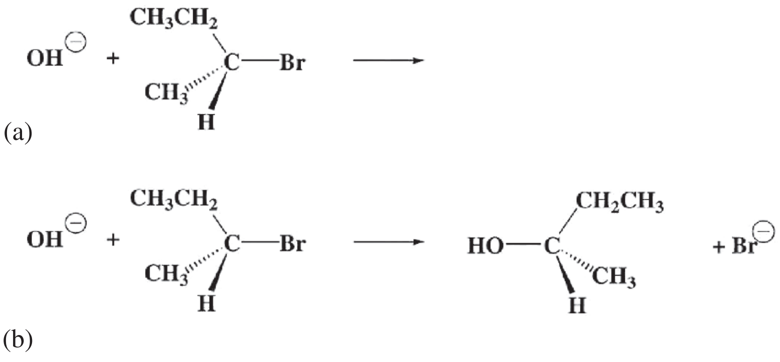


Fig. 1.13 (**a**) shows the task presented to students and (**b**) shows the dominant answer

By contrast, 17 other students were given the same task, except that they were given an equation in which the positions of the formulas of the two reactant species are reversed (Fig. 1.14(a)). Eight of the students drew a substitution product with-

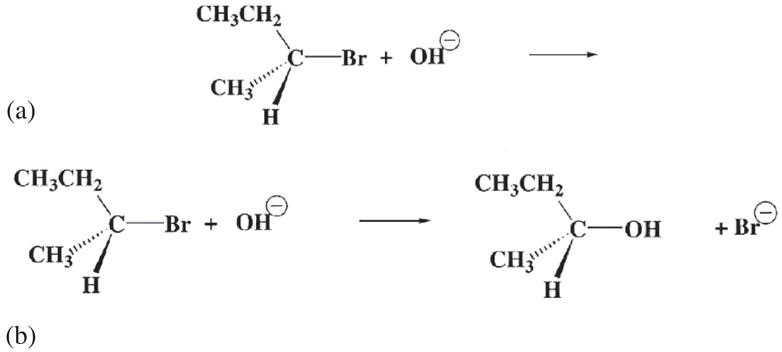


Fig. 1.14 The former shows the task presented to students and the latter shows the dominant answer

out inversion, as though the hydroxide and bromide had simply changed places (Fig. 1.14(b)) and only one of the others predicted inversion.

The predicted product shown in Fig. 1.14 is different from that shown in Fig. 1.13, even though the reactants are the same. Of course it is nonsense to think that the product of a reaction between two species could depend upon the relative positions of their formulas in a representation of a reaction equation. This is clear evidence that some students consider the juxtaposition of the written representations of the reactants on the page, rather than a visualisation of the reaction mixture at the sub-microscopic level. The quality of the predictions would have been greatly enhanced if the students had visualised a many-particle, probabilistic picture of the reaction mixture, as discussed earlier

Conclusion

On its own, the imagined world of sub-microscopic chemistry presents serious challenges for students and, therefore, for teachers. Not the least challenge is that it is indeed an imagined world. Given that this sub-microscopic world must be knitted into the kindred worlds of observable macroscopic behaviour and symbolic representations, the complexity of learning chemistry is revealed. There is a need for clear understanding of the conventions and styles of molecular representations and therefore the teaching of these conventions. Without such an understanding, students cannot then visualise spatial and structural features of a molecule nor consider implications of these features on reactivity. Perhaps the eventual seamless weaving of the three worlds of chemistry will be made easier for students if initially the distinction between them is explicitly emphasised. Starting from a sharp consciousness of the different worlds can lead to a more comfortable and effective operational mode than can be achieved from a condition of confusion or simply lack of recognition of these levels of chemistry.

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