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EDUCATIONAL SOFTWARE “ChimUniv” FOR CHEMICAL BONDS

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ABSTRACT: Chemical bonding is a topic found challenging by students, who commonly develop alternative conceptions which act as impediments to learning the scientific models. This article offers an introductory treatment of the topic. It is intended to support teaching that avoids encouraging the common misconceptions, and which supports progression through the secondary/college years. In particular, chemical bonding is here understood as part of a more general way of modeling the structure of matter at the scale of molecules. Space in this article only allows a cursory exploration of basic bonding ideas, but this should be sufficient for readers to get a feel for the strengths and weaknesses of this approach. Much of this presentation is supported by research into how students' ideas develop, and the misconceptions they often develop with current common approaches to teaching the topic.

KEYWORDS: chemical bonds, software, e-learning

❖ INTRODUCTION

Chemical bonding is one of the key concepts in the study of chemistry, and is important in understanding material structures, properties and reactions. Yet the notion of the chemical bond is purely theoretical, in the sense that it does not refer directly to any readily observable phenomenon. Rather the idea of the chemical bond is part of a conceptual framework developed by chemists to explain phenomena that can be observed in the laboratory in terms of an elaborate set of models of matter at a submicroscopic scale.

The key point of chemists' submicroscopic models that novices commonly fail to appreciate is that the macroscopic properties and behaviors of substances are explained in terms of the distinct properties of the submicroscopic entities. Unfortunately it is common for learners to misconstrue how these explanatory models work, and to think that the properties of substances are explained by assuming they are composed of tiny particles having those properties: eg that copper conducts because it is made up of copper atoms that are themselves conducting.

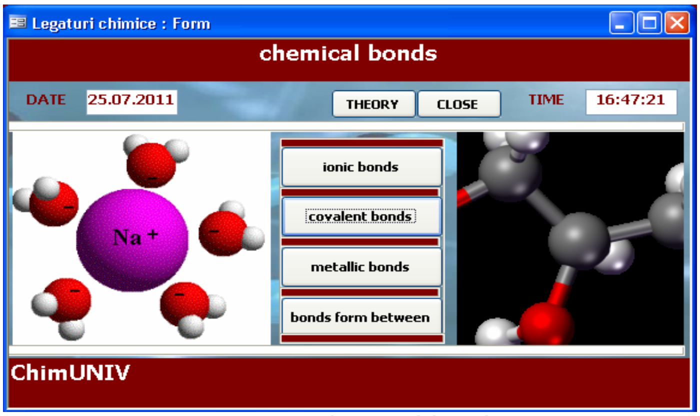

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Figure 1. Chemical bonds

❖ GETTING ON THE FIELD

A basic premise of the explanatory framework constructed by chemists is that apparently solid, continuous, matter is actually discontinuous and composed of myriad tiny components. That is, chemists use a quantum theory of matter. I will refer to the various components as 'quanticles'. Although these quanticles can be imagined as tiny particles, a bit like specks of dust or grains of salt, that is misleading as they have some properties very unlike familiar particles (like being impossible to localize in space, sometimes interpenetrating each other, and - under certain conditions - giving rise to interference patterns).

A key feature of these quanticles is that because some of them are charged, matter tends to bind together, and this is the basis of the explanation for why matter on the more familiar scale is held together. Unfortunately when 'particle theory' is first introduced in secondary schools, usually to explain the three states of matter, the emphasis on the arrangement of the 'particles' in solids, liquids and gases often leads to this key property being neglected, leaving learners with little rationale for why the condensed phases exist.

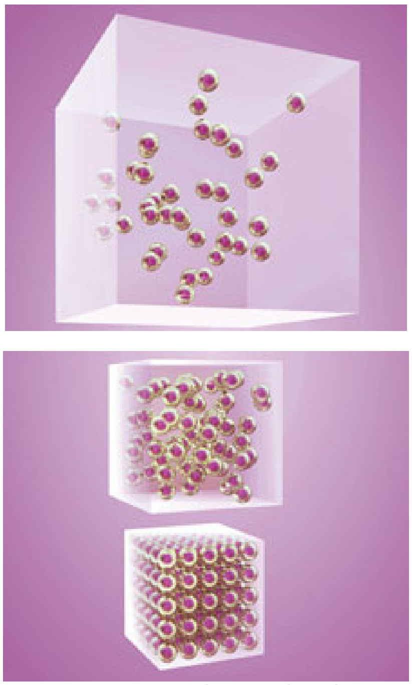


Figure 2. Particles in the three states of matter: gas (top), liquid (middle) and solid (bottom)

The central principle that matter binds together, but the bonding can be disrupted at high enough temperatures, applies at a range of levels (ie lattices, molecules, atoms, nuclei, hadrons) and can be introduced in the context of understanding why there are different states of matter, and why phase changes occur in association with heat flow into or away from the substance.

The most fundamental quanticles, for chemists at least, are the proton, neutron and electron, although other important quanticles are formed when these bind together. The protons and neutrons, collectively known as nucleons, can bind together through the strong nuclear force to produce aggregates termed nuclei. For most chemical purposes these aggregates can be considered stable.

Positively charged nuclei attract negatively charged electrons, so under normal conditions nuclei are surrounded by a swarm or 'cloud' of electrons, such that they tend to produce overall neutral, or nearly neutral, conglomerates.

This electrostatic model can be used as the basis of explaining a great deal of chemistry. Stable structures are in an equilibrium where the various forces balance out. In all the examples of bonding below, quanticles are attracted together until they reach a point where they are close enough for repulsions to balance attractions.

METALLIC BONDING

Some metals are found 'native', but these are not atomic, but rather consist of extensive lattices comprising atomic cores with enough delocalized electrons moving around them to give an overall neutral structure. The cores are the nuclei surrounded by one or more shells of electrons, held in the lattice by the electrical forces between the positive cores and the delocalized electrons. A consequence of this type of bonding, metallic, is the conductivity (electrical, but also thermal) associated with metals. Other properties of metals can also be related to the bonding and structure at the level of quanticles.

COVALENT BONDING

Other elements found native, like sulfur, oxygen, and nitrogen, are not metals. Their basic components at the quanticle level are comprised of a small number of cores surrounded by a sheath of sufficient electrons to give overall neutrality. These arrangements are called molecules.

In our simple model we find that in molecules there are electrons between any two cores - so that the attraction between electrons and cores balances the repulsion between the cores, and holds the structure together. This is called covalent bonding. Sometimes it is said that electron pairs are 'shared' between cores, but this figurative language can be taken a little too seriously by learners who will see the sharing - rather than the balance of electrical forces - as the explanation for the bond.

In the case of oxygen and nitrogen, hydrogen, fluorine and chlorine, the molecules each comprise two atomic cores with the surrounding sheath of electrons. However phosphorus often consists of molecules with four cores (arranged as the corners of a tetrahedron), and sulfur molecules consists of eight cores arranged in a ring - with each core having a covalent bond with each of its neighbors in the ring.

In some structures, such as diamond, there are extensive networks of cores linked through covalent bonding so that there is a giant structure, although the individual bonds comprise of electron pairs localised between adjacent cores.

INTERMOLECULAR BONDING

Phosphorus and sulfur are solids at room temperature, because the individual molecules are themselves bound together. On our simple model this can be explained in terms of the movements of electrons in the molecules leading to transient areas of positive and negative charge, which influence electrons distribution in adjacent molecules. The synchronization of the transient shifts in charge leads to an attraction between molecules that attract them together. This form of intermolecular bonding is an induced-dipole-induced-dipole interaction. Even the noble gases will condense due to these weak attractions when the temperature is low enough.

POLAR BONDING

Most material on earth is not in the form of elemental substances, and indeed there are a vast number of compounds, when the basic quanticles involved are cores of several different elements bound together. In covalent bonding, the electrons found between cores of the same atom are equally attracted towards both. However, when electrons are binding cores with different charges, the electron charge density pattern will reflect the different core charges.

So, for example, in water molecules, H_2O, the electron pairs between the hydrogen and oxygen cores are attracted more strongly to the oxygen cores (with their +6 charge) and so the 'average' position of the bonding electrons can be considered to be shifted towards the oxygen core. This type of bonding is called polar bonding. This gives molecules that have an asymmetrical distribution of charge and are themselves often polar. These polar molecules can align as the positive areas on one attract the negative areas of another (and vice versa).

Such permanent dipole interactions form another class of intermolecular bonding. This is particularly strong in water, and other compounds with hydrogen bonded to electronegative elements, when it is called hydrogen bonding. (Understanding the special nature of hydrogen bonding requires more sophisticated models.)

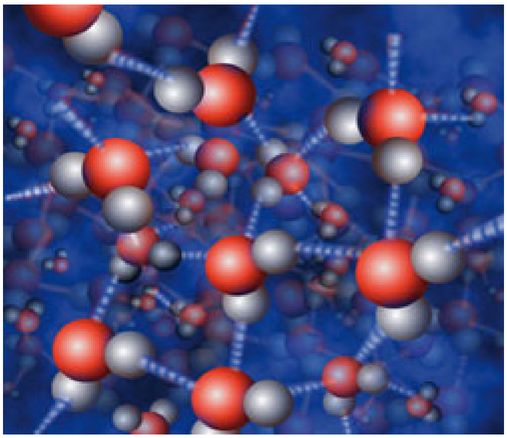
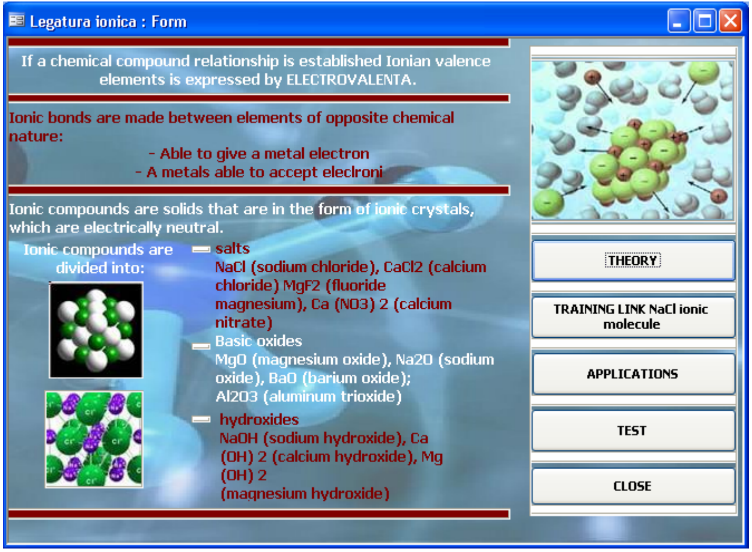


Figure 3. Hydrogen bonding in water molecule

❖ IONIC BONDING

Some compounds have a different kind of structure that is not molecular, but rather a crystalline lattice. This ionic structure is rather different to the metallic lattice, and leads to different properties. Substances with ionic bonding do not conduct electricity in the solid state, and can often be dissolved in solvents consisting of polar molecules.



If a chemical compound relationship is established Ionian valence elements is expressed by ELECTROVALENTA.

Ionic bonds are made between elements of opposite chemical nature:

- Able to give a metal electron
- A metals able to accept elecIroni

Ionic compounds are solids that are in the form of ionic crystals, which are electrically neutral.

Ionic compounds are divided into:

- salts
  NaCl (sodium chloride), CaCl2 (calcium chloride) MgF2 (fluoride magnesium), Ca (NO3) 2 (calcium nitrate)
- Basic oxides
  MgO (magnesium oxide), Na2O (sodium oxide), BaO (barium oxide); Al2O3 (aluminum trioxide)
- hydroxides
  NaOH (sodium hydroxide), Ca (OH) 2 (calcium hydroxide), Mg (OH) 2 (magnesium hydroxide)

Figure 4. Ionic bonding

Ionic bonding tends to occur between electropositive metals and electronegative non-metals. Simple ions are single atomic cores surrounded by shells of electrons (whereas molecular ions contain several cores). Cations are cores of metallic elements, as found in metallic lattices. However, some nonmetallic elements will form anions where 'excess' electrons give the ions net negative charge. Individual ions are not usually stable as discrete entities as their charges lead to them interacting with other species. In ionic compounds each cation is surrounded by several anions, and vice versa.

The interspersing of positive and negative ions allows the ions to come close together until the repulsions balance the attractions. The bonding is the attraction between the ions and their 'counter-ions' in the lattice. So for example, in sodium chloride, each ion is surrounded by six oppositely charged ions and is equally 'bonded' to each. Students often find this difficult to grasp, as they tend to think that the charge on an ion should limit how many bonds it can form, so often assume each ion in NaCl only forms one 'proper' bond.

❖ LIMITATIONS AND DEVELOPMENTS

The framework here offers a number of advantages for teachers. It provides an intellectually honest set of simplifications that (a) undermines common misconceptions and (b) can underpin more advanced understanding of bonding and related topics such as reactions, ionisation, and chemical stability. Most importantly, it bases chemical explanation on physical forces, whereas with traditional teaching approaches most students come to see the molecular world in terms of the actions of atoms trying to satisfy needs.

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