Road map of quantum aspects of general chemistry

Notes on General Chemistry

http://quantum.bu.edu/notes/GeneralChemistry/RoadMapOfQuantumAspectsOfGeneralChemistry.pdf
Last updated Wednesday, October 24, 2007 9:40:35-05:00

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An atom of chemical matter consists of a compact nucleus surrounded by a diffuse cloud of electrons. Atoms differ in mass, due to different numbers protons (elements) and of neutrons (isotopes) in their nuclei. Atoms differ in chemical properties according to the anatomy of their electron clouds. Atomic electrons clouds are about 10^{-10} meters in diameter, and nuclear diameters are 10,000 times smaller. Atoms are wisps of nothingness surrounding incredibly dense centers.

Structure of atoms

Electron clouds have an inner core region and an outer valence region. Chemical properties reflect the screening of nuclear charge by the electron cloud core and the fine details of the electron cloud valence region. Electrons clouds have a concentric shell-like structure and this accounts for periodicity of chemical properties

Electrons clouds in atoms are described by quantum waves of potentiality. These quantum waves are not physical objects but rather ingredients of recipes that tells us how electron clouds interact with one another and with light.

Quantum waves

Quantum waves are mathematical functions that oscillate in both space and time. The oscillations in space are similar to the sinusoidal patterns familiar from geometry. The oscillations in time are sinusoidal too, but with the crucial additional aspect that the oscillation contains a part that is imaginary, that is, proportional to $\sqrt{-1} = i$.

The different character of the oscillations in space and in time account for chemical bonding on the one hand and the way atoms interact with light on the other hand.

The spatial parts of quantum waves can combine just like water waves, to make bigger waves when they meet crest to crest, or cancel each other out when they meet crest to trough. Quantum waves combining crest to crest are the origin of the stickiness of atoms for one another, that is, chemical bonding (more on the below).

When the temporal parts of quantum waves combine, the result depends on whether the wave oscillate on time with the same frequency or with different frequencies.

If the waves oscillate with the same frequency, then electron cloud made by combining such quantum waves no longer changes with time at all—*the electron cloud does not move*.

If the waves oscillate with different frequencies, then electron clouds made by combining such quantum waves oscillates with frequency equal to the difference of the frequencies of the combining waves; that is, the electron cloud that results *jiggles in space with difference frequency*.

Stickiness of atoms: Bonding

Atoms combine by sharing electrons through merging of electron clouds. The extent of sharing reflects the relative holding power of each nucleus for its electron cloud. The more equal the sharing, the less polar (ionic), more covalent the bond. The more unequal the sharing, the more polar (ionic), less covalent the bond.

Sharing of electrons between atoms takes place at the level of quantum waves. Quantum waves on separate atoms can interact to form new *molecular* quantum waves extending over each of the atoms in three ways.

. to form a wave concentrated between the atoms, known as a *bonding* wave

. to form a wave split to the far sides of each atom, known as an *antibonding* wave

. to exactly cancel on another, known as a *non-bonding* wave

All three kinds of molecular quantum wave are necessary to understand how atoms *stick together* in molecules. The shapes of the molecular quantum waves account for the three dimensional shape of molecules.

Seeing electrons, atoms, and molecules: Spectroscopy

Because atoms are so small, we cannot see them directly and so we can only explore their structure indirectly. The primary tool is the way they interact with light. Light causes the electrons in atoms to jiggle, like Jell-O jiggling in a bowl. The reverse is true too: Anything that causes electrons to jiggle will result in light. The frequencies of the jiggling must match the frequencies of light that can interact with the atom. Working from the frequencies of jiggling to the structure of the atom is known as *spectroscopy*.

. Electron quantum waves in atoms jiggle at UV and higher (X-Ray, gamma ray) frequencies

Just as light interacts with atoms through jiggling of their electrons, light interacts with molecules by causing their electrons to jiggle.

. Electron quantum wave in molecules jiggle at visible and UV frequencies. The colors in dyes in clothes are due to such jiggling of molecular electron waves.

A new feature of molecules, however, is that the atoms can also jiggle as a group. Such group jiggling is vibration of atoms with respect to one another and rotations of the atoms as a group.

. Vibrational jiggling of atoms in molecules is at IR frequencies. Our sensation of warmth is due to such vibrational jiggling.

. Rotational jiggling of atoms in molecules is at microwave frequencies. Microwave ovens heat by causing the water molecules in food to rotate and then bump into neighboring particles.