THE HYDROGEN ATOM

As Viewed by Quantum Mechanics

VOL 14

SUMMARY:

A description of the atom that is in accord with quantum mechanics is presented. This description explains the energy levels and line spectrum of the hydrogen atom and furnishes the basis of contemporary theory of chemical bonding. The electron position in the atom is considered in terms of probability, and the meaning of a 1s orbital is clarified with a digital computer plot, two analogies, and animation. The principal quantum number, n, is introduced together with its relation to energy levels, number of orbitals, and the number of nodal surfaces.

PURPOSE:

To show that an orbital represents an electron in motion which may be located at various positions with respect to the nucleus, but whose details of motion can be described only in terms of probability.

OUTLINE:

1. *Obtaining experimental energies from hydrogen atoms.*

   A brief review is given, reminding the student that the hydrogen atom spectrum provides experimental evidence for the energy-level diagram of the H atom. The spectrum also provides experimental confirmation for quantum mechanics since quantum mechanics can calculate the energy levels for the hydrogen atom based entirely on theoretical principles. Agreement with experimental data, even in complex detail, is the triumph of the theory.

2. *Developing a model for the calculated energies of hydrogen atoms.*

   Beginning with the electron-proton interactions in a hydrogen atom, the potential energy and kinetic energy are added to give the total energy. Using the mathematical procedures of quantum mechanics, the calculated energies are found to be in exact agreement with the experimental energies. Computers can be used to speed up the calculations.

3. *Developing the meaning of probability.*

   Because of the good agreement between calculated and experimental energies, other aspects of the quantum mechanical model are considered to be useful. Chief among these is its designation of electron positions as probabilities, since positions can never be measured directly. A game of darts helps to introduce the concept of probability as it is needed to interpret the meaning of an orbital in quantum mechanics.

4. *Developing an analogy to the 1s orbital.*

   To help illustrate the quantum mechanical meaning of the 1s orbital of hydrogen, an analogy of a hummingbird is given. A record of the various flowers visited by the hummingbird is kept and their positions with respect to the nest are plotted. A probability plot is obtained that has the same meaning as the 1s orbital.

5. *Describing the properties of the 1s orbital.*

   Computing devices are used to prepare a two-dimensional plot of a 1s orbital as dictated by quantum mechanics. Animation is used to discuss the three-dimensional properties of the orbital. The "satellite model" of the hydrogen atom is analyzed and found to be less satisfactory than quantum mechanics in accounting for the experimental evidence of atomic behavior. (This "satellite model" is often referred to as the older, conceptually simpler, but incorrect, Bohr theory.)

6. *Discussion of nodes, energies, and number of orbitals.*

   The nodal properties of 1s, 2s, and 2p orbitals are explained. The possible energies of the hydrogen atom are related to the principal quantum number, n. As the principal quantum number, n, increases in value, there are n^2 different possible orbitals, each with n nodal surfaces. For each value of n, there is only one spherically symmetrical orbital. As n increases, the complexity of the spatial orientation of the possible orbitals increases.

SUPPLEMENTARY MATERIAL:

The energies of the photons early in the film, and ionization energy later can be easily converted from the kcal/mole given to kJoule/mole, if desired, using the conversion 1 kcal = 4.184 kJoule. Thus 43.6 kcal/mole for red wavelengths becomes 182 kJoule/mole, 58.5 kcal/mole for blue becomes 246 kJoule/mole, and 65.9 kcal/mole for violet is 276 kJoule/mole. The ionization energy of the hydrogen atom is 1312 kJoule/mole.

Some persons may be bothered by nodes in 2s or 2p orbitals as indicated by questions such as, "How does the electron get from one side of node to the other?" The answer is that the model provided by quantum mechanics does not describe the details of electron motion, but only describes the probability of finding the electron at a given position.

The trajectory is a concept carried over from classical mechanics, which is not able to explain the properties of electrons in atoms. Hence we should not be surprised that trajectory questions are not readily answered. Perhaps a better and more truthful way to resolve the "trajectory paradox" is to emphasize that quantum mechanics is based on the concept of the electron behaving in an atom as a wave rather than as a particle. The idea of an electron as a wave should not be totally unfamiliar to students. For example, most have heard about the electron microscope which uses a beam of electrons in a device based on the same principles of optics used in a conventional microscope for visible light.

The complex equations manipulated so elegantly and graphically by the computer are equations of wave behavior involving three variables for three-dimensional space. Solving these equations yields mathematical results (the square of the wave function) which have the physical significance of probabilities. Thus the interpretation of these results as defining an orbital does not need the idea that an electron particle moves from one location to another on some mysterious "trajectory."

20 MINUTES IN COLOR

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