Quantum Mechanical Model

The purpose of this unit is to familiarize the chemistry student with the history, development and structure of the quantum mechanical atomic model in an attempt to answer the three questions concerning the electron.

Wave Mechanical Model

The work of Planck, Einstein, and Compton led to the acceptance of the quantum theory of energy that stated light comes in discrete quanta called photons and though mostly wave it also has particle properties. Their work also inspired Bohr to develop an atomic model explaining the behavior of electrons. But Bohr's model was doomed to fail because he modified classical mechanics to make his ideas work. A new physics was needed to solve the problems of the electron.

Matter Waves

In 1924 a French graduate student, **Louis de Broglie**, was impressed with Einstein's 1905 discovery and the dual nature of light. So impressed, that in his graduate thesis, he suggested that since nature is often symmetric, matter which is mostly particle should also have wave properties. These waves were not electromagnetic but a new kind of wave, **matter waves**.

Louis de Broglie

Using Einstein's equation, de Broglie developed an equation for the wavelength of matter waves, but had no experimental evidence to support his proposal.

$$\lambda = \frac{h}{mv}$$ **de Broglie's equation**

Amazing!

In 1927, the American physicists Clinton J. Davisson and Lester H. Germer verified de Broglie's hypothesis experimentally and four months later G. P. Thomson independently confirmed it. They were able to diffract a beam of electrons in a crystal of nickel and only waves can be diffracted. Therefore, if an electron that is particle can be diffracted, it must have wave properties. De Broglie was right matter has wave properties.

Exercise: Calculate the wavelength (m) of an oxygen molecule that is moving at a velocity of 444 m/s. (1 amu = 1.6606 x 10^{-27} kg)

"If that turns out to be true, I'll quit physics." -Max Von Laue
(on de Broglie's thesis on electrons having wave properties.)

Standing Waves

E. Schrödinger

In 1926 **Erwin Schrödinger** proposed the electron was a 3-D waveform circling the nucleus in a <u>whole number of wavelengths</u> allowing the waveform to repeat itself as a stable **standing wave** representing the energy levels of the Bohr model.

A standing wave is one that does not transfer energy or move but it does undergo resonance. That is to say, it can absorb energy from a nearby source which is oscillating at a proper frequency. A standing wave must also have a wavelength such that a whole number of wave segments fit within its setting. If the number of wave segments isn't a whole number then the wave will collapse.

Schrödinger suggested that de Broglie was correct about matter waves and the electrons are located in the atomic space according to standing wave frequencies. Therefore, the **energy** needed to change from one standing wave to another must be quantized in order to maintain a whole number of wavelengths and avoid collapsing. In support of his hypothesis, Schrödinger developed a mathematical equation to describe the wave-like behavior of the electron. The **Schrödinger wave equation** not only gave the correct energy levels for the hydrogen atom, but also was somewhat useful in atoms with more than one electron. This mathematical description of the details of atomic behavior became known as the **Wave-mechanical model**.

$$-\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V\psi=E\psi$$

Schrödinger Equation

Exercise: (a) Draw a line that is 6.00 cm long, then using the ends of this line as the ends of a standing wave, draw a standing wave that has two nodes in addition to the nodes at the ends.

(b) What is the wavelength of the standing wave above?
(c) How many 1.00 cm wavelengths will fit between the ends of this line?

Although, the wave-mechanical model was an improvement over the Bohr model, it worked with only the simplest of atoms. There was still something missing from the puzzle.

"If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet." –Niels Bohr

The Uncertainty Principle

W. Heisenberg

In 1925, **Werner Heisenberg** proposed from a purely theoretical view that it was impossible to know both the position and momentum of the electron simultaneously. This idea, which became known as the **uncertainty principle**, dealt with the probability of an electron's position in a region of space rather than its exact position.

The uncertainty principle was hard for many scientists to accept. If they accepted this idea of uncertainty, it meant that man was not capable of all knowledge and science might not be able to explain everything. But not even Einstein, who objected to the idea of uncertainty, could find a suitable reason not to accept the new idea.

The Quantum Mechanical Model

Max Born

In view of the uncertainty principle, in 1926, **Max Born** proposed that the solutions to the Schrödinger wave equation be taken as a description of the probability of finding electrons in certain areas of space. These solutions in the form of numbers are called **quantum numbers**.

Quantum numbers not only describe specific **quantized energy states** for the electron but also a set of probabilities for the **position** of the electron in a given energy level. These probable positions known as **atomic orbitals** refer to a region in space where an electron might be found, whereas an orbit is a definite path in space. Since the orbital does not have definite boundaries, it is sometimes referred to as an **electron cloud.**

Three of the quantum numbers came directly from the Schrödinger equation. A fourth quantum number (m_s), independent of the other three, was proposed in 1925 by **George Uhlenbeck** and **Samuel Goudsmit** after they discovered the electron seems to have a spin. Oddly enough, the spin of the electron had been observed in 1920 by Otto Stern and Walter Gerlach years before the theoretical description was suggested and their experiment provided the empirical evidence for the electron's spin.

George Uhlenbeck

Paul Dirac

In 1930, **Paul Dirac** revised the Wave Equation to include relativity and the spin quantum number (m_s) arose naturally during the solution of **Dirac's Equation**. Together, these four quantum numbers can be used to describe the probable location of each electron. More importantly, quantum numbers can describe the **electron configurations** (electron arrangements) in all atoms. The Schrödinger equation, the Heisenberg Uncertainty Principle and the quantum numbers produced a purely mathematical view of the atom and the arrangement of the electrons. Thus, quantum physics was born.

"… the existence of uncertainty need not be a source of humiliation for science … If a tiny, but crucial, uncertainty is part of the fabric of the universe, it is a tribute to scientists to have discovered the fact." --Isaac Asimov

Think It Through

- What are three main questions about the electron?
- Why bother with the electron?
- What are matter waves?
- Do you know de Broglie equation?
- What is a standing wave?
- What is the Uncertainty Principle?
- What is Quantum Mechanics?
- What are atomic orbitals?
- What are quantum numbers?
- What is an electron configuration?
- How would you describe an atom, today?

Vocabulary

orbitals matter waves electron cloud standing wave

People

Louis de Broglie	Erwin Schrödinger	Werner Heisenberg
Paul Dirac	Max Born	George Uhlenbeck
Samuel Goudsmit		

Exercises

______________________ Calculate the velocity of a hydrogen molecule that has a wavelength of 1.120×10^{-10} m.

______________________ Calculate the wavelength (m) of an electron traveling at 1.24×10^{7} m/s. (electron = 9.11×10^{-31} kilograms)

______________________ Calculate the velocity of a neutron with a wavelength of 95.0 pm.

"What we observe as material bodies and forces are nothing but shapes and variations in the structure of space."
– Erwin Schrodinger