Chapter 6

Quantum Theory and the
Electronic Structure of Atoms
Part 1
Topics

- The nature of light
- Quantum theory
- Bohr’s theory of the hydrogen atom
- Wave properties of matter
- Quantum mechanics
- Quantum numbers
- Atomic orbitals
- Electron configuration
- Electron configuration and the periodic Table
6.1 The Nature of Light

- **electromagnetic radiation**: form of energy that acts as a wave as it travels
  - includes: X rays, Ultraviolet, visible light, infrared light, microwaves, and radio waves
  - It travels in waves at a speed of $2.9979 \times 10^8$ m/s in a vacuum

- All forms of EMR are combined to form electromagnetic spectrum
The whole range of frequencies is called "Spectrum". Visible light accounts for only a small part of the spectrum.
Electromagnetic Spectrum

Wavelength (nm)

$10^{-3}$ $10^{-1}$ 10 $10^{3}$ $10^{5}$ $10^{7}$ $10^{9}$ $10^{11}$ $10^{13}$

Frequency (Hz)

$10^{18}$ $10^{16}$ $10^{14}$ $10^{12}$ $10^{10}$ $10^{8}$ $10^{6}$ $10^{4}$

Type of radiation

- Gamma rays
- X rays
- Ultraviolet
- Visible
- Infrared
- Microwave
- Radio waves

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Wave Characteristics

Crest

Origin

Wavelength

Trough

Amplitude
Wavelength

- $\lambda =$ Greek letter lambda
- distance between points on adjacent waves (consecutive peaks or troughs)
- Units used are in nm ($10^9$nm = 1m)

Frequency

- $\nu =$ Greek letter nu
- number of wave cycles that passes a point in a second. $10^8$ cycles/s = $10^8$ s$^{-1}$
- $=10^8$ Hertz = $10^8$ Hz
- in 1/second (Hertz = Hz)

Amplitude

The vertical distance from the midline of waves to the top of the peak or the bottom of the trough
Electromagnetic radiation propagates through space as a wave moving at the speed of light.

Equation:

\[ c = \lambda \nu \]

\[ \nu = \frac{c}{\lambda} \]

- \( c \) = speed of light, a constant \((2.998 \times 10^8 \text{ m/s})\)
- \( \lambda \) (lambda) = wavelength, in meters
- \( \nu \) (nu) = frequency, in units of hertz (hz or sec\(^{-1}\))
Wave Calculation

The wavelength of a laser pointer is reported to be 663 nm. What is the frequency of this light?

\[ \nu = \frac{c}{\lambda} \]

\[ \lambda = 663 \text{ nm} \times \frac{10^{-9} \text{ m}}{\text{nm}} = 6.63 \times 10^{-7} \text{ m} \]

\[ \nu = \frac{3.00 \times 10^8 \text{ m/s}}{6.63 \times 10^{-7} \text{ m}} = 4.52 \times 10^{14} \text{ s}^{-1} \]
6.2 Quantum Theory

- According to the old views, matter could absorb or emit any quantity (frequency) of energy.

- Max Planck studied the radiation emitted by solid bodies heated to incandescence.

- Max Planck found that the cooling of hot objects couldn’t be explained by viewing energy as a wave.

- Max Planck postulated that energy can be gained (absorbed) or lost (emitted in discrete quantities.
Mack’s Planck suggested that an object absorbs or emits energy in the form of small packets of energy called quanta. That is the energy is quantized.

- **Quantum** - the minimum amount of energy that can be gained or lost by an atom (energy in each packet)

\[ E = h\nu \]

- \( h \) = Planck’s constant = 6.626 \times 10^{-34} \text{ J.s}

- Thus energy seems to have particulate properties
Photoelectric Effect

- Albert Einstein used Planck’s theory to explain photoelectric effect.
- Electrons ejected from a metal’s surface when exposed to light of certain frequency.
- Einstein suggested that a beam of light is really a stream of particles.
- Einstein called the particles of light photons (packets of light energy) and deduced that

\[ E_{\text{photon}} = h\nu \]
Only light with a frequency of photons such that $h\nu$ equals the energy that binds the electrons in the metal is sufficiently energetic to eject electrons.

If light of higher frequency (enough to break the electrons free) is used, electrons will be ejected and will leave the metal with additional kinetic energy.

$$h\nu = KE + W \text{ (the binding energy of electrons in the metal)}$$

Light of at least the threshold frequency and of greater intensity will eject more electrons.
Calculate the energy (in joules) of a photon with a wavelength of 700.0 nm

\[ \lambda = 700.0 \text{ nm} \times \frac{10^{-9} \text{ m}}{\text{nm}} = 7.00 \times 10^{-7} \text{ m} \]

\[ \nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m/s}}{7.00 \times 10^{-7} \text{ m}} = 4.29 \times 10^{14} \text{ s}^{-1} \]

\[ E = h \nu = (6.63 \times 10^{-34} \text{ J} \cdot \text{s})(4.29 \times 10^{14} \text{ s}^{-1}) \]

\[ E = 2.84 \times 10^{-19} \text{ J} \]
Example

Calculate the wavelength (in nm) of light with energy 7.83x $10^{-19}$ J per photon. In what region of the electromagnetic radiation does this light fall?

\[
\nu = \frac{7.83 \times 10^{-19} \text{ J}}{6.63 \times 10^{-34} \text{ J} \cdot \text{s}} = 1.18 \times 10^{15} \text{ s}^{-1}
\]

\[
\lambda = \frac{3.00 \times 10^{8} \text{ m} \cdot \text{s}^{-1}}{1.18 \times 10^{15} \text{ s}^{-1}} = 2.53 \times 10^{-7} \text{ m} \quad \text{or} \quad 253 \text{ nm}
\]

Ultraviolet region
Light possesses wave and particle properties

- Dilemma caused by Einestien’s theory - is light a wave or particle?
- Conclusion: Light must have particle characteristics as well as wave characteristics
- This concept is found to be applicable for all matter.
6.3 Bohr’s Theory of the Hydrogen Atom

- Planck’s theory along with Einstein’s ideas not only explained the photoelectric effect, but also made it possible for scientists to unravel the idea of atomic line spectra.
Emission Spectrum

Main experiments led to the information related to atom:

- Thompson discovery of electron
- Rutherford discovery of nucleus
- Study of emission of spectrum

- The emission spectrum of a substance can be seen by energizing a sample of material with either a thermal energy or other some form of energy

- The glow of a red–hot object is the emitted radiation in the visible region

- The emission spectrum of the sun or the heated solid is continuous that is all wavelengths of visible light are present in each spectrum
When sunlight is dispersed by rain drops the rainbow is produced; that is a **continuous spectrum** is produced.

- continuous spectrum contains all colors; that is all wavelengths of the visible light
The Continuous Spectrum

The different colors of light correspond to different wavelengths and frequencies.

- $\lambda \sim 650$ nm
- $\lambda \sim 575$ nm
- $\lambda \sim 500$ nm
- $\lambda \sim 480$ nm
- $\lambda \sim 450$ nm
Atomic Line Spectra

- **Line spectra**: emission of light only at specific wavelengths
- Every element has a unique emission spectrum
- Often referred to as “fingerprints” of the element
Atomic Line Spectra

[Diagram showing a discharge tube, slit, prism, and photographic plate with a line spectrum.]
- Line spectrum
- Unique to each element, like fingerprints!
- Very useful for identifying elements
Bright-line Spectra

![Diagram of bright-line spectra for various elements including Lithium (Li), Sodium (Na), Potassium (K), Calcium (Ca), Strontium (Sr), Barium (Ba), Hydrogen (H), Helium (He), Neon (Ne), and Argon (Ar).]
The Line Spectrum of Hydrogen

Main experiments led to the information related to atom:
- Thompson discovery of electron
- Rutherford discovery of nucleus
- Study of emission of light by excited hydrogen atom

When $H_2$ molecules absorb energy, some H-H bonds are broken and excited H-atoms will be produced.

The excited H-atoms release energy by emitting light at various wavelengths that is known as emission spectrum of H-atoms.
Spectroscopic analysis of the hydrogen spectrum...

H receives a high energy spark

H-H bonds are broken and H atoms are excited

Hydrogen emission spectrum is called “line spectrum”
Line Spectrum of Hydrogen

- **The Rydberg equation**

\[ \frac{1}{\lambda} = R_\infty \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \]

- **Balmer** (initially) and **Rydberg** (later) developed the equation to calculate all spectral lines in the hydrogen spectrum

- **Rydberg constant** = 1.09737316 m⁻¹

- \( n_1 \) and \( n_2 \) are positive integers where \( n_2 > n_1 \).
Significance of the line spectrum of H-atom

- Only **certain energies are allowed** for the electron in the hydrogen atom.

- That is, the energy of an electron in a hydrogen atom is **quantized**.

- Changes in energy between discrete energy levels in hydrogen will produce only certain wavelengths of emitted light.

- **The discrete line spectrum of hydrogen shows that only certain energies are possible.**

- The electron energy levels are **quantized**. If all energy levels are allowed the spectrum would be continuous.
The Bohr Model

- Niels Bohr (Danish physicist) 1885-1962
- Developed a quantum model for H atom that explained the emission line spectrum
- Electron moves around the nucleus only in certain allowed circular paths called orbits, in which it has a certain amount of energy
- The electrons were attracted to the nucleus because of opposite charges.
- But electron does not fall in to the nucleus because it is moving around and it does not radiate energy.
The Bohr Atom

- Only valid energies for hydrogen’s electron are allowed with the following equation:

- The energies that the electron in a hydrogen atom can possess is given by the equation:

\[ E_n = -2.18 \times 10^{-18} J \left( \frac{1}{n^2} \right) \]

- Negative sign means that the energy of electron bound to nucleus is lower than it would be if it were at infinite distance \((n=\infty)\) from the nucleus.

- The energy of an electron in an atom is lower than that of the free electron.

\( n \) is an integer = 1, 2, 3, ..
The quantity of energy absorbed or emitted depends on the difference of energy levels between initial and final state.

The higher the excited state, the farther away the electron from nucleus and the less tightly is held by nucleus.

$E=0$ is set at an distance of $\infty$ away from the nucleus and becomes more negative as the electron comes closer to the nucleus.

$$E_n = -2.18 \times 10^{-18} J \left( \frac{1}{\infty^2} \right) = 0$$
- An electron can pass only from one orbit to another. **Absorption or emission** of $E$ will occur.

- **Putting Energy** into the atom moves the electron away from the nucleus.
  - From **ground state** to **excited state**.

- When it returns to ground state it **gives off (emits)** light of a certain energy.

- Ground state is the most stable one. The stability diminishes when $(n)$ increases.

- Wavelength of a photon released or absorbed can be calculated by using the equation

$$\Delta E = h\nu = h\frac{c}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E}$$
For a mole of hydrogen atom in the ground state

\[ E_n = -2.178 \times 10^{-18} \frac{J}{\text{particle}} \times 6.02 \times 10^{23} \frac{\text{particles}}{1\text{mol}} \times \frac{1\text{kJ}}{1000\text{J}} \times \frac{1}{n^2} = -1312 \frac{\text{kJ}}{\text{mol}} \]

\[ E_n = \frac{-1312 \text{kJ}}{n^2 \text{ mole}} \]
Bohr’s theory explains the line spectrum of hydrogen

- Each spectral line in the hydrogen spectrum corresponds to a specific transition from one orbit to another.
- Electrons moving from ground state to higher states require energy; an electron falling from a higher to a lower state releases energy.