Electronic Structure of Atoms

AP Chemistry Lecture Outline

**Electronic structure**: the arrangement of electrons in an atom

**Quantum mechanics**: the physics that correctly describes atoms

**Electromagnetic radiation** (i.e., light)

--- waves of oscillating electric (E) and magnetic (B) fields

--- source is vibrating electric charges

**Characteristics of a Wave**

- Crest
- Amplitude, A
- Wavelength, \( \lambda \)
- Trough

**Frequency**: the number of cycles per unit time (usually sec)

--- unit is Hz, or \( s^{-1} \)

**Electromagnetic spectrum**: contains all of the “types” of light that vary according to frequency and wavelength

--- radio, microwaves, infrared, visible, ultraviolet, X rays, gamma rays, cosmic rays

--- visible spectrum ranges only from ~400 to 700 nm (a very narrow band of spectrum)

The speed of light in a vacuum (and in air) is constant: \( c = 3.00 \times 10^8 \text{ m/s} \)

--- Equation:

In 1900, Max Planck assumed that energy can be absorbed or released only in certain discrete amounts, which he called **quanta**. Later, Albert Einstein dubbed a light “particle” that carried a quantum of energy a **photon**.

--- Equation:
EX. A laser used in eye surgery to fuse detached retinas emits radiation with a frequency of \(4.69 \times 10^{14}\) Hz. Find the wavelength of this radiation and the energy of one of its photons.

In 1905, Einstein explained the photoelectric effect using Planck’s quantum idea. 

-- only light at or above a threshold freq. will cause \(e^-\) to be ejected from a metal surface

Einstein also expanded Planck’s idea, saying that energy \textbf{exists} only in quanta.

Light has both wavelike and particle-like qualities, and...

\textbf{Line Spectra}

Ordinary white light is dispersed by a prism into a...

From the gas in a nearly-evacuated gas-discharge tube, we instead get a...

Niels Bohr took Planck’s quantum idea and applied it to the \(e^-\) in atoms.

--

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-- Bohr’s assumed his circular orbits had particular energies, given by:

\[
R_H = \text{Rydberg constant} = 2.18 \times 10^{-18} \text{ J}
\]

\[
n = 1, 2, 3, \ldots \ (the \text{ principal quantum number})
\]

The more (\(\sim\)) an electron’s energy is...

The less (\(\sim\)) an electron’s energy is...

When \(n\) is very large, \(E_n\) goes to zero, which is larger than anything (\(\sim\)).

-- Bohr stated that \(e^-\) could “jump” from one level to another, absorbing light of a particular freq. to “jump up” and releasing light of a particular freq. to “fall down.”

Equation:

-- Bohr’s model only worked for atoms with a single \(e^-\).

EX. Calculate the wavelength of the hydrogen emission line that corresponds to the transition of an electron from the \(n = 5\) to \(n = 2\) state.
The Wave Behavior of Matter

Since light (traditionally thought of as a wave) behaves as both a wave and a particle, Louis de Broglie suggested that matter (traditionally thought of as particles) might also behave like both a wave and a particle. He called these matter waves.

-- The wavelength of a sample of matter is given by:

EX. At what velocity must a proton be moving for it to exhibit a wavelength of 800 pm?

A wave is smeared out through space, i.e., its location is not precisely defined. Since matter exhibits wave characteristics, there are limits to how precisely we can define an e\(^-\)'s location.

-- the limitation also applies to...

-- Heisenberg's uncertainty principle:

Schroedinger’s wave equation (1926) accounts for both wave and particle behaviors of e\(^-\)s.

-- Solutions to the wave equation yield wave functions, symbolized by \(\Psi\), which have no physical meaning, but \(\Psi^2\) at any point in space gives the probability that you’ll find an e\(^-\) at that point. \(\Psi^2\) is called the probability density, which gives the electron density.

-- Orbitals describe a specific distribution of electron density in space.

    Each orbital has a characteristic shape and energy.
Quantum numbers are used to describe where an e\textsuperscript{−} is in an atom.

1. principal quantum number, \( n \)
   -- integers 1, 2, 3,...
   -- correspond to the energy level of the electrons
   -- all orbitals having the same \( n \) are called an electron shell (e.g., 2s and 2p)

2. azimuthal quantum number, \( l \)
   -- integers from 0 up to \((n - 1)\)
   -- this number defines the shape of the orbital
   -- \( s = 0, \ p = 1, \ d = 2, \ f = 3 \)
   -- you should know the shapes and orientations of the s, p, and d orbitals
     \( s, \ p_x, \ p_y, \ p_z, \ d_{yz}, \ d_{xz}, \ d_{xy}, \ d_{x^2−y^2}, \ d_{z^2} \)
   -- degenerate orbitals have the same energy (e.g., all five 4d orbitals)
   -- In general, for a given shell, the energies of orbitals go: \( s < p < d < f \)

3. magnetic quantum number, \( m_l \)
   -- integers from \(-l\) to \( l\)
   -- describes the orientation of an orbital in space

4. electron spin quantum number, \( m_s \)
   -- only two values: \( +\frac{1}{2} \) or \(-\frac{1}{2} \) (sometimes called “spin-up” and “spin-down”)
   -- Pauli exclusion principle: no two electrons in an atom may have the same set
     of four quantum numbers (i.e., an orbital may hold only two electrons,
     and they must have opposite spins)

EX.  (a) Predict the number of subshells in the third shell.
(b) Give the label for each of these subshells.
(c) How many orbitals are in each of these subshells?

EX.  What are the values of \( n \) and \( l \) for the following sublevels?
     \( 2s \quad 3d \quad 4p \quad 5s \quad 4f \)

EX.  List the first three quantum numbers for the highest-energy electron in each of the
     following atoms, assuming each atom is in its ground state.
     \( Al \quad Zr \quad Kr \quad Eu \)
In a many-electron atom, each e\textsuperscript{−} is attracted to the nucleus and repelled by the other e\textsuperscript{−}.

--- effective nuclear charge, \( Z_{\text{eff}} \): the net (+) charge attracting an e\textsuperscript{−}

Equation:

\[ Z_{\text{eff}} = \text{effective nuclear charge} \]

-- Within a given electron shell, s e\textsuperscript{−}s have the greatest \( Z_{\text{eff}} \), f e\textsuperscript{−}s the least.
-- The (+) charge “felt” by the outer e\textsuperscript{−} is always less than the nuclear charge.

This effect, due to the core (or kernel)\textsuperscript{ electrons}, is called the...

**Electron Configurations**: Where are the e\textsuperscript{−}? (probably)

\[
\begin{array}{ll}
H & \text{Al} \\
He & \text{Ti} \\
Li & \text{As} \\
N & \text{Xe}
\end{array}
\]

**Aufbau Principle**: e\textsuperscript{−} will take the lowest-energy orbital that is available

**Hund’s Rule**: for degenerate orbitals, each must have one e\textsuperscript{−} before any take a second

**Orbital Diagrams**…show spins of e\textsuperscript{−} and which orbital each is in

\[
\begin{array}{cccccccc}
O & & & & & & & \\
& 1s & 2s & 2p & 3s & 3p & & \\
& \text{paired e}\textsuperscript{−} & & & & & \text{unpaired e}\textsuperscript{−} \\
P & & & & & & & \\
& 1s & 2s & 2p & 3s & 3p & & \\
& \text{valence e}\textsuperscript{−}: & & & & & \\
\end{array}
\]

**Sections of Periodic Table to Know**: s-block, p-block, d-block, f-block

**Shorthand Electron Configuration** (S.E.C.)

1. Put symbol of noble gas that precedes element in brackets.
2. Continue writing e\textsuperscript{−} configuration from that point.

\[
\begin{array}{ll}
S & \text{Co}
\end{array}
\]
Brief Review of the Periodic Table

alkali metals:
alkaline-earth metals:
transition elements/metals:
chalcogens:
halogens:
noble gases:
lanthanide elements:
actinide elements:
representative (main block) elements:

EX. What family of elements has an $ns^2$ valence electron configuration?

Anomalies in the Electron Configurations
Your best guide to writing electron configurations is the periodic table. There are, however, a few exceptions.

e.g., Cr:

Cu:

These exceptions are due to the closeness in energy of the upper-level orbitals. Other exceptions are Nb, Mo, Ru, Rh, and Ag. Note that all of the above exceptions have a single valence-level s electron.