Atomic Model

Line Spectra of Atomic Gases
Emission spectra of gases of atoms are composed of discrete lines (i.e., the wavelengths of the emitted light from the atoms are discrete).

Why?

Neon (Ne)
Mercury (Hg)
Solar absorption spectrum

Emission spectra of gases of atoms are composed of discrete lines (i.e., the wavelengths of the emitted light from the atoms are discrete).

Lyman series
Balmer series
Paschen series

Rydb erg’s description for the Line Spectrum of Hydrogen
Lyman series
Balmer series
Paschen series

where \( R = 1.097 \times 10^7 \text{m}^{-1} \) is the Rydberg constant.

Observed Line Spectra of Hydrogen

Energy of an Atom

\[ E = K + U = \frac{1}{2}mv^2 - \frac{kZe^2}{r} \]

Centripetal force
Electric force

But this doesn’t lead to quantization of \( E \). To proceed, we need some hypotheses.
Bohr’s Model of Atom
Bohr hypothesized that the angular momentum of electrons in an atom is quantized:

\[ mvr_n = \frac{nh}{2\pi} \quad n = 1, 2, 3, \ldots \]

De Broglie suggested standing particle waves as an explanation for Bohr’s angular momentum assumption.

\[ 2\pi r_n = n\lambda = n\frac{h}{\cancel{p}} = \frac{nh}{mv_n} \]

which leads to Bohr’s hypothesis given above.

Bohr’s Model for Hydrogen-like Atoms
By using \( \frac{mv_n}{2\pi} \) (p. 7), \( mv^2 = \frac{kZe^2}{r} \) and \( E = -\frac{kZe^2}{2r} \) (p. 6), Bohr derived an expression for the energy levels of an atom with atomic no. \( Z \):

\[ E_n = \left( \frac{2\pi^2 mk^2 \phi^4 \lambda^4}{\hbar^2} \right) \frac{Z^2}{n^2} \quad n = 1, 2, 3, \ldots \]

\[ E_n = -\left( 2.18 \times 10^{-18} J \right) \frac{Z^2}{n^2} \quad n = 1, 2, 3, \ldots \]

\[ = -\left( 13.6 \text{ eV} \right) \frac{Z^2}{n^2} \]

Ionization Energy of \( \text{Li}^{2+} \)
\( \text{Li}^{2+} \) is a lithium atom (\( Z=3 \)) with only one electron. What is the ionization energy of \( \text{Li}^{2+} \) in the ground state? (n.b. Ionization energy is the minimum energy required to just free an electron from its atom.)

1. -13.6 eV)(3^2/12)
2. +(13.6 eV)(3^2/12)
3. -(13.6 eV)(3^2/2^2)
4. +(13.6 eV)(3^2/2^2)
5. Cannot be determined

Ionization Energy of \( \text{Li}^{2+} \)
Ionization energy is the minimum energy required to just free an electron from its atom. So the final state of the electron should have zero total energy (i.e., \( K = U = 0 \).) Thus, the ionization energy is \( 0 - E_n = -E_n \).

Because an \( \text{Li}^{2+} \) ion has only one orbiting electron, it is like a hydrogen atom with a nuclear charge of +3e. We can use Bohr’s model to find the ground state energy, \( E_1 \):

\[ E_n = -\left( 13.6 \text{ eV} \right) \frac{Z^2}{n^2} = -\left( 13.6 \text{ eV} \right) \frac{3^2}{1^2} = -122 \text{ eV} \]

Ionization energy = +122 eV

Four Quantum Numbers of an Atom
The full quantum mechanical description of atoms actually involves solving the Schrödinger’s equation named after Erwin Schrödinger who shared the Nobel Prize in 1933 for his contribution leading to quantum mechanics. The solution to Schrödinger’s equation reveals that four different quantum numbers are required to describe the electronic state of an atom.

1. The principal quantum number \( n \). This number determines the total energy of the atom and can have only integer values. It is the same \( n \) that appears in Bohr’s Energy Levels.

\[ n = 1, 2, 3, \ldots \]

2. The orbital quantum number \( \ell \).

This number determines the orbital angular momentum, \( L \), of the electron by:

\[ L = \sqrt{\ell(\ell+1)} \frac{\hbar}{2\pi} \]
Four Quantum Numbers of an Atom

3. The magnetic quantum number $m_l$

This number characterizes the orientation (or the $z$ component) of the angular momentum vector of the electron.

$$L_z = m_l \frac{\hbar}{2\pi}$$

$m_l = -\ell, \ldots, -2, -1, 0, 1, 2, \ldots, +\ell$

Note that there are $2\ell + 1$ values of $m_l$.

Pauli Exclusion Principle

No two electrons can be in the same quantum state. In other words, no two electrons can possess the same set of four quantum numbers.

The consequence of the Pauli Exclusion Principle is that when we fill the energy levels of an atom with electrons (where there are $Z$ of them), we can only fill one electron in each distinguishable slot (i.e., sub-orbital and spin state) available in an energy level at a time, from low to high energies.

Number-letter-number notation for electronic configuration of atoms

The number of filled electron states for the $l$ orbital. The maximum of this number is $2(2l + 1)$.

A letter representing the value of $l$ (see table below)

<table>
<thead>
<tr>
<th>Value of $l$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Letter</td>
<td>s</td>
<td>p</td>
<td>d</td>
<td>f</td>
<td>g</td>
<td>h</td>
<td>i</td>
</tr>
</tbody>
</table>

Filling the electrons – Shell Model

The no. of electrons an atom possesses is $Z$. By filling the electrons of an atom according to the Shell Model, which is based on the four quantum numbers, we can understand the chemical properties of the elements as grouped in the periodic table. From the periodic table, the chemical property of an atom is largely determined by its “outermost shell” electrons.

<table>
<thead>
<tr>
<th>Shell no. (n)</th>
<th>Max. no. of e</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>32</td>
</tr>
<tr>
<td>5</td>
<td>50</td>
</tr>
<tr>
<td>6</td>
<td>72</td>
</tr>
<tr>
<td>7</td>
<td>98</td>
</tr>
</tbody>
</table>
### Filling the electrons – Shell Model

The table shows some examples of electronic configurations of elements successfully predicted by the Shell Model.

These are what would give the lowest possible energy the atoms can have and so is called the **ground-state**. If the electronic configuration of an atom deviates from that of the ground-state, the atom is in an **excited state**. De-excitation of an atom leads to emissions.

<table>
<thead>
<tr>
<th>Element</th>
<th>Number of Electrons</th>
<th>Configuration of the Electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen (H)</td>
<td>1</td>
<td>1s^1</td>
</tr>
<tr>
<td>Helium (He)</td>
<td>2</td>
<td>1s^2</td>
</tr>
<tr>
<td>Lithium (Li)</td>
<td>3</td>
<td>1s^2 2s^1</td>
</tr>
<tr>
<td>Beryllium (Be)</td>
<td>4</td>
<td>1s^2 2s^2 2p^2</td>
</tr>
<tr>
<td>Boron (B)</td>
<td>5</td>
<td>1s^2 2s^2 2p^3</td>
</tr>
<tr>
<td>Carbon (C)</td>
<td>6</td>
<td>1s^2 2s^2 2p^2 2p^6</td>
</tr>
<tr>
<td>Nitrogen (N)</td>
<td>7</td>
<td>1s^2 2s^2 2p^3 2p^5</td>
</tr>
<tr>
<td>Oxygen (O)</td>
<td>8</td>
<td>1s^2 2s^2 2p^4 2p^6</td>
</tr>
<tr>
<td>Flouorne (F)</td>
<td>9</td>
<td>1s^2 2s^2 2p^5 2p^6</td>
</tr>
<tr>
<td>Neon (Ne)</td>
<td>10</td>
<td>1s^2 2s^2 2p^6</td>
</tr>
<tr>
<td>Sodium (Na)</td>
<td>11</td>
<td>1s^2 2s^2 2p^6 3s^1</td>
</tr>
<tr>
<td>Magnesium (Mg)</td>
<td>12</td>
<td>1s^2 2s^2 2p^6 3p^6 3s^2</td>
</tr>
<tr>
<td>Aluminum (Al)</td>
<td>13</td>
<td>1s^2 2s^2 2p^6 3p^6 3s^2 3p^3</td>
</tr>
</tbody>
</table>