**Inorganic Chemistry 1**

**QUANTUM THEORY**

## QUANTUM NUMBERS

***Principle Quantum Number, $n$: Orbital Shape / Azimuthal Quantum Number, $l$ : Orbital-Orientation / Magnetic Quantum Number, $m_l$ : Spin-Orientation Quantum Number, $m_s$***

1. The Schrödinger equation has solutions only for specific energy values. In other words, the energy of an atom is restricted to certain values (quantized)

2. The three dimensional region in which an electron can be found within an atom is known as an orbital.

3. An orbit is two-dimensional (circle or ellipse) - the path where the electron circulate around the nucleus.

4. Just as energy is quantized, orbitals have specific shapes and orientations.

5. Each electron in an atom has 3 quantum number that describes a particular energy, orbital shape and orbital orientation. A fourth quantum number with a value of $+\frac{1}{2}$ or $-\frac{1}{2}$ describes spin orientation.

Quantum Numbers
- Principal Quantum number, $n$
- Azimuthal Quantum number, $l$ (orbital-Shape Quantum number)
- Magnetic Quantum number, $m_l$ (orbital-Orientation Quantum number)
- Spin Orientation Quantum number, $m_s$

a) Principal Quantum number, $n$

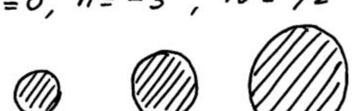
- determining the energy of an electron.
- $n = 1, 2, 3, 4, \ldots$

$n = 1$ ($E_1$) ; $n = 2$ ($E_2$); etc.

* The most stable energy of an electron corresponds to $n = 1$ (ground state)

* $n$ must be a positive integer (ie $n = 1, 2, 3 \ldots 8, 9$ etc)

$n = 0$, $n = -3$, $n = 5/2$ - not acceptable



$n=1$ $n=2$ $n=3$

← size of atomic orbitals

Each $n$, can accommodate a maximum number of $2n^2$ electrons

* The principal quantum numbers tells us something about the size of an atomic orbital. That is, the more energy the electron has, the more it is spread out in space.
* The higher the principal quantum number, the more energy the electron has and the greater its average distance from the nucleus.
* As $n$ increases, the energy of the electron increases as well and the electron, on average is farther away from the nucleus and is not as tightly bound to it.

## b) Azimuthal Quantum Number, $l$

* The shape of the orbital is determined by the value of $l$.
* The value of $l$ are limited by the value of $n$
* The value of $l$ can be zero or any positive integer smaller than $n$

  i.e. $l = 0, 1, 2, \ldots (n-1)$

  eg. If $n = 3$ : $l = 0$, $l = 1$, and $l = 2$ (3 subshells)

  If $n = 4$ : $l = 0$, $l = 1$, $l = 2$, and $l = 3$ (4 subshells)

| $l$ value | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| subshell | s | p | d | f |

If $n = 3$ $l = 0$ : the subshell is 3s

$n = 3$ $l = 2$ : the subshell is 3d

$n = 2$ $l = 1$ : the subshell is 2p

| $n$ | 1 | 2 | | 3 | | | 4 | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $l$ | 0 | 0 | 1 | 0 | 1 | 2 | 0 | 1 | 2 | 3 |
| level | 1s | 2s | 2p | 3s | 3p | 3d | 4s | 4p | 4d | 4f |

* The number of orbital types within a principal energy level equals $n$.

  $n = 3$ : 3p, 3s, 3d (3 subshells)

  $n = 4$ : 4s, 4p, 4d, 4f (4 subshells)

Review Exercises

$Q_1$. Give the subshell designation for an electron with the quantum numbers

(a) $n = 6$, $l = 1$ (b) $n = 4$; $l = 3$ (c) $n = 6$; $l = 2$

$Q_2$. Explain the following:

a) 2d is an incorrect subshell designation

b) $n = 3$; $l = 3$ is incorrect for a subshell.

c) $n = 4$; $l = 4$ is incorrect for a subshell.

d) 3f doesnot exist.

c) Magnetic Quantum Number, $m_l$

* $m_l$ relates to its orientation.
* $m_l$ can be any integral value, including zero, between $l$ and $-l$.

ie $m_l = l, \ldots\ldots +1, 0, -1, \ldots\ldots -l$

* $l$ values limits the orientations, $m_l$
* The total number of orbitals/orientations in a shell equals $n^2$.

eg. $n = 3$ : there are $3^2$ orbitals = 9 orbitals

$n = 3$ $l = 0$ $m_l = 0$ } 3s (1 orbital) $(2\times0)+1 = 1$

$l = 1$: $m_l = +1$, $m_l = 0$, $m_l = -1$ } 3p (3 orbitals) $(2l+1) = (2\times1)+1 = 3$

$l = 2$: $m_l = +2$, $m_l = +1$, $m_l = 0$, $m_l = -1$, $m_l = -2$ } 3d (5 orbitals) $(2l+1) = (2\times2)+1 = 5$

Total = 9 orbitals

* For each value of $l$:
No. of orbital $= (2l+1)$

$l = 2$ (d orbital) : total no. of orbital $= 2(2)+1 = 5$

$l = 3$ (f orbital) : total no. of orbital $= 2(3)+1 = 7$

**SUMMARY**

1. $n = 1, 2, 3, \ldots$ (energy level)

2. Within each $n$ – there are $n$ subshells.
   - designated as $s\ (l=0)$, $p\ (l=1)$, $d\ (l=2)$, $f\ (l=3)$

3. Each subshells of $s, p, d, f$ – there are number of orbitals. ie one $s$ orbital; three $p$ orbitals ($p_x, p_y, p_z$); five $d$ orbitals ($d_{xy}, d_{xz}, d_{yz}, d_{z^2}, d_{x^2-y^2}$)

   * Total no. of orbitals in shell equals $n^2$.

- Subshells (sublevels) are $s, p, d, f, g \ldots$

  $l=0$ is an $s$-sublevel ($s$ = sharp/shape)
  $l=1$ is an $p$-sublevel ($p$ = principal)
  $l=2$ is an $d$-sublevel ($d$ = diffuse)
  $l=3$ is an $f$-sublevel ($f$ = fundamental)

$s$-sublevel has one orbital $s$

$p$-sublevel has three orbital $p_x$, $p_y$ and $p_z$

$d$-sublevel has five orbital $d_{xy}, d_{xz}, d_{yz}, d_{x^2-y^2}$ and $d_{z^2}$

4. Each allowed combination of $n$, $l$ and $m_l$ values specifies one of the atom's orbitals.

eg. $n=2,\ l=0,\ m_l=0$ : for 2s orbital

$n=3,\ l=1;\ m_l=+1$ : for 3p orbital

3d sublevel has 5 orbitals:

| | $d_{xy}$ | $d_{xz}$ | $d_{yz}$ | $d_{z^2}$ | $d_{x^2-y^2}$ |
|---|---|---|---|---|---|
| $m_l$ | +2 | +1 | 0 | −1 | −2 |

for d-orbital

$$\left.\begin{array}{lll} n=3 & l=2 & m_l=+2 \\ n=3 & l=2 & m_l=+1 \\ n=3 & l=2 & m_l=-1 \\ n=3 & l=2 & m_l=-2 \\ n=3 & l=2 & m_l=0 \end{array}\right\}\ \text{5 orbitals}$$

* $2n^2$ = no. of e's in each $n$.
* $n^2$ = total no. of orbital in each $n$.
* $(2l+1)$ = total no. of orbitals in each sublevel ($s, p, d \ldots$
* for each $n$: No. of sublevel, $l = 0, 1, 2 \ldots (n-1)$

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