The Third Quantum Number: Describing Orbital Orientation

The magnetic quantum number \( m_s \) is an integer with values ranging from \(-\frac{1}{2}\) to \(+\frac{1}{2}\), including 0. This quantum number describes the orientation of the orbital in the space around the nucleus. The value of \( m_s \) can be limited by the value of \( \ell \). If \( \ell = 0, m_s \) can be only 0. In other words, for a given value of \( n \), there is only one orbital, of \( s \) type \( (\ell = 0) \). If \( \ell = 1, m_s \) may have one of three values: \(-1, 0, \) or \(+1\). In other words, for a given value of \( n \), there are three orbitals of \( p \) type \( (\ell = 1) \). Each of these \( p \) orbitals has the same shape and energy, but a different orientation around the nucleus. Notice that for any given value of \( \ell \), there are \((2\ell + 1)\) values for \( m_s \).

The total number of orbitals for any energy level \( n \) is given by \( n^2 \).

For example, if \( n = 2 \), it has a total of 4 orbitals (an \( s \) orbital and three \( p \) orbitals). The Sample Problem below shows further use of this calculation.

### Concept Organizer

The Relationship Among the First Three Quantum Numbers

- **Principal quantum number, \( n \)**
  - Describes size and energy of an orbital
  - Allowed values: 1, 2, 3, ...

- **Orbital shape quantum number, \( \ell \)**
  - Describes shape of an orbital
  - Allowed values: 0 to \((n - 1)\)

- **Magnetic quantum number, \( m_s \)**
  - Describes orientation of orbital
  - Allowed values: \(-\frac{1}{2}, 0, +\frac{1}{2}\)

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### Quantum Numbers

#### Physical Interpretation

<table>
<thead>
<tr>
<th>QUANTUM NUMBER</th>
<th>PHYSICAL INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )</td>
<td>Distance from nucleus</td>
</tr>
<tr>
<td></td>
<td>to maximum in the radial distribution</td>
</tr>
<tr>
<td>( \ell )</td>
<td>Angular momentum</td>
</tr>
<tr>
<td></td>
<td>orbital shape</td>
</tr>
<tr>
<td>( m_s )</td>
<td>Magnetic quantum number</td>
</tr>
<tr>
<td></td>
<td>Projection of the angular momentum vector with respect to an external field direction</td>
</tr>
<tr>
<td>( m_l )</td>
<td>Spin quantum number</td>
</tr>
<tr>
<td></td>
<td>Spin angular momentum</td>
</tr>
<tr>
<td></td>
<td>clockwise = 1</td>
</tr>
</tbody>
</table>

### Mathematical limitations

\[ n = 0, 1, 2, 3, 4, \ldots \] (any positive integer)

\[ \ell = 0 \text{ to } \ell = n - 1 \]

For any \( n \), \( +\frac{1}{2} \leq m_s \leq -\frac{1}{2} \)

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### Instructional Master

#### Quantum Numbers

- **Principal quantum number, \( n \)**
- **Orbital shape quantum number, \( \ell \)**
- **Magnetic quantum number, \( m_s \)**

**SUMMARY**

- Energy levels are not to scale
- All electrons in an atom must have the same quantum numbers
- For a given \( n \), \( \ell \) and \( m_s \) values are limited

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### LSM 3.5-1
ENERGY LEVELS AND ORBITAL CONFIGURATIONS

An energy level is a given amount of energy that an electron can possess.
An orbital is a region of space that an electron can occupy.
(it has definite energy)
In the first period the max. number of electrons is $2n^2 = 2$.
There are 2 elements in the first period. The first period has 1 energy level and 1 orbital; (s).

ELECTRON CONFIGURATIONS

$$
\begin{align*}
\text{H} & : 1s^1 \\
\text{He} & : 1s^2 \\
\end{align*}
$$

When an orbital is filled it has 2 electrons in it and is more stable than an orbital that has only one electron.

Lithium is in the second period ($n = 2$). Like hydrogen it forms an ion with a charge of $1^+$. Thus it’s outer electronic configuration must be similar to hydrogen’s. Then, lithium has one electron in an “s” orbital.

$$
\text{Li} \text{ (3 electrons)} \quad 1s^2 \ 2s^1 \quad \text{or} \quad [\text{He}] \ 2s^1
$$

Beryllium has one more electron than Li

$$
\text{Be} \text{ (4 electrons)} \quad 1s^2 \ 2s^2 \quad \text{or} \quad [\text{He}] \ 2s^2
$$

This fills the 2s orbital.

$$
\text{Ca} \quad [\text{Ar}] \ 4s^2 \\
\text{Ca} \quad 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6 \ 4s^2
$$
There are 6 more elements in the second period. There must be 6 more electrons in the second energy level ie. \(2n^2 = 8\). Since 2 electrons can occupy 1 orbital there must be 3 more orbitals in the second energy level.

These orbitals are called "p" orbitals \((p_x, p_y, p_z)\). They all have the same energy. Thus, the electronic configuration for boron is:

\[
\text{B} \quad 1s^2 \ 2s^2 \ 2p^1 \ 
\]\n
or

\[
1s^2 \ 2s^2 \ 2p^2
\]

For carbon the next electron goes into a different "p" orbital, to reduce electronic repulsion (Hund's rule)

\[
\text{C} \quad 1s^2 \ 2s^2 \ 2p_x^1 \ 2p_y^1 \ 
\]\n
or

\[
1s^2 \ 2s^2 \ 2p^2
\]

Similarly,

\[
\text{N} \quad 1s^2 \ 2s^2 \ 2p_x^1 \ 2p_y^1 \ 2p_z^1 \ 
\]\n
or

\[
1s^2 \ 2s^2 \ 2p^3
\]

When one looks at the chart for I.E., nitrogen is higher than both C and O. The greater effective nuclear charge accounts for the increase from C, but it must be some other factor to account for the decrease in I.E. to oxygen. This must be electronic repulsion.
The Aufbau Principal – each additional electron that is added to an electron configuration will always occupy the lowest available energy level.

Hund’s Rule – Electrons must be distributed in an orbital so that as many electrons are unpaired as possible. Thus orbitals will always \( \frac{1}{2} \) fill first. If there are three electrons in a set of orbitals, they must be placed in separate orbitals and must have the same value for the spin quantum numbers.

\[
\begin{align*}
\sqrt{ \frac{1}{p_x} } & \quad \frac{1}{p_y} & \quad \frac{1}{p_z} \\
\sqrt{ \frac{1}{p_x} } & \quad \frac{1}{p_y} & \quad \frac{1}{p_z} \\
X & \quad \frac{1}{p_x} & \quad \frac{1}{p_y} & \quad \frac{1}{p_z}
\end{align*}
\]
Oxygen, then fills one of the “p” orbitals

\[
\begin{align*}
\text{O} & : 1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1 \quad \text{or} \quad 1s^2 2s^2 2p^4 \\
\text{F} & : 1s^2 2s^2 2p_x^2 2p_y^2 2p_z^1 \quad \text{or} \quad 1s^2 2s^2 2p^5 \\
\text{Ne} & : 1s^2 2s^2 2p_x^2 2p_y^2 2p_z^2 \quad \text{or} \quad 1s^2 2s^2 2p^6
\end{align*}
\]

Stability occurs when an orbital series is filled (He, Be, Ne) or each orbital has 1e (N)

**Prediction:** for period 3, maxima in I.E. will occur at these elements.

\[
\begin{align*}
\text{Mg} & : 1s^2 2s^2 2p^6 3s^2 \quad \text{or} \quad [\text{Ne}] 3s^2 \\
\text{P} & : 1s^2 2s^2 2p^6 3s^2 3p^3 \quad \text{or} \quad [\text{Ne}] 3s^2 3p^3 \\
\text{Ar} & : 1s^2 2s^2 2p^6 3s^2 3p^6 \quad \text{or} \quad [\text{Ne}] 3s^2 3p^6
\end{align*}
\]

**Check:** I.E. peaks at Mg, P, Ar

For \( n = 2 \) there are \( n^2 = 4 \) orbitals; one s, three p and \( 2n^2 = 18 \).

We have already accounted for 4 orbitals; s, p, so now we need 5 more.
Since potassium and calcium have similar properties to group IA and IIA, they must fill 4s
THE 1s ORBITAL

Probability of finding an electron at radius \( r \) in any direction from the nucleus

\[ a_o \quad \text{Radius of first orbit in Bohr atom} \]
Probability of finding an electron at radius \( r \) in any direction from the nucleus.