Worksheet 10 - Electronic Structure of Atoms

The Schrödinger equation defines wave equations which describe the distribution of electrons around the nucleus. The wave functions that satisfy the Schrödinger equation are called atomic orbitals. They define the allowed energy states of the electrons.

The energy levels are described by three quantum numbers, \( n \), \( l \) and \( m_l \).

\( n \) is the principal quantum number and has values of 1, 2, 3, ...
The value of \( n \) determines the size of the orbital and the energy of electrons in that orbital.

\( l \) is the angular momentum quantum number as has values of 0 through \( n - 1 \). The value of \( l \) determines the shape of the orbital.

\( m_l \) is the magnetic quantum number and has values of \(-l\) through \(+l\) and determines the orientation of the orbital.

1. Complete the first two columns of the chart shown below for \( n = 1 \) through \( n = 4 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( l )</th>
<th>( m_l )</th>
<th>orbital name</th>
<th># e(^-)</th>
<th>total e(^-) in level ( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1s</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>2s</td>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>1</td>
<td>-1, 0, 1</td>
<td></td>
<td>2p</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3s</td>
<td>2</td>
<td>18</td>
</tr>
<tr>
<td>1</td>
<td>-1, 0, 1</td>
<td></td>
<td>3p</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-2, -1, 0, 1, 2</td>
<td></td>
<td>3d</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>4s</td>
<td>2</td>
<td>32</td>
</tr>
<tr>
<td>1</td>
<td>-1, 0, 1</td>
<td></td>
<td>4p</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-2, -1, 0, 1, 2</td>
<td></td>
<td>4d</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-3, -2, -1, 0, 1, 2, 3</td>
<td></td>
<td>4f</td>
<td>14</td>
<td></td>
</tr>
</tbody>
</table>

The \( l = 0 \) orbitals are called \textbf{s} orbitals. The \( l = 1 \) orbitals are called \textbf{p} orbitals. For \( l = 2 \), 3 and 4, they are called \textbf{d}, \textbf{f} and \textbf{g} orbitals. Each orbital can contain a maximum of 2 electrons.

2. Fill in the orbital names and the number of electrons per orbital and per energy level in the chart.

3. How many orbitals are present in each of the principal levels?

\[
\begin{array}{ccccc}
\text{n = 1} & \text{n = 2} & \text{n = 3} & \text{n = 4} & \text{n = 5} \\
1 & 4 & 9 & 16 & 25 & (\text{always } n^2)
\end{array}
\]
The s orbitals are **spherical**. They increase in size with increasing values of n.

The p orbitals are dumbbell shaped. Each of the three p orbitals is oriented differently in space, as shown below.

Again, size of these orbitals increases with n.

The shapes of the d and f orbitals are more complex and are shown in the textbook.

4. Which of the following orbitals **can not** exist?

<table>
<thead>
<tr>
<th>n = 3, ℓ = 0</th>
<th>n = 3, ℓ = 2</th>
<th>n = 3, ℓ = 3</th>
<th>n = 5, ℓ = 0</th>
<th>n = 3, ℓ = 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>3s</td>
<td>3d</td>
<td>doesn’t exist</td>
<td>5s</td>
<td>3p</td>
</tr>
</tbody>
</table>

5. Name the **allowed** orbitals described by the following quantum numbers (e.g. n = 2, ℓ = 1 would be 2p)

   - n = 3, ℓ = 0
   - n = 3, ℓ = 2
   - n = 3, ℓ = 3
   - n = 5, ℓ = 0
   - n = 3, ℓ = 1

6. How many orbitals in an atom can have the designation:

<table>
<thead>
<tr>
<th>5p</th>
<th>3s</th>
<th>n=4</th>
<th>4d</th>
<th>n=3</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
<td>16</td>
<td>5</td>
<td>9</td>
</tr>
</tbody>
</table>
The importance of these orbitals is apparent when we look at the Periodic Table. Period 1 (H and He) is the n = 1 energy level. This means that there is only one orbital (1s) available. H has 1 electron and He has 2, completely filling the 1s orbital. Electrons in the same orbital must have different spin states (a 4th quantum number), either spin up (↑) or spin down (↓).

So, the electron configuration for H is 1s\(^1\) and He is 1s\(^2\), since each s orbital can hold two electrons.

These can also be drawn out as:

H: 1s\(^\uparrow\) and He: 1s\(^\uparrow\uparrow\)

In He, the electrons are paired, one spin up and one down. Parallel spins are not allowed in an orbital. Electron spin is the 4\(^{th}\) quantum number, \(m_s\), with values of +½ and -½.

The next element is Li with 3 electrons or 1s\(^2\) 2s\(^1\)

The 2s orbital is higher in energy than the 1s orbital

Li: 2s\(^\uparrow\)

1s\(^\uparrow\uparrow\)

7. The next element is Be with 4 electrons.

What is its electron configuration? 1s\(^2\) 2s\(^2\)

Energy level diagram? 2s\(^\uparrow\uparrow\)

1s\(^\uparrow\uparrow\)
8. Which element has 5 electrons? **boron (B)**

Which block is it part of? **p**

Write its electron configuration and draw its energy level diagram. Remember that the number of orbitals changes with \( l \).

\[
\begin{align*}
2p & \quad \uparrow \quad \uparrow \quad \uparrow \\
2s & \quad \uparrow \\
1s & \quad \uparrow 
\end{align*}
\]

9. Carbon has 6 electrons, \( 1s^2 \ 2s^2 \ 2p^2 \). When we put a second electron in the \( p \) orbitals, **Hund's rule** states that the electrons should have parallel spins (remain unpaired) if possible. Add the electrons to the energy level diagram of C.

\[
\begin{align*}
2p & \quad \uparrow \quad \uparrow \quad \uparrow \\
2s & \quad \uparrow \\
1s & \quad \uparrow 
\end{align*}
\]

10. What is the electron configuration of oxygen? **\( 1s^22s^22p^4 \)**

Draw the energy level diagram for oxygen.

\[
\begin{align*}
2p & \quad \uparrow \quad \uparrow \quad \uparrow \\
2s & \quad \uparrow \\
1s & \quad \uparrow 
\end{align*}
\]

Notice that oxygen has **unpaired electrons**. This means that oxygen is **paramagnetic**, and will interact with magnetic fields.

11. Write out the electron configurations for Ne, Na and Al:

- **Ne**: \( 1s^22s^22p^6 \)
- **Na**: \( 1s^22s^22p^63s^1 \)
- **Al**: \( 1s^22s^22p^63s^23p^1 \)

You may have noticed that a lot of the electron configuration is repetitive. Every atom has 1s electrons. Comparing Ne, Na and Al shows that they are very similar up to the configuration of Ne. There is a **shorthand** notation that can be used. Na is basically \([\text{Ne}] \ 3s^1\) and Al is \([\text{Ne}] \ 3s^2 \ 3p^1\). The previous **noble gas** is used as a summary of lower state electrons.

12. In shorthand notation, what is the electron configuration for Ca? **\([\text{Ar}]4s^2\)**
13. The next element is scandium. Which block is it in? Write the shorthand electron configuration for Sc. (Hint: look at the table in question 1 to determine orbitals)

d block

Draw an energy level diagram for Sc.

\[
\begin{align*}
3d & \uparrow \quad \_\_ \quad \_\_ \quad \_\_ \\
4s & \_\_\_\_\_\_ \\
3p & \_\_\_\_\_\_ \\
3s & \_\_\_\_\_\_ \\
2p & \_\_\_\_\_\_ \\
2s & \_\_\_\_\_\_ \\
1s & \_\_\_\_\_\_ \\
\end{align*}
\]

14. Write the shorthand notation for the electron configuration of arsenic, As.

\[[\text{Ar}]4s^23d^{10}4p^3\]

15. Arrange the following orbitals in order of increasing energy. (Hint: use the Periodic Table for help).

\[1s \quad 3s \quad 4s \quad 3d \quad 4f \quad 3p \quad 7s \quad 5d \quad 5p\]

\[1s \quad 3s \quad 3p \quad 4s \quad 3d \quad 5p \quad 4f \quad 5d \quad 7s\]

16. Write the shorthand electron configuration for \( \text{Cl}^- \). (How many electrons are present?)

\( \text{Cl}^- \) has 18 electrons, so it is isoelectronic with argon

\[[\text{Ar}]\]
Shown below are four different electronic configurations of carbon:

\[ \begin{array}{cccccc}
\psi & \psi & \psi & \psi & \psi & \psi \\
\text{excited state 3} \\
\psi & \psi & \psi & \psi & \psi & \psi \\
\text{excited state 2} \\
\psi & \psi & \psi & \uparrow & \psi & \psi \\
\text{excited state 1} \\
1s & 2s & 2p & 3s \\
\text{ground state} \\
\end{array} \]

The bottom configuration is the **ground state** (lowest energy) configuration. The others are **excited state** (higher energy) configurations.

17. Describe how each excited state is different from the ground state.

1 – the 2p electrons have opposite spins
2 – the 2p electrons are paired together
3 – one of the 2p electrons has been excited to the 3s orbital

What is wrong with the configuration shown below? Is it an excited state?

\[ \begin{array}{cccc}
\psi & \psi & \psi & \psi \\
1s & 2s & 2p & 3s \\
\end{array} \]

The 2p electrons both have the same set of 4 quantum numbers \((n=2, l=1, m_l=-1, m_s=+\frac{1}{2})\). This is NOT an excited state. This state is **forbidden**.

18. Which of the following correspond to an excited state? Identify the atoms and write the ground state configuration if needed.

a) \(1s^2 2s^2 2p^1\) \(\text{B}\)

b) \(1s^2 2s^2 2p^6\) \(\text{Ne}\)

c) \(1s^2 2s^2 2p^4 3s^1\) excited F; ground is \(1s^2 2s^2 2p^5\)

d) \([\text{Ar}] 4s^2 3d^5 4p^1\) excited Fe; ground is \([\text{Ar}] 4s^2 3d^6\)
We will only be looking at the first row of the transition metals.

19. Write the shorthand electron configuration and energy level diagram for V.

\[ \text{[Ar]}4s^23d^3 \]

\[
\begin{array}{cccccccc}
1s & 2s & 2p & 3s & 3p & 4s & 3d \\
\end{array}
\]

20. The expected shorthand electron configuration and energy level diagram for Cr is:

\[ \text{[Ar]}4s^23d^4 \]

\[
\begin{array}{cccccccc}
1s & 2s & 2p & 3s & 3p & 4s & 3d \\
\end{array}
\]

This is not what is observed. Instead, one of the 4s electrons occupies one of the 3d orbitals.

21. Write the observed shorthand electron configuration and energy diagram for Cr.

\[ \text{[Ar]}4s^13d^5 \]

\[
\begin{array}{cccccccc}
1s & 2s & 2p & 3s & 3p & 4s & 3d \\
\end{array}
\]

Notice that this puts 5 electrons in the 3d orbitals, leaving them \( \frac{1}{2} \) full. There seems to be a special stability associated with the half-full orbitals.

This also happens when the 3d orbitals are full. Zn has 10 electrons in the 3d orbitals. Cu should have only 9 electrons in the 3d orbitals.

22. Write the shorthand electron configuration and energy diagram of Cu with 10 electrons in the 3d orbitals, which is actually observed.

\[ \text{[Ar]}4s^13d^{10} \]

\[
\begin{array}{cccccccc}
1s & 2s & 2p & 3s & 3p & 4s & 3d \\
\end{array}
\]