Worksheet 11 - Electronic Structure of Atoms

The Schroedinger equation defines wave equations which describe the distribution of electrons around the nucleus. The wave functions that satisfy the Schroedinger 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 mₗ.

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.

mₗ 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>mₗ</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>2p</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>-1, 0, 1</td>
<td></td>
<td>3s</td>
<td>3</td>
<td>18</td>
</tr>
<tr>
<td>2</td>
<td>-2, -1, 0, 1, 2</td>
<td></td>
<td>3p</td>
<td>6</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 s orbitals. The ℓ = 1 orbitals are called p orbitals.
For ℓ = 2, 3 and 4, they are called d, f and 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?

n = 1: 1
n = 2: 4
n = 3: 9
n = 4: 16
n = 5: 25

n²

n²

n²

n²

n²
The s orbitals are spherical. They increase in size with increasing values of n.

\[ 1s \quad 2s \quad 3s \]

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

\[ \text{p}_x \quad \text{p}_y \quad \text{p}_z \]

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?

\[
\begin{array}{cccc}
1s & 3p & 1s & 3s \\
\text{OK} & \text{OK} & \text{NO} & \text{OK} \\
& & (3s) & (3s, 3p) \\
& & \text{OK} & \text{OK} \\
7d & 3f & 4s & 2s \quad 2p \\
\text{OK} & \text{NO} & \text{OK} & \text{OK}
\end{array}
\]

5. Name the 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

\[
\begin{array}{cccc}
3s & 3d & \text{impossible} & 5s \quad 13p
\end{array}
\]

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

\[
\begin{array}{cccc}
5p & 3s & n=4 & 4d & n=3 \\
3 & 1 & 16 & 5 & 9
\end{array}
\]

\[
\begin{array}{cccc}
\text{s, p, d, f} & \text{1, 3, 5} & \text{1, 3, 5} & \text{i, j, l}
\end{array}
\]
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 \( \text{He} \) has 2, completely filling the \( 1s \) orbital. Electrons in the same orbital must have different spin states (a 4th quantum number), either spin up (\( \uparrow \)) or spin down (\( \downarrow \)).

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

These can also be drawn out as:

\[
\begin{align*}
\text{H} & \quad 1s \uparrow \\
\text{He} & \quad 1s \uparrow \downarrow 
\end{align*}
\]

In \( \text{He} \), the electrons are paired, one spin up and one down. Parallel spins are not allowed in an orbital. **Electron spin** is the 4th quantum number, \( m_s \), with values of \( +\frac{1}{2} \) and \( -\frac{1}{2} \).

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

The \( 2s \) orbital is higher in energy than the \( 1s \) orbital.

\[
\begin{align*}
\text{Li} & \quad 2s \uparrow \\
& \quad 1s \uparrow \downarrow 
\end{align*}
\]

7. The next element is \( \text{Be} \) with 4 electrons.

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

Energy level diagram?

\[
\begin{align*}
2s & \uparrow \\
1s & \uparrow \downarrow 
\end{align*}
\]
8. Which element has 5 electrons? B
Which block is it part of? p-block

Write its electron configuration and draw its energy level diagram.
Remember that the number of orbitals changes with r.
\[ \begin{align*}
1s^2 & \quad 2s^2 \quad 2p^1 & \quad 1s^2 & \quad 2s^2 \quad 2p^1 \\
& \quad 2s & \quad 1s & \quad 2s & \quad 1s
\end{align*} \]

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.
\[ \begin{align*}
2p & \quad \frac{\hspace{1em} 1}{4} \\
2s & \quad \frac{\hspace{1em} 1}{4} \\
1s & \quad \frac{\hspace{1em} 1}{4}
\end{align*} \]

10. What is the electron configuration of oxygen? 6e- 1s^2 2s^2 2p^4
Draw the energy level diagram for oxygen.
\[ \begin{align*}
2p & \quad \frac{\hspace{1em} 1}{4} \\
2s & \quad \frac{\hspace{1em} 1}{4} \\
1s & \quad \frac{\hspace{1em} 1}{4}
\end{align*} \]
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:
\[ \begin{align*}
\text{Ne} = 10\text{e}^- & \quad 1s^2 2s^2 2p^6 \\
\text{Na} = 11\text{e}^- & \quad 1s^2 2s^2 2p^6 3s^1 \\
\text{Al} = 13\text{e}^- & \quad 1s^2 2s^2 2p^6 3s^1 3p^1
\end{align*} \]
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 [Ne] 3s^1 and Al is [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?

\[ \text{Ca}^{2+} \quad [\text{Ar}]4s^2 \]

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

\([\text{Ar}]4s^2\, 3d^1\]

Draw an energy level diagram for Sc. 21 electrons

\[ 3d, 4s, 4p \]

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

\([\text{Ar}]4s^2\, 3d^{10}\, 4p^3\]

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

\[ 1s < (2s) < (2p) < 3s < 3p < 4s < 3d < (4p) < (5s) < (4d) < 5p < (6s) < 4f < 5d < (6p) < 7s \]

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

\[ \text{Cl}^- = 18\, e^- \quad [\text{Ar}] \]

18 electrons with Ar configuration.
Shown below are four different electronic configurations of carbon:

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

The bottom configuration is the \textbf{ground state} (lowest energy) configuration. The others are \textbf{excited state} (higher energy) configurations.

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

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

\[
\begin{array}{cccc}
1s & 2s & 2p & 4s \\
\text{two c-will same} \\
\text{quartet numbers} \\
\text{not an excited state} \\
\text{will m}\not\text{=}\frac{1}{2} \\
\end{array}
\]

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

a) \[1s^2 \ 2s^2 \ 3p^1\] ground state B

b) \[1s^2 \ 2s^2 \ 2p^5\] ground state Ne

c) \[1s^2 \ 2s^2 \ 2p^4 \ 3s^1\] excited state

ground state \[1s^2 \ 2s^2 \ 2p^5\]

d) \[[Ar] \ 4s^2 \ 3d^5 \ 4p^1\] excited state

\[26e^- \ Fe\] \[[Ar] \ 4s^2 \ 3d^6\]
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.

\[ 23e^- \text{ [Ar]} 4s^2 \ 3d^3 \]

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

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

\[ 24e^- \text{ [Ar]} 4s^2 \ 3d^4 \]

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

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.

\[ 24e^- \text{ [Ar]} 4s^1 \ 3d^5 \]

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

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.

\[ 29e^- \]

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

Notice that this configuration has a full set of 10 electrons in the 3d orbitals.