Electron Configurations, Orbital Notation and Quantum Numbers
Understanding Electron Arrangement and Oxidation States

Chemical properties depend on the number and arrangement of electrons in an atom. Usually, only the valence or outermost electrons are involved in chemical reactions. The electron cloud is compartmentalized. We model this compartmentalization through the use of electron configurations and orbital notations. The compartmentalization is as follows, energy levels have sublevels which have orbitals within them. We can use an apartment building as an analogy. The atom is the building, the floors of the apartment building are the energy levels, the apartments on a given floor are the orbitals and electrons reside inside the orbitals. There are two governing rules to consider when assigning electron configurations and orbital notations. Along with these rules, you must remember electrons are lazy and they hate each other, they will fill the lowest energy states first AND electrons repel each other since like charges repel.

Rule 1: The Pauli Exclusion Principle
In 1925, Wolfgang Pauli stated: No two electrons in an atom can have the same set of four quantum numbers. This means no atomic orbital can contain more than TWO electrons and the electrons must be of opposite spin if they are to form a pair within an orbital.

Rule 2: Hund’s Rule
The most stable arrangement of electrons is one with the maximum number of unpaired electrons. It minimizes electron-electron repulsions and stabilizes the atom. Here is an analogy. In large families with several children, it is a luxury for each child to have their own room. There is far less fussing and fighting if siblings are not forced to share living quarters. The entire household experiences a lower, less frazzled energy state. Electrons find each other very repulsive, so they too, are in a lower energy state if each “gets their own room” or in this case orbital. Electrons will fill an orbital singly, before pairing up in order to minimize electron-electron repulsions. All of the electrons that are single occupants of orbitals have parallel (same direction) spins and are assigned an up arrow. The second electron to enter the orbital, thus forming an electron pair, is assigned a down arrow to represent opposite spin.

PURPOSE
In this activity you will acquire an ability to write electron configurations, orbital notations and a set of quantum numbers for electrons within elements on the periodic table. You will also be able to justify oxidation or valence states using electron configurations and orbital notations.
MATERIALS
Periodic Table found at the end of this activity

To write electron configurations and orbital notations successfully, you must formulate a plan of attack—learn the following relationships:

ELECTRON CONFIGURATIONS
1. Each main energy level has \( n \) sublevels, where \( n \) equals the number of the energy level. That means the first energy level has one sublevel, the second has two, the third has three….

2. The sublevels are named s, p, d, f, g . . . and continue alphabetically. The modern periodic table does not have enough elements to necessitate use of sublevels beyond f. Why s, p, d, f? Early on in the development of this model, the names of the sublevels came from sharp, principle, diffuse and fundamental, words used in describing spectral lines of hydrogen.

3. It may be easier for you to understand this by studying the table presented below:

<table>
<thead>
<tr>
<th>Energy level</th>
<th>Number of sublevels</th>
<th>Names of sublevels</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>s</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>s, p</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>s, p, d</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>s, p, d, f</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>s, p, d, f, g</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sublevel Name</th>
<th>Number of Orbitals</th>
<th>Maximum number of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>p</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>d</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>f</td>
<td>7</td>
<td>14</td>
</tr>
</tbody>
</table>

4. Each sublevel has increasing odd numbers of orbitals available. \( s = 1, p = 3, d = 5, f = 7 \). Each orbital can hold only two electrons and they must be of opposite spin. An s-sublevel holds 2 electrons, a p-sublevel holds 6 electrons, a d-sublevel holds 10 electrons, and an f-sublevel holds 14 electrons.
5. The filling of the orbitals is related to energy. Remember, electrons are lazy, much like us! Just as you would place objects on a bottom shelf in an empty store room rather than climb a ladder to place them on a top shelf, expending more energy—electrons fill the lowest sublevel available to them. Use the diagonal rule as your map as you determine the outermost or valence electron configurations for any of the elements.

Using the diagonal rule you can quickly determine the electron configuration for the outermost valence electron in sulfur. First locate sulfur on the periodic table and notice that the atomic number of sulfur is 16. That means it has 16 protons and 16 electrons in a neutral atom. The first two electrons go into the 1s sublevel and fill it, the next two go into the 2s sublevel and fill it. That leaves 12 more electrons to place. The next six go into the 2p sublevel, filling it and leaving six more. Two of them go into the 3s sublevel, filling it and the remaining four go into the 3p sublevel. The completed electron configuration looks like this: \( 1s^22s^22p^63s^23p^4 \).

6. Complete the electron configuration portion of the table on your student answer sheet.

**ORBITAL NOTATION**

Orbital notation is a drawing of the electron configuration. It is very useful in determining electron pairing and thus predicting oxidation numbers. The orbital notation for sulfur would be represented as follows:

\[
\begin{array}{ccccccccccccc}
1 & 2 & 3 & 4 & 5 & 8 & 6 & 9 & 7 & 10 & 11 & 12 & 13 & 16 & 14 & 15 \\
\uparrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \uparrow & \uparrow \\
\end{array}
\]

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

The electrons are numbered as to the filling order. Notice electrons 5, 6, and 7 went into their own orbitals before electrons 8, 9, and 10 forced a pairing to fill the 2p sublevel. This is an application of Hund’s rule which minimizes electron-electron repulsions. The same filling order is repeated in the 3p sublevel.

It’s time to get the lingo straight!
Electron Configurations

Group the 1’s, 2’s, etc. TOGETHER and it looks like this:

\[ 1s^2 2s^2 2p^4 \]

Which element has this electron configuration?

Orbital notations

Use blanks to represent orbitals and arrows to represent electrons and looks like this:

\[
\begin{array}{cccccc}
1 & 2 & 3 & 4 & 5 & 8 \\
\uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow & \uparrow & \\
1s & 2s & 2p & \\
\end{array}
\]

The electrons are numbered as to the filling order. Notice electrons 5, 6, 7 went into their own orbitals before electron 8 forced a pairing. This minimizes repulsion.

Which element has this orbital notation?

7. Complete the orbital notation column on your student answer page.

JUSTIFYING OXIDATION STATES

Elements in compounds have oxidation states. These oxidation states determine their behavior in the company of other elements. Your understanding of oxidation states will become very important as you learn to write correct chemical formulas for compounds. Some elements have only one oxidation state, while others have several. In general, the representative elements, those groups or families numbered as 1 - 8A have the oxidation states listed on the periodic table below.

The transition metals generally have several oxidation states possible.

Learn the following; it will help you make your predictions:

- Metals (found to the left of the stair-step line) lose electrons to either minimize electron-electron repulsions or eliminate their valence electrons entirely.
- Nonmetals tend to gain electrons to acquire an octet of electrons. An octet means the atom has eight valence electrons arranged as \( ns^2 np^6 \) where \( n \) corresponds to the main energy level.
• Transition metals generally have an oxidation state of +2 since they lose the s\(^2\) that was filled just before the d-sublevel began filling.
• Electrons in the d-sublevels are very similar in energy to those in the s-sublevel preceding them. This means that 3d electrons are similar in energy to 4s electrons and 4d are similar to 5s, etc.
• Noble gases have an octet naturally, so they generally do not react.

Let’s practice.
• Sulfur has many oxidation states. Use an orbital notation to justify its most common -2 oxidation state:

Sulfur has a valence electron configuration of 3s\(^2\)3p\(^4\). Start by drawing its orbital notation for the outermost, valence electrons.

\[
\text{[Ne]} \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \\
3s \quad 3p
\]

Sulfur is a nonmetal and tends to gain electrons, creating the -2 charge. Gaining two electrons gives it an octet of 3s\(^2\)3p\(^6\).

• Copper has two common oxidation states, +1 and +2. Justify both oxidation states:

Copper has an ending electron configuration of 4s\(^2\)3d\(^9\). Start by drawing its orbital notation for the outermost, valence electrons.

\[
\text{[Ar]} \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \uparrow \\
4s \quad 3d
\]

Since copper is a transition metal, the +2 oxidation state comes from losing the 4s electrons leaving 4s\(^0\)3d\(^9\). Almost all of the transition metals lose the s sublevel and have an oxidation state of +2. [Silver is an exception and only makes an oxidation state of +1.] The +1 oxidation state for copper comes from transferring one of the s electrons to the d orbitals to fill that sublevel and then losing the remaining s electron to form 4s\(^0\)3d\(^10\).

8. Complete the conclusion questions that justify oxidation states on your student answer page.
## QUANTUM NUMBERS AND ATOMIC ORBITALS

<table>
<thead>
<tr>
<th><strong>Principal quantum number (n)</strong>&lt;br&gt;1, 2, 3, 4, 5, etc.</th>
<th>Determines the total energy of the electron. Describes the energy level of the electron and refers to the average distance of the electron from the nucleus. $2n^2$ electrons may be assigned to an energy level. For $n = 1$, 2 electrons. For $n = 2$, 8 electrons, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Angular momentum or azimuthal quantum number ($\ell$)</strong>&lt;br&gt;0, 1, 2, 3…</td>
<td>Refers to the sublevels that occur within each principal level and determines the shape of the orbital. Corresponds to the s, p, d, f [in order of increasing energy]. Each $\ell$ is a different orbital shape or orbital type. This quantum number has integral values from 0 up to n-1.</td>
</tr>
<tr>
<td><strong>Magnetic quantum number ($m_\ell$)</strong>&lt;br&gt;…-2, -1, 0, 1, 2, …</td>
<td>Specifies which orbital within a sublevel you are likely to find the electron. It determines the orientation of the orbital in space relative to the other orbitals in the atom. This quantum number has values from $-\ell$ through zero to $+\ell$.</td>
</tr>
<tr>
<td><strong>Spin quantum number ($m_s$)</strong>&lt;br&gt;+½ or -½</td>
<td>Specifies the value for the spin. Only two possibilities: $+\frac{1}{2}$ and $-\frac{1}{2}$. No more than two electrons can occupy an orbital. In order for two electrons to occupy an orbital, they must have opposite spins.</td>
</tr>
</tbody>
</table>

### Determining Quantum Numbers

Now that we know the electron configuration of the valence electron in sulfur is $3p^4$ based on its position in the periodic table, and we have a picture of how those p electrons are filling the p sublevel, the set of quantum numbers for this valence electron are extremely easy to obtain. First, $n = 3$ since it is a $3p$ electron. Next it is a $p$ electron and p sublevels have an $\ell$ value of 1. So far we know 3,1. To get the $m_\ell$ quantum number we go back to the orbital notation for the valence electron and focus on the 3p sublevel alone. It looks like this: \[
\text{↑↓} \quad \text{↑} \\
-1 \quad 0 \quad +1
\]

Simply number the blanks with a zero assigned to the center blank and increasing negative numbers to the left and increasing positive to the right of the zero. The last electron was number 16 and “landed” in the first blank as a down arrow. This picture gives us the last two quantum numbers of $m_\ell = -1$ and $m_s = -\frac{1}{2}$ since it is the second electron to be placed in the orbital.
In summary:

<table>
<thead>
<tr>
<th>Energy Level</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7,….</th>
</tr>
</thead>
<tbody>
<tr>
<td># of sublevels</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7,….</td>
</tr>
<tr>
<td>Names of sublevels</td>
<td>s</td>
<td>s, p</td>
<td>s,p,d</td>
<td>s,p,d,f</td>
<td>s,p,d,f,g</td>
<td>s,p,d,f,g,h</td>
<td>s,p,d,f,g,h,i</td>
</tr>
<tr>
<td>n, principal quantum number</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7,….</td>
</tr>
<tr>
<td>Name of sublevel</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7,….</td>
</tr>
<tr>
<td>ℓ, angular momentum quantum number [= n-1]</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td># of orbitals [= -ℓ to +ℓ]</td>
<td>1</td>
<td>3</td>
<td>5</td>
<td>7</td>
<td>9</td>
<td>11</td>
<td>13</td>
</tr>
<tr>
<td>(m_ℓ) for each orbital within a sublevel</td>
<td>(0)</td>
<td>(-1)</td>
<td>(0)</td>
<td>(+1)</td>
<td>(-2)</td>
<td>(-1)</td>
<td>(0)</td>
</tr>
</tbody>
</table>

And so on, just pretend you’re in elementary school and make a number line with ZERO in the middle and obviously, negative numbers to the left and positive to the right. Make as many blanks as there are orbitals for a given sublevel.

For assigning \(m_s\), the first electron placed in an orbital [the up arrow] gets the \(+\frac{1}{2}\) and the second one [the down arrow] gets the \(-\frac{1}{2}\).

Try working backwards. Which element has this set of quantum numbers 5, 1, -1, -\(\frac{1}{2}\)? First think about the electron configuration. \(n = 5\) and \(ℓ = 1\), so it must be a 5 p electron. The \(m_s\) quantum number corresponds to this orbital notation picture ↓. Be sure and number the blanks and realize that the \(-\frac{1}{2}\) means it is a pairing electron, so the orbital had to be half-filled before pairing could occur, thus for the electron to occupy the -1 position, it must be a p\(^4\) electron. The element has a configuration of 5p\(^4\) so it must be Tellurium.

Quantum numbers are a set of the 4 numbers that describe an electron’s position within an atom. They are quite easy to determine if you start with the electron configuration. The set of quantum numbers for the 2p\(^4\) electron would be 2, 1, -1, +\(\frac{1}{2}\). Each electron in the atom has a set of quantum numbers, but you will most often be asked for the set describing the valence electron.
**Electron Configurations, Orbital Notation and Quantum Numbers**

**Understanding Electron Arrangement and Oxidation States**

**ANALYSIS**

Complete this table:

<table>
<thead>
<tr>
<th>Element</th>
<th>Electron configuration</th>
<th>Valence Orbital notation [only the outermost orbitals are drawn]</th>
<th>Set of Quantum Numbers for the LAST Valence electron to fill</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>1s^22s^22p^3</td>
<td>↑↓</td>
<td>↑↓</td>
</tr>
<tr>
<td>Br</td>
<td>[Ar] 4s^23d^8</td>
<td>↑↓</td>
<td></td>
</tr>
<tr>
<td>P</td>
<td>1s^22s^22p^6</td>
<td>↑↓</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>[Kr] 5s^24d^10</td>
<td>↑↓</td>
<td></td>
</tr>
<tr>
<td>W</td>
<td>[Rn] 7s^2</td>
<td>↑↓</td>
<td></td>
</tr>
<tr>
<td>Pu</td>
<td>1s^22s^22p^3</td>
<td>↑↓</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>4s^23s^2</td>
<td>↑↓</td>
<td></td>
</tr>
</tbody>
</table>

*Laying the Foundation in Chemistry*
CONCLUSION QUESTIONS

1. Iron has two common oxidation states, +2 and +3. Justify each of these oxidation states. Draw the orbital notation of the neutral atom and each oxidation state as part of your justification.

2. Nitrogen has a common oxidation state of -3. Justify this oxidation state. Draw the orbital notation for the neutral atom and oxidation state as part of your justification.

3. Silver has only one oxidation state, +1. Justify this oxidation state even though most transition metals have an oxidation state of +2 among others. Draw the orbital notation for the neutral atom and oxidation state as part of your justification.

4. Manganese has a common oxidation state of +7. Justify this oxidation state. Draw the orbital notation for the neutral atom and oxidation state as part of your justification.
The Diagonal Rule or Aufbau Series

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f
6s 6p 6d
7s 7p
**Electron Configurations, Orbital Notation and Quantum Numbers**

Laying the Foundation in Chemistry

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<table>
<thead>
<tr>
<th>Period</th>
<th>Group 1A</th>
<th>Group 2A</th>
<th>Group 13A</th>
<th>Group 14A</th>
<th>Group 15A</th>
<th>Group 16A</th>
<th>Group 17A</th>
<th>Group 18A</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H</td>
<td>Na</td>
<td>Li</td>
<td>Be</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Al</td>
<td>K</td>
<td>Mg</td>
<td>Si</td>
<td>P</td>
<td>S</td>
<td>Cl</td>
<td>Ar</td>
</tr>
<tr>
<td>3</td>
<td>B</td>
<td>Al</td>
<td>Ga</td>
<td>Ge</td>
<td>As</td>
<td>Se</td>
<td>Br</td>
<td>Kr</td>
</tr>
<tr>
<td>4</td>
<td>C</td>
<td>Si</td>
<td>In</td>
<td>Sn</td>
<td>Te</td>
<td>I</td>
<td>Xe</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>N</td>
<td>P</td>
<td>Tl</td>
<td>Pb</td>
<td>Bi</td>
<td>Po</td>
<td>At</td>
<td>Rn</td>
</tr>
</tbody>
</table>

---

**Lanthanides**
- La
- Ce
- Pr
- Nd
- Pm
- Sm
- Eu
- Gd
- Tb
- Dy
- Ho
- Er
- Tm
- Yb

**Actinides**
- Ac
- Th
- Pa
- U
- Np
- Pu
- Am
- Cm
- Bk
- Cf
- Es
- Fm
- Md
- No

---

Noble gases
- Ne
- Ar
- Kr
- Xe
- Rn