

AUCHE 212 GENERAL CHEMISTRY II PART 1



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CHAPTER OVERVIEW

1: Review- VSEPR Theory

1.1: VSPER Theory - Predicting Molecular Geometries

1.2: VSEPR Theory - The Five Basic Shapes

1.3: VSPER Theory- The Effect of Lone Pairs

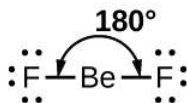
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1.1: VSEPR Theory - Predicting Molecular Geometries

Valence shell electron-pair repulsion theory (VSEPR theory) enables us to predict the molecular structure, including approximate bond angles around a central atom, of a molecule from an examination of the number of bonds and lone electron pairs in its Lewis structure. The VSEPR model assumes that electron pairs in the valence shell of a central atom will adopt an arrangement that minimizes repulsions between these electron pairs by maximizing the distance between them. The electrons in the valence shell of a central atom form either bonding pairs of electrons, located primarily between bonded atoms, or lone pairs. The electrostatic repulsion of these electrons is reduced when the various regions of high electron density assume positions as far from each other as possible.

VSEPR theory predicts the arrangement of electron pairs around each central atom and, usually, the correct arrangement of atoms in a molecule. We should understand, however, that the theory only considers electron-pair repulsions. Other interactions, such as nuclear-nuclear repulsions and nuclear-electron attractions, are also involved in the final arrangement that atoms adopt in a particular molecular structure.

As a simple example of VSEPR theory, let us predict the structure of a gaseous BeF_2 molecule. The Lewis structure of BeF_2 (Figure 1.1.2) shows only two electron pairs around the central beryllium atom. With two bonds and no lone pairs of electrons on the central atom, the bonds are as far apart as possible, and the electrostatic repulsion between these regions of high electron density is reduced to a minimum when they are on opposite sides of the central atom. The bond angle is 180° (Figure 1.1.2).



A Lewis structure is shown. A fluorine atom with three lone pairs of electrons is single bonded to a beryllium atom which is single bonded to a fluorine atom with three lone pairs of electrons. The angle of the bonds between the two fluorine atoms and the beryllium atom is labeled, "180 degrees."

Figure 1.1.2: The BeF_2 molecule adopts a linear structure in which the two bonds are as far apart as possible, on opposite sides of the Be atom.

Figure 1.1.3 illustrates this and other electron-pair geometries that minimize the repulsions among regions of high electron density (bonds and/or lone pairs). Two regions of electron density around a central atom in a molecule form a linear geometry; three regions form a trigonal planar geometry; four regions form a tetrahedral geometry; five regions form a trigonal bipyramidal geometry; and six regions form an octahedral geometry.

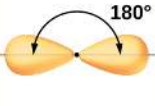
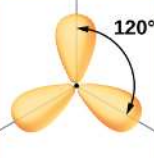
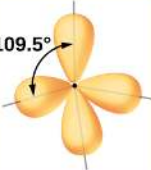
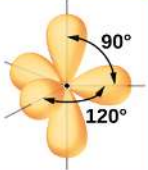
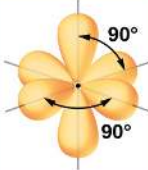
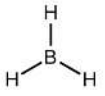
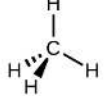
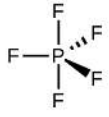
Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement					
Line-dash-wedge notation	$\text{H}-\text{Be}-\text{H}$				
Electron pair geometry	Linear; 180° angle	Trigonal planar; all angles 120°	Tetrahedral; all angles 109.5°	Trigonal bipyramidal; angles of 90° or 120° An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).	Octahedral; all angles 90° or 180°

Figure 1.1.3: The basic electron-pair geometries predicted by VSEPR theory maximize the space around any region of electron density (bonds or lone pairs).

In this table summarizing the geometries proposed by VSEPR Theory, the number of regions along with spatial arrangement, line-dash-wedge notation, and electron pair geometry are shown.

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1.2: VSEPR Theory - The Five Basic Shapes

Learning Objectives

- To use the VSEPR model to predict molecular geometries.
- To predict whether a molecule has a dipole moment.

The Lewis electron-pair approach can be used to predict the number and types of bonds between the atoms in a substance, and it indicates which atoms have lone pairs of electrons. This approach gives no information about the actual arrangement of atoms in space, however. We continue our discussion of structure and bonding by introducing the **valence-shell electron-pair repulsion** (VSEPR) model (pronounced “vesper”), which can be used to predict the shapes of many molecules and polyatomic ions. Keep in mind, however, that the VSEPR model, like any model, is a limited representation of reality; the model provides no information about bond lengths or the presence of multiple bonds.

The VSEPR Model

The VSEPR model can predict the structure of nearly any molecule or polyatomic ion in which the central atom is a nonmetal, as well as the structures of many molecules and polyatomic ions with a central metal atom. The premise of the VSEPR theory is that electron pairs located in bonds and lone pairs repel each other and will therefore adopt the geometry that places electron pairs as far apart from each other as possible. This theory is very simplistic and does not account for the subtleties of orbital interactions that influence molecular shapes; however, the simple VSEPR counting procedure accurately predicts the three-dimensional structures of a large number of compounds, which cannot be predicted using the Lewis electron-pair approach.

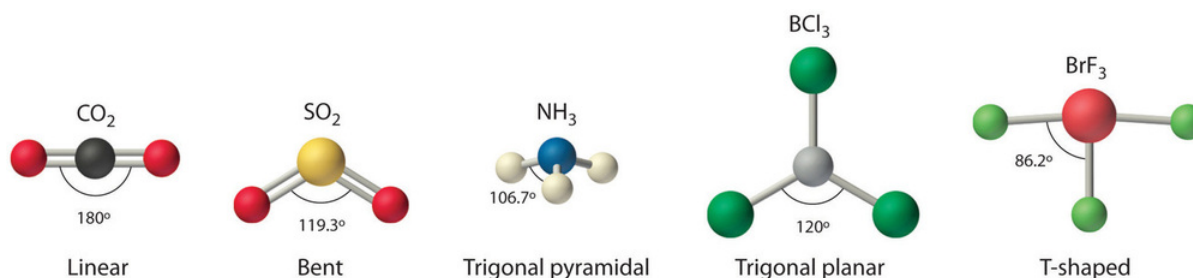


Figure 1.2.1: Common Structures for Molecules and Polyatomic Ions That Consist of a Central Atom Bonded to Two or Three Other Atoms. (CC BY-NC-SA; anonymous)

We can use the VSEPR model to predict the geometry of most polyatomic molecules and ions by focusing only on the number of electron pairs around the *central atom*, ignoring all other valence electrons present. According to this model, valence electrons in the Lewis structure form *groups*, which may consist of a single bond, a double bond, a triple bond, a lone pair of electrons, or even a single unpaired electron, which in the VSEPR model is counted as a lone pair. Because electrons repel each other electrostatically, the most stable arrangement of electron groups (i.e., the one with the lowest energy) is the one that minimizes repulsions. Groups are positioned around the central atom in a way that produces the molecular structure with the lowest energy, as illustrated in Figures 1.2.1 and 1.2.2.

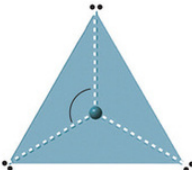
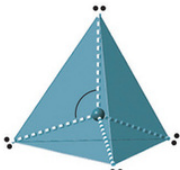
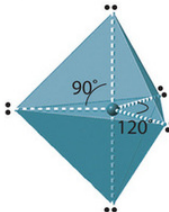
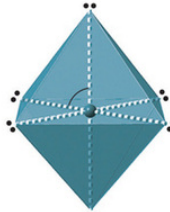
Electron Groups	2	3	4	5	6
Geometry	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
					
Predicted Bond Angles	180°	120°	109.5°	90°, 120°	90°

Figure 1.2.2: Electron Geometries for Species with Two to Six Electron Groups. Groups are placed around the central atom in a way that produces a molecular structure with the lowest energy, that is, the one that minimizes repulsions. (CC BY-NC-SA; anonymous)

In the VSEPR model, the molecule or polyatomic ion is given an AX_mE_n designation, where A is the central atom, X is a bonded atom, E is a nonbonding valence electron group (usually a lone pair of electrons), and m and n are integers. Each group around the central atom is designated as a bonding pair (BP) or lone (nonbonding) pair (LP). From the BP and LP interactions we can predict both the relative positions of the atoms and the angles between the bonds, called the bond angles. Using this information, we can describe the molecular geometry, the arrangement of the *bonded atoms* in a molecule or polyatomic ion.

VSEPR Procedure to predict Molecular geometry

This VSEPR procedure is summarized as follows:

1. Draw the Lewis electron structure of the molecule or polyatomic ion.
2. Determine the electron group arrangement around the central atom that minimizes repulsions.
3. Assign an AX_mE_n designation; then identify the LP–LP, LP–BP, or BP–BP interactions and predict deviations from ideal bond angles.
4. Describe the molecular geometry.

We will illustrate the use of this procedure with several examples, beginning with atoms with two electron groups. In our discussion we will refer to Figure 1.2.2 and Figure 1.2.3, which summarize the common molecular geometries and idealized bond angles of molecules and ions with two to six electron groups.

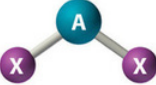
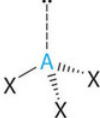
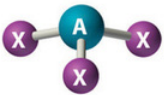
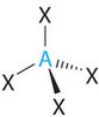
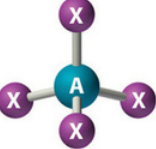
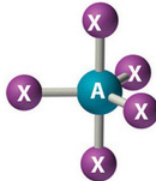
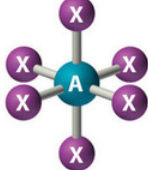
AX_mE_n Notation	AX_2	AX_2E	AX_3	AX_3E
Geometry	Linear $X-A-X$ 	Bent (V-shaped)  	Trigonal planar  	Trigonal pyramidal  
Idealized Bond Angles	180°	$<180^\circ$	120°	$<120^\circ$
AX_mE_n Notation	AX_4E_2	AX_4	AX_5	AX_6
Geometry	Square planar  	Tetrahedral  	Trigonal bipyramidal  	Octahedral  
Idealized Bond Angles	90°	109.5°	$90^\circ, 120^\circ$	90°

Figure 1.2.3: Common Molecular Geometries for Species with Two to Six Electron Groups. Lone pairs are shown using a dashed line. (CC BY-NC-SA; anonymous)

Linear, bent, trigonal planar, trigonal pyramidal, square planar, tetrahedral, trigonal bipyramidal, octahedral.

Two Electron Groups

Our first example is a molecule with two bonded atoms and no lone pairs of electrons, BeH_2 .

AX_2 Molecules: BeH_2

1. The central atom, beryllium, contributes two valence electrons, and each hydrogen atom contributes one. The Lewis electron structure is



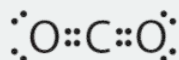
Lewis structure

Figure 1.2.2 that the arrangement that minimizes repulsions places the groups 180° apart. (CC BY-NC-SA; anonymous)

3. Both groups around the central atom are bonding pairs (BP). Thus BeH_2 is designated as AX_2 .
4. From Figure 1.2.3 we see that with two bonding pairs, the molecular geometry that minimizes repulsions in BeH_2 is *linear*.

AX₂ Molecules: CO₂

1. The central atom, carbon, contributes four valence electrons, and each oxygen atom contributes six. The Lewis electron structure is



2. The carbon atom forms two double bonds. Each double bond is a group, so there are two electron groups around the central atom. Like BeH₂, the arrangement that minimizes repulsions places the groups 180° apart.

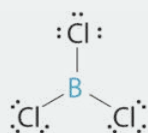
3. Once again, both groups around the central atom are bonding pairs (BP), so CO₂ is designated as AX₂.

4. VSEPR only recognizes groups around the *central* atom. Thus the lone pairs on the oxygen atoms do not influence the molecular geometry. With two bonding pairs on the central atom and no lone pairs, the molecular geometry of CO₂ is linear (Figure 1.2.3). The structure of CO₂ is shown in Figure 1.2.1.

Three Electron Groups

AX₃ Molecules: BCl₃

1. The central atom, boron, contributes three valence electrons, and each chlorine atom contributes seven valence electrons. The Lewis electron structure is



Lewis structure

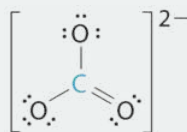
Figure 1.2.2): (CC BY-NC-SA; anonymous)

3. All electron groups are bonding pairs (BP), so the structure is designated as AX₃.

4. From Figure 1.2.3 we see that with three bonding pairs around the central atom, the molecular geometry of BCl₃ is *trigonal planar*, as shown in Figure 1.2.2.

AX₃ Molecules: CO₃²⁻

1. The central atom, carbon, has four valence electrons, and each oxygen atom has six valence electrons. As you learned previously, the Lewis electron structure of one of three resonance forms is represented as



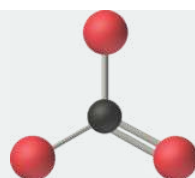
Lewis structure

Figure 1.2.2).

The three oxygens are arranged in a triangular shape with carbon at the center. Two of the oxygens have three lone pairs. One oxygen has 2 lone pairs and is double bonded to the carbon. The molecule has a minus 2 charge.

3. All electron groups are bonding pairs (BP). With three bonding groups around the central atom, the structure is designated as AX₃.

4. We see from Figure 1.2.3 that the molecular geometry of CO₃²⁻ is trigonal planar with bond angles of 120°.



Molecular geometry
(trigonal planar)

In our next example we encounter the effects of lone pairs and multiple bonds on molecular geometry for the first time.

AX₂E Molecules: SO₂

1. The central atom, sulfur, has 6 valence electrons, as does each oxygen atom. With 18 valence electrons, the Lewis electron structure is shown below.

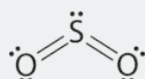


Figure 1.2.2): (CC BY-NC-SA; anonymous)

The two oxygens are double bonded to the sulfur. The oxygens have 2 lone pairs while sulfur had one lone pair.

3. There are two bonding pairs and one lone pair, so the structure is designated as AX₂E. This designation has a total of three electron pairs, two X and one E. Because a lone pair is not shared by two nuclei, it occupies more space near the central atom than a bonding pair (Figure 1.2.4). Thus bonding pairs and lone pairs repel each other electrostatically in the order BP–BP < LP–BP < LP–LP. In SO₂, we have one BP–BP interaction and two LP–BP interactions.

4. The molecular geometry is described only by the positions of the nuclei, *not* by the positions of the lone pairs. Thus with two nuclei and one lone pair the shape is *bent*, or *V shaped*, which can be viewed as a trigonal planar arrangement with a missing vertex (Figures 1.2.2 and 1.2.3). The O–S–O bond angle is expected to be *less than* 120° because of the extra space taken up by the lone pair.

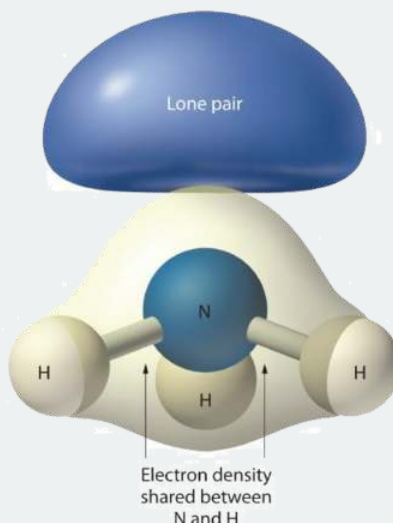
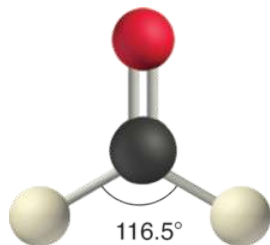


Figure 1.2.4: The Difference in the Space Occupied by a Lone Pair of Electrons and by a Bonding Pair. (CC BY-NC-SA; anonymous)

As with SO₂, this composite model of electron distribution and negative electrostatic potential in ammonia shows that a lone pair of electrons occupies a larger region of space around the nitrogen atom than does a bonding pair of electrons that is shared with a hydrogen atom.

Like lone pairs of electrons, multiple bonds occupy more space around the central atom than a single bond, which can cause other bond angles to be somewhat smaller than expected. This is because a multiple bond has a higher electron density than a single bond, so its electrons occupy more space than those of a single bond. For example, in a molecule such as CH₂O (AX₃), whose

structure is shown below, the double bond repels the single bonds more strongly than the single bonds repel each other. This causes a deviation from ideal geometry (an H–C–H bond angle of 116.5° rather than 120°).

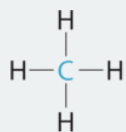


Four Electron Groups

One of the limitations of Lewis structures is that they depict molecules and ions in only two dimensions. With four electron groups, we must learn to show molecules and ions in three dimensions.

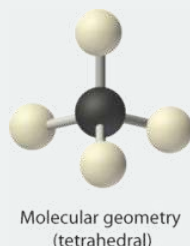
AX₄ Molecules: CH₄

1. The central atom, carbon, contributes four valence electrons, and each hydrogen atom has one valence electron, so the full Lewis electron structure is



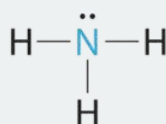
Lewis structure

2. There are four electron groups around the central atom. As shown in Figure 1.2.2, repulsions are minimized by placing the groups in the corners of a tetrahedron with bond angles of 109.5° .
3. All electron groups are bonding pairs, so the structure is designated as AX₄.
4. With four bonding pairs, the molecular geometry of methane is *tetrahedral* (Figure 1.2.3).



AX₃E Molecules: NH₃

1. In ammonia, the central atom, nitrogen, has five valence electrons and each hydrogen donates one valence electron, producing the Lewis electron structure



Lewis structure

2. There are four electron groups around nitrogen, three bonding pairs and one lone pair. Repulsions are minimized by directing each hydrogen atom and the lone pair to the corners of a tetrahedron.
3. With three bonding pairs and one lone pair, the structure is designated as AX₃E. This designation has a total of four electron pairs, three X and one E. We expect the LP–BP interactions to cause the bonding pair angles to deviate significantly from the

angles of a perfect tetrahedron.

4. There are three nuclei and one lone pair, so the molecular geometry is *trigonal pyramidal*. In essence, this is a tetrahedron with a vertex missing (Figure 1.2.3). However, the H–N–H bond angles are less than the ideal angle of 109.5° because of LP–BP repulsions (Figure 1.2.3 and Figure 1.2.4).

AX₂E₂ Molecules: H₂O

1. Oxygen has six valence electrons and each hydrogen has one valence electron, producing the Lewis electron structure

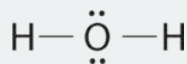
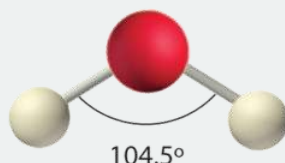


Figure 1.2.2: (CC BY-NC-SA; anonymous)

3. With two bonding pairs and two lone pairs, the structure is designated as AX₂E₂ with a total of four electron pairs. Due to LP–LP, LP–BP, and BP–BP interactions, we expect a significant deviation from idealized tetrahedral angles.

4. With two hydrogen atoms and two lone pairs of electrons, the structure has significant lone pair interactions. There are two nuclei about the central atom, so the molecular shape is *bent*, or *V shaped*, with an H–O–H angle that is even less than the H–N–H angles in NH₃, as we would expect because of the presence of two lone pairs of electrons on the central atom rather than one. This molecular shape is essentially a tetrahedron with two missing vertices.



Five Electron Groups

In previous examples it did not matter where we placed the electron groups because all positions were equivalent. In some cases, however, the positions are not equivalent. We encounter this situation for the first time with five electron groups.

AX₅ Molecules: PCl₅

1. Phosphorus has five valence electrons and each chlorine has seven valence electrons, so the Lewis electron structure of PCl₅ is

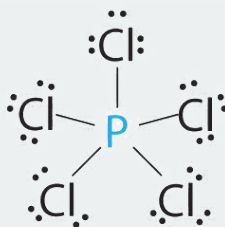
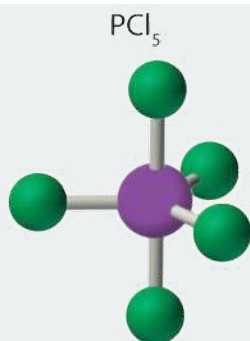


Figure 1.2.2: (CC BY-NC-SA; anonymous)

3. All electron groups are bonding pairs, so the structure is designated as AX₅. There are no lone pair interactions.

4. The molecular geometry of PCl₅ is *trigonal bipyramidal*, as shown in Figure 1.2.3. The molecule has three atoms in a plane in *equatorial* positions and two atoms above and below the plane in *axial* positions. The three equatorial positions are separated by 120° from one another, and the two axial positions are at 90° to the equatorial plane. The axial and equatorial positions are not chemically equivalent, as we will see in our next example.



AX₄E Molecules: SF₄

1. The sulfur atom has six valence electrons and each fluorine has seven valence electrons, so the Lewis electron structure is



Lewis structure

Four fluorenes are bonded to a central sulfur. Each fluorine has three lone pairs. Sulfur has one lone pair.

With an expanded valence, this species is an exception to the octet rule.

2. There are five groups around sulfur, four bonding pairs and one lone pair. With five electron groups, the lowest energy arrangement is a trigonal bipyramid, as shown in Figure 1.2.2.

3. We designate SF₄ as AX₄E; it has a total of five electron pairs. However, because the axial and equatorial positions are not chemically equivalent, where do we place the lone pair? If we place the lone pair in the axial position, we have three LP–BP repulsions at 90°. If we place it in the equatorial position, we have two 90° LP–BP repulsions at 90°. With fewer 90° LP–BP repulsions, we can predict that the structure with the lone pair of electrons in the *equatorial position* is *more stable than the one with the lone pair in the axial position*. We also expect a deviation from ideal geometry because a lone pair of electrons occupies more space than a bonding pair.

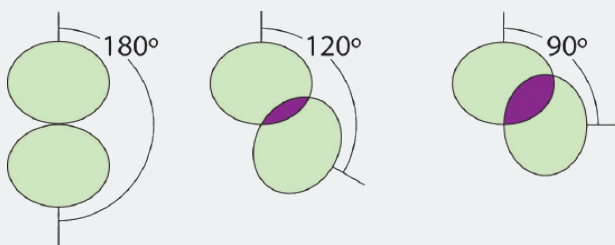
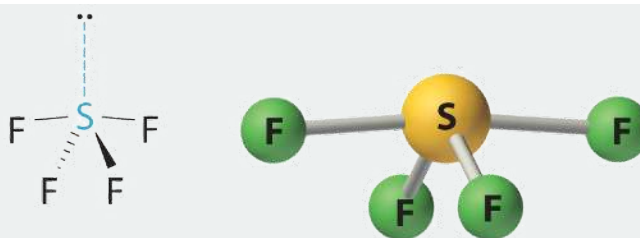


Figure 1.2.5: Illustration of the Area Shared by Two Electron Pairs versus the Angle between Them

180 degree angle has no shared space between two electron pairs. 120 degree angle has some shared area between two electron pairs. 90 degree angle has more shared space than 120.

At 90°, the two electron pairs share a relatively large region of space, which leads to strong repulsive electron–electron interactions.

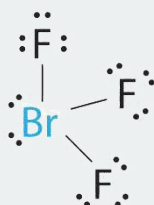
4. With four nuclei and one lone pair of electrons, the molecular structure is based on a trigonal bipyramid with a missing equatorial vertex; it is described as a *seesaw*. The F_{axial}–S–F_{axial} angle is 173° rather than 180° because of the lone pair of electrons in the equatorial plane.



Molecular geometry (seesaw)

AX₃E₂ Molecules: BrF₃

1. The bromine atom has seven valence electrons, and each fluorine has seven valence electrons, so the Lewis electron structure is



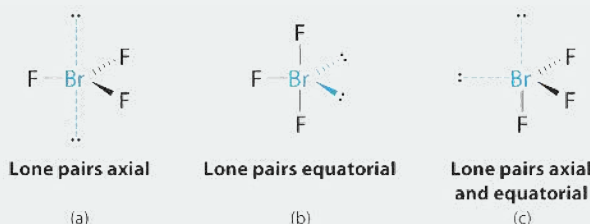
Lewis structure

Three fluorines are bonded to a central bromine. Each fluorine has three lone pairs, Bromine has two lone pairs.

Once again, we have a compound that is an exception to the octet rule.

2. There are five groups around the central atom, three bonding pairs and two lone pairs. We again direct the groups toward the vertices of a trigonal bipyramid.

3. With three bonding pairs and two lone pairs, the structural designation is AX₃E₂ with a total of five electron pairs. Because the axial and equatorial positions are not equivalent, we must decide how to arrange the groups to minimize repulsions. If we place both lone pairs in the axial positions, we have six LP–BP repulsions at 90°. If both are in the equatorial positions, we have four LP–BP repulsions at 90°. If one lone pair is axial and the other equatorial, we have one LP–LP repulsion at 90° and three LP–BP repulsions at 90°:



Interactions

90° LP–LP	0	0	1
90° LP–BP	6	4	3

If the lone pairs are axial, the 90 degree LP–LP interactions are 0 and the 90 degree LP–BP interaction is zero. If the lone pairs are equatorial there are zero 90 degree LP–LP interactions and four 90 degree LP–BP interactions. If the lone pairs are axial and equatorial there is one 90 degree LP–LP interaction and three 90 degree LP–BP interaction.

Structure (c) can be eliminated because it has a LP–LP interaction at 90°. Structure (b), with fewer LP–BP repulsions at 90° than (a), is lower in energy. However, we predict a deviation in bond angles because of the presence of the two lone pairs of electrons.

4. The three nuclei in BrF₃ determine its molecular structure, which is described as *T shaped*. This is essentially a trigonal bipyramid that is missing two equatorial vertices. The F_{axial}–Br–F_{axial} angle is 172°, less than 180° because of LP–BP repulsions (Figure 1.2.2.1).

Because lone pairs occupy more space around the central atom than bonding pairs, electrostatic repulsions are more important for lone pairs than for bonding pairs.

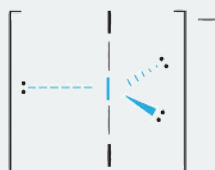
AX₂E₃ Molecules: I₃⁻

1. Each iodine atom contributes seven electrons and the negative charge one, so the Lewis electron structure is



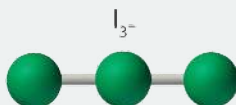
2. There are five electron groups about the central atom in I₃⁻, two bonding pairs and three lone pairs. To minimize repulsions, the groups are directed to the corners of a trigonal bipyramid.

3. With two bonding pairs and three lone pairs, I₃⁻ has a total of five electron pairs and is designated as AX₂E₃. We must now decide how to arrange the lone pairs of electrons in a trigonal bipyramid in a way that minimizes repulsions. Placing them in the axial positions eliminates 90° LP-LP repulsions and minimizes the number of 90° LP-BP repulsions.



The three lone pairs of electrons have equivalent interactions with the three iodine atoms, so we do not expect any deviations in bonding angles.

4. With three nuclei and three lone pairs of electrons, the molecular geometry of I₃⁻ is linear. This can be described as a trigonal bipyramid with three equatorial vertices missing. The ion has an I-I-I angle of 180°, as expected.



Six Electron Groups

Six electron groups form an *octahedron*, a polyhedron made of identical equilateral triangles and six identical vertices (Figure 1.2.2.)

AX₆ Molecules: SF₆

1. The central atom, sulfur, contributes six valence electrons, and each fluorine atom has seven valence electrons, so the Lewis electron structure is



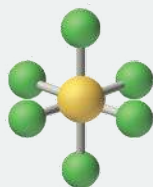
Lewis structure

With an expanded valence, this species is an exception to the octet rule.

2. There are six electron groups around the central atom, each a bonding pair. We see from Figure 1.2.2 that the geometry that minimizes repulsions is *octahedral*.

3. With only bonding pairs, SF₆ is designated as AX₆. All positions are chemically equivalent, so all electronic interactions are equivalent.

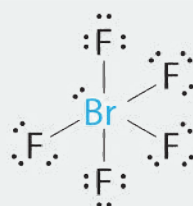
4. There are six nuclei, so the molecular geometry of SF_6 is octahedral.



Molecular geometry
(octahedral)

AX₅E Molecules: BrF_5

1. The central atom, bromine, has seven valence electrons, as does each fluorine, so the Lewis electron structure is

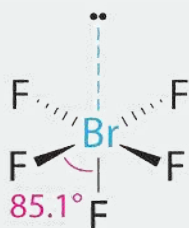


Lewis structure

Five fluorines are bonded to a central bromine. Each fluorine has three lone pairs, Bromine has one lone pair.

With its expanded valence, this species is an exception to the octet rule.

2. There are six electron groups around the Br, five bonding pairs and one lone pair. Placing five F atoms around Br while minimizing BP–BP and LP–BP repulsions gives the following structure:



3. With five bonding pairs and one lone pair, BrF_5 is designated as AX_5E ; it has a total of six electron pairs. The BrF_5 structure has four fluorine atoms in a plane in an equatorial position and one fluorine atom and the lone pair of electrons in the axial positions. We expect all $\text{F}_{\text{axial}}\text{--Br--F}_{\text{equatorial}}$ angles to be less than 90° because of the lone pair of electrons, which occupies more space than the bonding electron pairs.

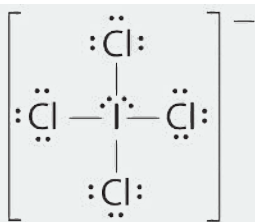
4. With five nuclei surrounding the central atom, the molecular structure is based on an octahedron with a vertex missing. This molecular structure is *square pyramidal*. The $\text{F}_{\text{axial}}\text{--Br--F}_{\text{equatorial}}$ angles are 85.1° , less than 90° because of LP–BP repulsions.



Molecular geometry
(square pyramidal)

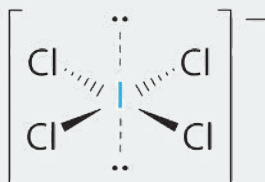
AX₄E₂ Molecules: ICl_4^-

1. The central atom, iodine, contributes seven electrons. Each chlorine contributes seven, and there is a single negative charge. The Lewis electron structure is



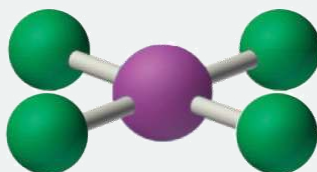
Four chlorines are bonded to a central iodine. Each chlorine has three electron pairs. The iodine has two electron pairs. The molecule is negatively charged.

2. There are six electron groups around the central atom, four bonding pairs and two lone pairs. The structure that minimizes LP-LP, LP-BP, and BP-BP repulsions is



3. ICl_4^- is designated as AX_4E_2 and has a total of six electron pairs. Although there are lone pairs of electrons, with four bonding electron pairs in the equatorial plane and the lone pairs of electrons in the axial positions, all LP-BP repulsions are the same. Therefore, we do not expect any deviation in the Cl-I-Cl bond angles.

4. With five nuclei, the ICl_4^- ion forms a molecular structure that is *square planar*, an octahedron with two opposite vertices missing.



The relationship between the number of electron groups around a central atom, the number of lone pairs of electrons, and the molecular geometry is summarized in Figure 1.2.6.

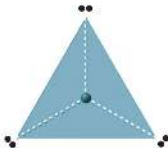
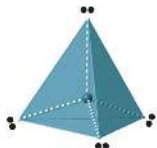
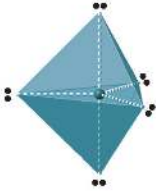
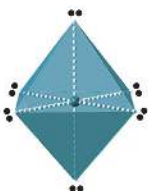
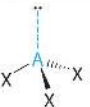
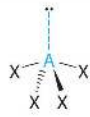
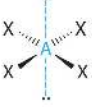
Electron Groups	2	3	4	5	6
Molecular Geometry	 Linear	 Trigonal planar	 Tetrahedral	 Trigonal bipyramidal	 Octahedral
Zero Lone Pairs	 Linear AX_2	 Trigonal planar AX_3	 Tetrahedral AX_4	 Trigonal bipyramidal AX_5	 Octahedral AX_6
One Lone Pair		 Bent (V-shaped) AX_2E	 Trigonal pyramidal AX_3E	 Seesaw AX_5E One axial lone pair	 Square pyramidal AX_5E
Two Lone Pairs			 Bent (V-shaped) AX_2E_2	 T-shaped AX_3E_2 Two axial lone pairs	 Square planar AX_4E_2
Three Lone Pairs				 Linear AX_3E_3 Three axial lone pairs	

Figure 1.2.6: Overview of Molecular Geometries



✓ Example 1.2.1

Using the VSEPR model, predict the molecular geometry of each molecule or ion.

1. PF_5 (phosphorus pentafluoride, a catalyst used in certain organic reactions)
2. H_3O^+ (hydronium ion)

Given: two chemical species

Asked for: molecular geometry

Strategy:

- Draw the Lewis electron structure of the molecule or polyatomic ion.
- Determine the electron group arrangement around the central atom that minimizes repulsions.
- Assign an AX_mE_n designation; then identify the LP–LP, LP–BP, or BP–BP interactions and predict deviations in bond angles.
- Describe the molecular geometry.

Solution:

- A** The central atom, P, has five valence electrons and each fluorine has seven valence electrons, so the Lewis structure of PF_5 is

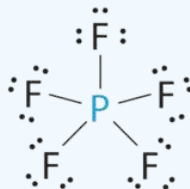
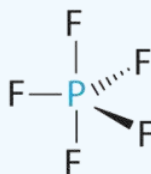


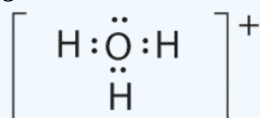
Figure 1.2.6): (CC BY-NC-SA; anonymous)

C All electron groups are bonding pairs, so PF_5 is designated as AX_5 . Notice that this gives a total of five electron pairs. With no lone pair repulsions, we do not expect any bond angles to deviate from the ideal.

D The PF_5 molecule has five nuclei and no lone pairs of electrons, so its molecular geometry is trigonal bipyramidal.



- A** The central atom, O, has six valence electrons, and each H atom contributes one valence electron. Subtracting one electron for the positive charge gives a total of eight valence electrons, so the Lewis electron structure is

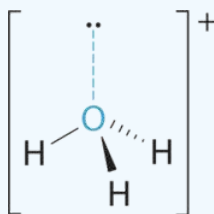


Three hydrogens are bonded to a central oxygen. The oxygen has two lone pairs. The molecule has a charge of plus one.

B There are four electron groups around oxygen, three bonding pairs and one lone pair. Like NH_3 , repulsions are minimized by directing each hydrogen atom and the lone pair to the corners of a tetrahedron.

C With three bonding pairs and one lone pair, the structure is designated as AX_3E and has a total of four electron pairs (three X and one E). We expect the LP–BP interactions to cause the bonding pair angles to deviate significantly from the angles of a perfect tetrahedron.

D There are three nuclei and one lone pair, so the molecular geometry is *trigonal pyramidal*, in essence a tetrahedron missing a vertex. However, the H–O–H bond angles are less than the ideal angle of 109.5° because of LP–BP repulsions:



? Exercise 1.2.1

Using the VSEPR model, predict the molecular geometry of each molecule or ion.

- XeO_3
- PF_6^-
- NO_2^+

Answer a

trigonal pyramidal

Answer b

octahedral

Answer c

linear

✓ Example 1.2.2

Predict the molecular geometry of each molecule.

- XeF_2
- SnCl_2

Given: two chemical compounds

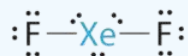
Asked for: molecular geometry

Strategy:

Use the strategy given in Example 1.2.1.

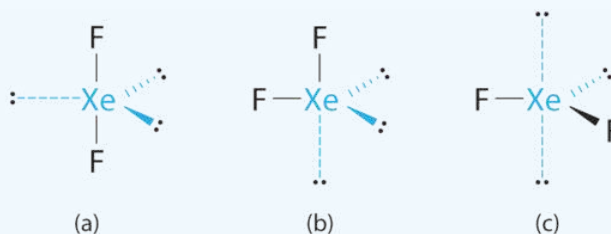
Solution:

- A** Xenon contributes eight electrons and each fluorine seven valence electrons, so the Lewis electron structure is



B There are five electron groups around the central atom, two bonding pairs and three lone pairs. Repulsions are minimized by placing the groups in the corners of a trigonal bipyramid.

C From B, XeF_2 is designated as AX_2E_3 and has a total of five electron pairs (two X and three E). With three lone pairs about the central atom, we can arrange the two F atoms in three possible ways: both F atoms can be axial, one can be axial and one equatorial, or both can be equatorial:



Interactions

90 LP-LP

0

2

2

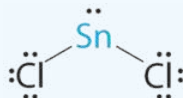
If the two F atoms are axial there are zero 90 LP-LP interactions. If the two F atoms are axial and equatorial or just equatorial, there are 2 90 LP-LP interactions.

The structure with the lowest energy is the one that minimizes LP-LP repulsions. Both (b) and (c) have two 90° LP-LP interactions, whereas structure (a) has none. Thus both F atoms are in the axial positions, like the two iodine atoms around

the central iodine in I_3^- . All LP–BP interactions are equivalent, so we do not expect a deviation from an ideal 180° in the F–Xe–F bond angle.

D With two nuclei about the central atom, the molecular geometry of XeF_2 is linear. It is a trigonal bipyramid with three missing equatorial vertices.

2. **A** The tin atom donates 4 valence electrons and each chlorine atom donates 7 valence electrons. With 18 valence electrons, the Lewis electron structure is



Two chlorines are bonded to a central tin. Each chlorine has three lone pairs. Tin has one lone pair.

B There are three electron groups around the central atom, two bonding groups and one lone pair of electrons. To minimize repulsions the three groups are initially placed at 120° angles from each other.

C From **B** we designate SnCl_2 as AX_2E . It has a total of three electron pairs, two X and one E. Because the lone pair of electrons occupies more space than the bonding pairs, we expect a decrease in the Cl–Sn–Cl bond angle due to increased LP–BP repulsions.

D With two nuclei around the central atom and one lone pair of electrons, the molecular geometry of SnCl_2 is bent, like SO_2 , but with a Cl–Sn–Cl bond angle of 95° . The molecular geometry can be described as a trigonal planar arrangement with one vertex missing.

? Exercise 1.2.2

Predict the molecular geometry of each molecule.

- SO_3
- XeF_4

Answer a

trigonal planar

Answer b

square planar

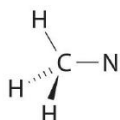


Molecules with No Single Central Atom

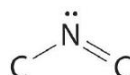
The VSEPR model can be used to predict the structure of somewhat more complex molecules with no single central atom by treating them as linked AX_mE_n fragments. We will demonstrate with methyl isocyanate ($\text{CH}_3\text{–N=C=O}$), a volatile and highly toxic molecule that is used to produce the pesticide Sevin. In 1984, large quantities of Sevin were accidentally released in Bhopal, India,

when water leaked into storage tanks. The resulting highly exothermic reaction caused a rapid increase in pressure that ruptured the tanks, releasing large amounts of methyl isocyanate that killed approximately 3800 people and wholly or partially disabled about 50,000 others. In addition, there was significant damage to livestock and crops.

We can treat methyl isocyanate as linked AX_mE_n fragments beginning with the carbon atom at the left, which is connected to three H atoms and one N atom by single bonds. The four bonds around carbon mean that it must be surrounded by four bonding electron pairs in a configuration similar to AX_4 . We can therefore predict the CH_3-N portion of the molecule to be roughly tetrahedral, similar to methane:



The nitrogen atom is connected to one carbon by a single bond and to the other carbon by a double bond, producing a total of three bonds, $C-N=C$. For nitrogen to have an octet of electrons, it must also have a lone pair:



One carbon bonded to nitrogen and another carbon double bonded to the nitrogen. The nitrogen has one lone pair.

Because multiple bonds are not shown in the VSEPR model, the nitrogen is effectively surrounded by three electron pairs. Thus according to the VSEPR model, the $C-N=C$ fragment should be bent with an angle less than 120° .

The carbon in the $-N=C=O$ fragment is doubly bonded to both nitrogen and oxygen, which in the VSEPR model gives carbon a total of two electron pairs. The $N=C=O$ angle should therefore be 180° , or linear. The three fragments combine to give the following structure:

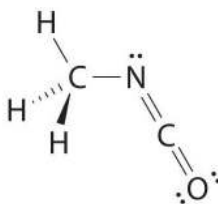


Figure 1.2.7).

Three hydrogens are bonded to a carbon. The carbon is also bonded to a nitrogen. The nitrogen is double bonded to another carbon. The second carbon is double bonded to an oxygen. The nitrogen has one lone pair. The oxygen has two lone pairs.

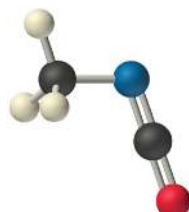


Figure 1.2.7: The Experimentally Determined Structure of Methyl Isocyanate

Certain patterns are seen in the structures of moderately complex molecules. For example, carbon atoms with four bonds (such as the carbon on the left in methyl isocyanate) are generally tetrahedral. Similarly, the carbon atom on the right has two double bonds that are similar to those in CO_2 , so its geometry, like that of CO_2 , is linear. Recognizing similarities to simpler molecules will help you predict the molecular geometries of more complex molecules.

✓ Example 1.2.3

Use the VSEPR model to predict the molecular geometry of propyne ($H_3C-C\equiv CH$), a gas with some anesthetic properties.

Given: chemical compound

Asked for: molecular geometry

Strategy:

Count the number of electron groups around each carbon, recognizing that in the VSEPR model, a multiple bond counts as a single group. Use Figure 1.2.3 to determine the molecular geometry around each carbon atom and then deduce the structure of the molecule as a whole.

Solution:

Because the carbon atom on the left is bonded to four other atoms, we know that it is approximately tetrahedral. The next two carbon atoms share a triple bond, and each has an additional single bond. Because a multiple bond is counted as a single bond in the VSEPR model, each carbon atom behaves as if it had two electron groups. This means that both of these carbons are linear, with $\text{C}-\text{C}\equiv\text{C}$ and $\text{C}\equiv\text{C}-\text{H}$ angles of 180° .

? Exercise 1.2.3

Predict the geometry of allene ($\text{H}_2\text{C}=\text{C}=\text{CH}_2$), a compound with narcotic properties that is used to make more complex organic molecules.

Answer

The terminal carbon atoms are trigonal planar, the central carbon is linear, and the $\text{C}-\text{C}-\text{C}$ angle is 180° .

Molecular Dipole Moments

You previously learned how to calculate the **dipole moments** of simple diatomic molecules. In more complex molecules with polar covalent bonds, the three-dimensional geometry and the compound's symmetry determine whether there is a net dipole moment. Mathematically, dipole moments are *vectors*; they possess both a *magnitude* and a *direction*. The dipole moment of a molecule is therefore the *vector sum* of the dipole moments of the individual bonds in the molecule. If the individual bond dipole moments cancel one another, there is no net dipole moment. Such is the case for CO_2 , a linear molecule (Figure 1.2.8a). Each $\text{C}-\text{O}$ bond in CO_2 is polar, yet experiments show that the CO_2 molecule has no dipole moment. Because the two $\text{C}-\text{O}$ bond dipoles in CO_2 are equal in magnitude and oriented at 180° to each other, they cancel. As a result, the CO_2 molecule has no *net* dipole moment even though it has a substantial separation of charge. In contrast, the H_2O molecule is not linear (Figure 1.2.8b); it is bent in three-dimensional space, so the dipole moments do not cancel each other. Thus a molecule such as H_2O has a net dipole moment. We expect the concentration of negative charge to be on the oxygen, the more electronegative atom, and positive charge on the two hydrogens. This charge polarization allows H_2O to hydrogen-bond to other polarized or charged species, including other water molecules.

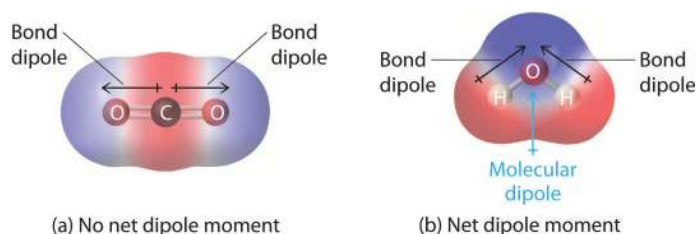


Figure 1.2.8: How Individual Bond Dipole Moments Are Added Together to Give an Overall Molecular Dipole Moment for Two Triatomic Molecules with Different Structures. (a) In CO_2 , the $\text{C}-\text{O}$ bond dipoles are equal in magnitude but oriented in opposite directions (at 180°). Their vector sum is zero, so CO_2 therefore has no net dipole. (b) In H_2O , the $\text{O}-\text{H}$ bond dipoles are also equal in magnitude, but they are oriented at 104.5° to each other. Hence the vector sum is not zero, and H_2O has a net dipole moment.

Other examples of molecules with polar bonds are shown in Figure 1.2.9. In molecular geometries that are highly symmetrical (most notably tetrahedral and square planar, trigonal bipyramidal, and octahedral), individual bond dipole moments completely cancel, and there is no net dipole moment. Although a molecule like CHCl_3 is best described as tetrahedral, the atoms bonded to carbon are not identical. Consequently, the bond dipole moments cannot cancel one another, and the molecule has a dipole moment. Due to the arrangement of the bonds in molecules that have V-shaped, trigonal pyramidal, seesaw, T-shaped, and square pyramidal geometries, the bond dipole moments cannot cancel one another. Consequently, molecules with these geometries always have a nonzero dipole moment. Molecules with asymmetrical charge distributions have a net dipole moment.

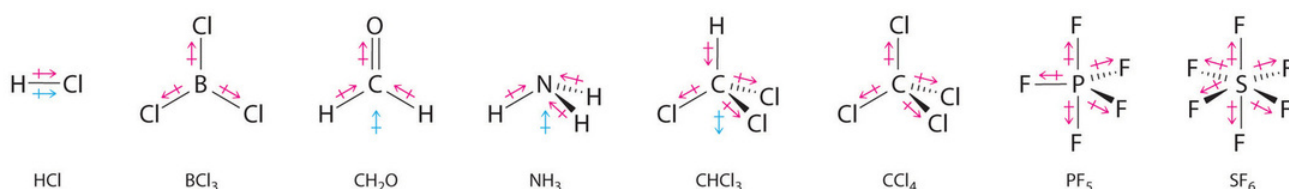


Figure 1.2.9: Molecules with Polar Bonds. Individual bond dipole moments are indicated in red. Due to their different three-dimensional structures, some molecules with polar bonds have a net dipole moment (HCl , CH_2O , NH_3 , and CHCl_3), indicated in blue, whereas others do not because the bond dipole moments cancel (BCl_3 , CCl_4 , PF_5 , and SF_6).



✓ Example 1.2.4

Which molecule(s) has a net dipole moment?

- H_2S
- NHF_2
- BF_3

Given: three chemical compounds

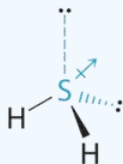
Asked for: net dipole moment

Strategy:

For each three-dimensional molecular geometry, predict whether the bond dipoles cancel. If they do not, then the molecule has a net dipole moment.

Solution:

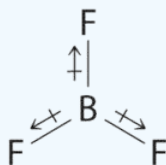
- The total number of electrons around the central atom, S, is eight, which gives four electron pairs. Two of these electron pairs are bonding pairs and two are lone pairs, so the molecular geometry of H_2S is bent (Figure 1.2.6). The bond dipoles cannot cancel one another, so the molecule has a net dipole moment.



- Difluoroamine has a trigonal pyramidal molecular geometry. Because there is one hydrogen and two fluorines, and because of the lone pair of electrons on nitrogen, the molecule is not symmetrical, and the bond dipoles of NHF_2 cannot cancel one another. This means that NHF_2 has a net dipole moment. We expect polarization from the two fluorine atoms, the most electronegative atoms in the periodic table, to have a greater affect on the net dipole moment than polarization from the lone pair of electrons on nitrogen.



3. The molecular geometry of BF_3 is trigonal planar. Because all the B–F bonds are equal and the molecule is highly symmetrical, the dipoles cancel one another in three-dimensional space. Thus BF_3 has a net dipole moment of zero:



? Exercise 1.2.4

Which molecule(s) has a net dipole moment?

- CH_3Cl
- SO_3
- XeO_3

Answer

CH_3Cl and XeO_3

Summary

Lewis electron structures give no information about **molecular geometry**, the arrangement of bonded atoms in a molecule or polyatomic ion, which is crucial to understanding the chemistry of a molecule. The **valence-shell electron-pair repulsion (VSEPR) model** allows us to predict which of the possible structures is actually observed in most cases. It is based on the assumption that pairs of electrons occupy space, and the lowest-energy structure is the one that minimizes electron pair–electron pair repulsions. In the VSEPR model, the molecule or polyatomic ion is given an AX_mE_n designation, where A is the central atom, X is a bonded atom, E is a nonbonding valence electron group (usually a lone pair of electrons), and m and n are integers. Each group around the central atom is designated as a bonding pair (BP) or lone (nonbonding) pair (LP). From the BP and LP interactions we can predict both the relative positions of the atoms and the angles between the bonds, called the **bond angles**. From this we can describe the **molecular geometry**. The VSEPR model can be used to predict the shapes of many molecules and polyatomic ions, but it gives no information about bond lengths and the presence of multiple bonds. A combination of VSEPR and a bonding model, such as Lewis electron structures, is necessary to understand the presence of multiple bonds.

Molecules with polar covalent bonds can have a *dipole moment*, an asymmetrical distribution of charge that results in a tendency for molecules to align themselves in an applied electric field. Any diatomic molecule with a polar covalent bond has a dipole moment, but in polyatomic molecules, the presence or absence of a net dipole moment depends on the structure. For some highly symmetrical structures, the individual bond dipole moments cancel one another, giving a dipole moment of zero.

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1.3: VSEPR Theory- The Effect of Lone Pairs

Learning Objectives

- To use the VSEPR model to predict molecular geometries.
- To predict whether a molecule has a dipole moment.

The Lewis electron-pair approach can be used to predict the number and types of bonds between the atoms in a substance, and it indicates which atoms have lone pairs of electrons. This approach gives no information about the actual arrangement of atoms in space, however. We continue our discussion of structure and bonding by introducing the **valence-shell electron-pair repulsion** (VSEPR) model (pronounced “vesper”), which can be used to predict the shapes of many molecules and polyatomic ions. Keep in mind, however, that the VSEPR model, like any model, is a limited representation of reality; the model provides no information about bond lengths or the presence of multiple bonds.

The VSEPR Model

The VSEPR model can predict the structure of nearly any molecule or polyatomic ion in which the central atom is a nonmetal, as well as the structures of many molecules and polyatomic ions with a central metal atom. The premise of the VSEPR theory is that electron pairs located in bonds and lone pairs repel each other and will therefore adopt the geometry that places electron pairs as far apart from each other as possible. This theory is very simplistic and does not account for the subtleties of orbital interactions that influence molecular shapes; however, the simple VSEPR counting procedure accurately predicts the three-dimensional structures of a large number of compounds, which cannot be predicted using the Lewis electron-pair approach.

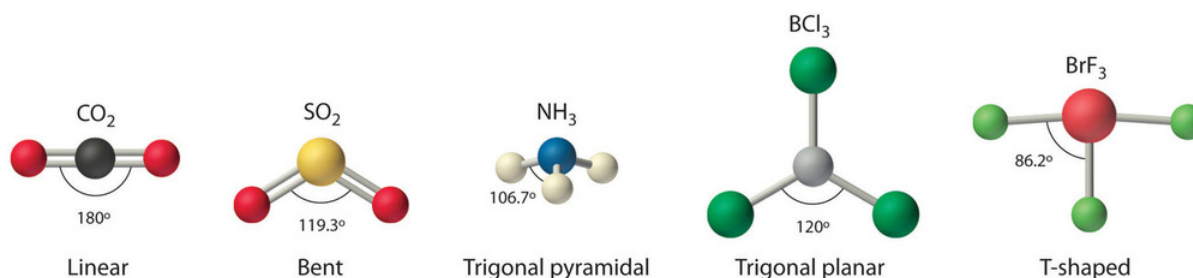


Figure 1.3.1: Common Structures for Molecules and Polyatomic Ions That Consist of a Central Atom Bonded to Two or Three Other Atoms. (CC BY-NC-SA; anonymous)

We can use the VSEPR model to predict the geometry of most polyatomic molecules and ions by focusing only on the number of electron pairs around the *central atom*, ignoring all other valence electrons present. According to this model, valence electrons in the Lewis structure form *groups*, which may consist of a single bond, a double bond, a triple bond, a lone pair of electrons, or even a single unpaired electron, which in the VSEPR model is counted as a lone pair. Because electrons repel each other electrostatically, the most stable arrangement of electron groups (i.e., the one with the lowest energy) is the one that minimizes repulsions. Groups are positioned around the central atom in a way that produces the molecular structure with the lowest energy, as illustrated in Figures 1.3.1 and 1.3.2.

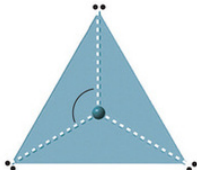
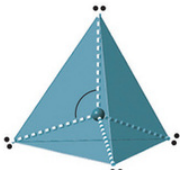
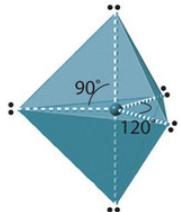
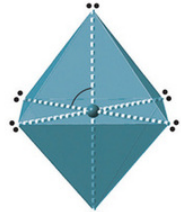
Electron Groups	2	3	4	5	6
Geometry	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
					
Predicted Bond Angles	180°	120°	109.5°	90°, 120°	90°

Figure 1.3.2: Electron Geometries for Species with Two to Six Electron Groups. Groups are placed around the central atom in a way that produces a molecular structure with the lowest energy, that is, the one that minimizes repulsions. (CC BY-NC-SA; anonymous)

In the VSEPR model, the molecule or polyatomic ion is given an AX_mE_n designation, where A is the central atom, X is a bonded atom, E is a nonbonding valence electron group (usually a lone pair of electrons), and m and n are integers. Each group around the central atom is designated as a bonding pair (BP) or lone (nonbonding) pair (LP). From the BP and LP interactions we can predict both the relative positions of the atoms and the angles between the bonds, called the bond angles. Using this information, we can describe the molecular geometry, the arrangement of the *bonded atoms* in a molecule or polyatomic ion.

VSEPR Produce to predict Molecular geometry

This VSEPR procedure is summarized as follows:

1. Draw the Lewis electron structure of the molecule or polyatomic ion.
2. Determine the electron group arrangement around the central atom that minimizes repulsions.
3. Assign an AX_mE_n designation; then identify the LP–LP, LP–BP, or BP–BP interactions and predict deviations from ideal bond angles.
4. Describe the molecular geometry.

We will illustrate the use of this procedure with several examples, beginning with atoms with two electron groups. In our discussion we will refer to Figure 1.3.2 and Figure 1.3.3, which summarize the common molecular geometries and idealized bond angles of molecules and ions with two to six electron groups.

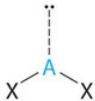
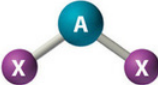
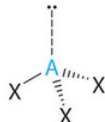
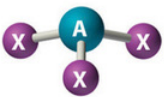
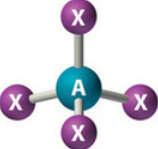
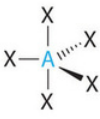
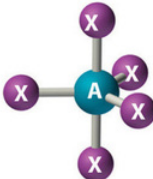
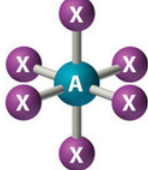
AX_mE_n Notation	AX_2	AX_2E	AX_3	AX_3E
Geometry	Linear $X-A-X$ 	Bent (V-shaped)  	Trigonal planar  	Trigonal pyramidal  
Idealized Bond Angles	180°	$<180^\circ$	120°	$<120^\circ$
AX_mE_n Notation	AX_4E_2	AX_4	AX_5	AX_6
Geometry	Square planar  	Tetrahedral  	Trigonal bipyramidal  	Octahedral  
Idealized Bond Angles	90°	109.5°	$90^\circ, 120^\circ$	90°

Figure 1.3.3: Common Molecular Geometries for Species with Two to Six Electron Groups. Lone pairs are shown using a dashed line. (CC BY-NC-SA; anonymous)

Linear, bent, trigonal planar, trigonal pyramidal, square planar, tetrahedral, trigonal bipyramidal, octahedral.

Two Electron Groups

Our first example is a molecule with two bonded atoms and no lone pairs of electrons, BeH_2 .

AX_2 Molecules: BeH_2

1. The central atom, beryllium, contributes two valence electrons, and each hydrogen atom contributes one. The Lewis electron structure is



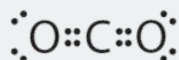
Lewis structure

Figure 1.3.2 that the arrangement that minimizes repulsions places the groups 180° apart. (CC BY-NC-SA; anonymous)

3. Both groups around the central atom are bonding pairs (BP). Thus BeH_2 is designated as AX_2 .
4. From Figure 1.3.3 we see that with two bonding pairs, the molecular geometry that minimizes repulsions in BeH_2 is *linear*.

AX₂ Molecules: CO₂

1. The central atom, carbon, contributes four valence electrons, and each oxygen atom contributes six. The Lewis electron structure is



2. The carbon atom forms two double bonds. Each double bond is a group, so there are two electron groups around the central atom. Like BeH₂, the arrangement that minimizes repulsions places the groups 180° apart.

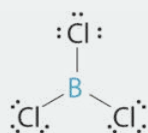
3. Once again, both groups around the central atom are bonding pairs (BP), so CO₂ is designated as AX₂.

4. VSEPR only recognizes groups around the *central* atom. Thus the lone pairs on the oxygen atoms do not influence the molecular geometry. With two bonding pairs on the central atom and no lone pairs, the molecular geometry of CO₂ is linear (Figure 1.3.3). The structure of CO₂ is shown in Figure 1.3.1.

Three Electron Groups

AX₃ Molecules: BCl₃

1. The central atom, boron, contributes three valence electrons, and each chlorine atom contributes seven valence electrons. The Lewis electron structure is



Lewis structure

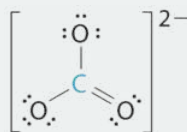
Figure 1.3.2): (CC BY-NC-SA; anonymous)

3. All electron groups are bonding pairs (BP), so the structure is designated as AX₃.

4. From Figure 1.3.3 we see that with three bonding pairs around the central atom, the molecular geometry of BCl₃ is *trigonal planar*, as shown in Figure 1.3.2.

AX₃ Molecules: CO₃²⁻

1. The central atom, carbon, has four valence electrons, and each oxygen atom has six valence electrons. As you learned previously, the Lewis electron structure of one of three resonance forms is represented as



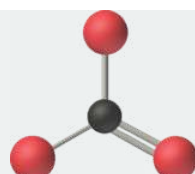
Lewis structure

Figure 1.3.2).

The three oxygens are arranged in a triangular shape with carbon at the center. Two of the oxygens have three lone pairs. One oxygen has 2 lone pairs and is double bonded to the carbon. The molecule has a minus 2 charge.

3. All electron groups are bonding pairs (BP). With three bonding groups around the central atom, the structure is designated as AX₃.

4. We see from Figure 1.3.3 that the molecular geometry of CO₃²⁻ is trigonal planar with bond angles of 120°.



Molecular geometry
(trigonal planar)

In our next example we encounter the effects of lone pairs and multiple bonds on molecular geometry for the first time.

AX₂E Molecules: SO₂

1. The central atom, sulfur, has 6 valence electrons, as does each oxygen atom. With 18 valence electrons, the Lewis electron structure is shown below.

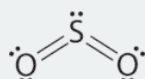


Figure 1.3.2): (CC BY-NC-SA; anonymous)

The two oxygens are double bonded to the sulfur. The oxygens have 2 lone pairs while sulfur had one lone pair.

3. There are two bonding pairs and one lone pair, so the structure is designated as AX₂E. This designation has a total of three electron pairs, two X and one E. Because a lone pair is not shared by two nuclei, it occupies more space near the central atom than a bonding pair (Figure 1.3.4). Thus bonding pairs and lone pairs repel each other electrostatically in the order BP–BP < LP–BP < LP–LP. In SO₂, we have one BP–BP interaction and two LP–BP interactions.

4. The molecular geometry is described only by the positions of the nuclei, *not* by the positions of the lone pairs. Thus with two nuclei and one lone pair the shape is *bent*, or *V shaped*, which can be viewed as a trigonal planar arrangement with a missing vertex (Figures 1.3.2 and 1.3.3). The O–S–O bond angle is expected to be *less than* 120° because of the extra space taken up by the lone pair.

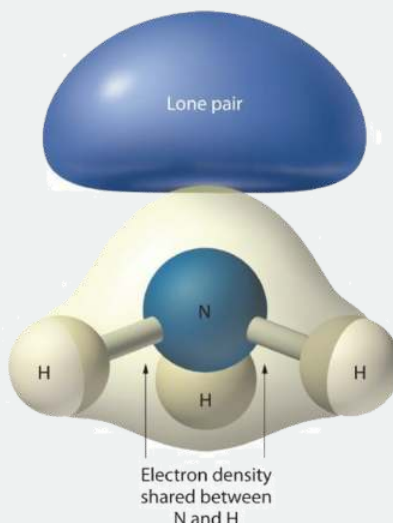
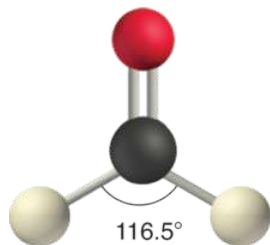


Figure 1.3.4: The Difference in the Space Occupied by a Lone Pair of Electrons and by a Bonding Pair. (CC BY-NC-SA; anonymous)

As with SO₂, this composite model of electron distribution and negative electrostatic potential in ammonia shows that a lone pair of electrons occupies a larger region of space around the nitrogen atom than does a bonding pair of electrons that is shared with a hydrogen atom.

Like lone pairs of electrons, multiple bonds occupy more space around the central atom than a single bond, which can cause other bond angles to be somewhat smaller than expected. This is because a multiple bond has a higher electron density than a single bond, so its electrons occupy more space than those of a single bond. For example, in a molecule such as CH₂O (AX₃), whose

structure is shown below, the double bond repels the single bonds more strongly than the single bonds repel each other. This causes a deviation from ideal geometry (an H–C–H bond angle of 116.5° rather than 120°).

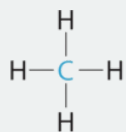


Four Electron Groups

One of the limitations of Lewis structures is that they depict molecules and ions in only two dimensions. With four electron groups, we must learn to show molecules and ions in three dimensions.

AX₄ Molecules: CH₄

1. The central atom, carbon, contributes four valence electrons, and each hydrogen atom has one valence electron, so the full Lewis electron structure is



Lewis structure

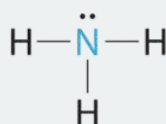
2. There are four electron groups around the central atom. As shown in Figure 1.3.2, repulsions are minimized by placing the groups in the corners of a tetrahedron with bond angles of 109.5° .
3. All electron groups are bonding pairs, so the structure is designated as AX₄.
4. With four bonding pairs, the molecular geometry of methane is *tetrahedral* (Figure 1.3.3).



Molecular geometry
(tetrahedral)

AX₃E Molecules: NH₃

1. In ammonia, the central atom, nitrogen, has five valence electrons and each hydrogen donates one valence electron, producing the Lewis electron structure



Lewis structure

2. There are four electron groups around nitrogen, three bonding pairs and one lone pair. Repulsions are minimized by directing each hydrogen atom and the lone pair to the corners of a tetrahedron.
3. With three bonding pairs and one lone pair, the structure is designated as AX₃E. This designation has a total of four electron pairs, three X and one E. We expect the LP–BP interactions to cause the bonding pair angles to deviate significantly from the

angles of a perfect tetrahedron.

4. There are three nuclei and one lone pair, so the molecular geometry is *trigonal pyramidal*. In essence, this is a tetrahedron with a vertex missing (Figure 1.3.3). However, the H–N–H bond angles are less than the ideal angle of 109.5° because of LP–BP repulsions (Figure 1.3.3 and Figure 1.3.4).

AX₂E₂ Molecules: H₂O

1. Oxygen has six valence electrons and each hydrogen has one valence electron, producing the Lewis electron structure

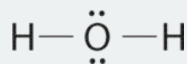


Figure 1.3.2: (CC BY-NC-SA; anonymous)

3. With two bonding pairs and two lone pairs, the structure is designated as AX₂E₂ with a total of four electron pairs. Due to LP–LP, LP–BP, and BP–BP interactions, we expect a significant deviation from idealized tetrahedral angles.

4. With two hydrogen atoms and two lone pairs of electrons, the structure has significant lone pair interactions. There are two nuclei about the central atom, so the molecular shape is *bent*, or *V shaped*, with an H–O–H angle that is even less than the H–N–H angles in NH₃, as we would expect because of the presence of two lone pairs of electrons on the central atom rather than one. This molecular shape is essentially a tetrahedron with two missing vertices.



Five Electron Groups

In previous examples it did not matter where we placed the electron groups because all positions were equivalent. In some cases, however, the positions are not equivalent. We encounter this situation for the first time with five electron groups.

AX₅ Molecules: PCl₅

1. Phosphorus has five valence electrons and each chlorine has seven valence electrons, so the Lewis electron structure of PCl₅ is

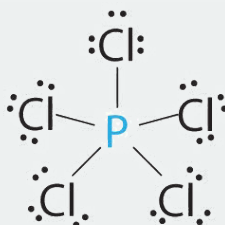
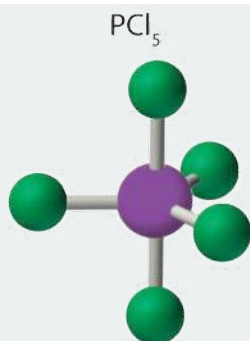


Figure 1.3.2: (CC BY-NC-SA; anonymous)

3. All electron groups are bonding pairs, so the structure is designated as AX₅. There are no lone pair interactions.

4. The molecular geometry of PCl₅ is *trigonal bipyramidal*, as shown in Figure 1.3.3. The molecule has three atoms in a plane in *equatorial* positions and two atoms above and below the plane in *axial* positions. The three equatorial positions are separated by 120° from one another, and the two axial positions are at 90° to the equatorial plane. The axial and equatorial positions are not chemically equivalent, as we will see in our next example.



AX₄E Molecules: SF₄

1. The sulfur atom has six valence electrons and each fluorine has seven valence electrons, so the Lewis electron structure is



Lewis structure

Four fluorenes are bonded to a central sulfur. Each fluorine has three lone pairs. Sulfur has one lone pair.

With an expanded valence, this species is an exception to the octet rule.

2. There are five groups around sulfur, four bonding pairs and one lone pair. With five electron groups, the lowest energy arrangement is a trigonal bipyramid, as shown in Figure 1.3.2.

3. We designate SF₄ as AX₄E; it has a total of five electron pairs. However, because the axial and equatorial positions are not chemically equivalent, where do we place the lone pair? If we place the lone pair in the axial position, we have three LP–BP repulsions at 90°. If we place it in the equatorial position, we have two 90° LP–BP repulsions at 90°. With fewer 90° LP–BP repulsions, we can predict that the structure with the lone pair of electrons in the *equatorial position* is *more stable than the one with the lone pair in the axial position*. We also expect a deviation from ideal geometry because a lone pair of electrons occupies more space than a bonding pair.

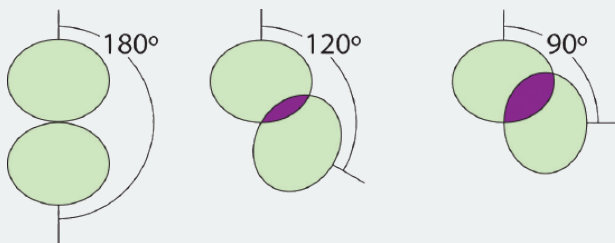
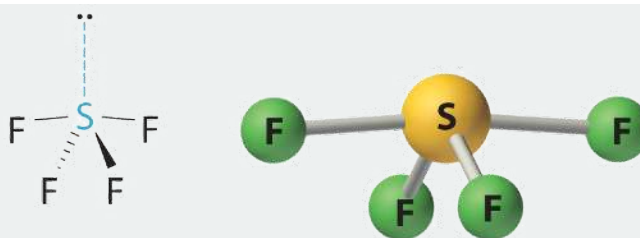


Figure 1.3.5: Illustration of the Area Shared by Two Electron Pairs versus the Angle between Them

180 degree angle has no shared space between two electron pairs. 120 degree angle has some shared area between two electron pairs. 90 degree angle has more shared space than 120.

At 90°, the two electron pairs share a relatively large region of space, which leads to strong repulsive electron–electron interactions.

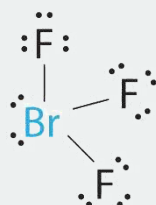
4. With four nuclei and one lone pair of electrons, the molecular structure is based on a trigonal bipyramid with a missing equatorial vertex; it is described as a *seesaw*. The F_{axial}–S–F_{axial} angle is 173° rather than 180° because of the lone pair of electrons in the equatorial plane.



Molecular geometry (seesaw)

AX₃E₂ Molecules: BrF₃

1. The bromine atom has seven valence electrons, and each fluorine has seven valence electrons, so the Lewis electron structure is



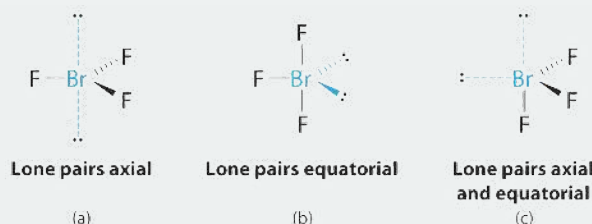
Lewis structure

Three fluorines are bonded to a central bromine. Each fluorine has three lone pairs, Bromine has two lone pairs.

Once again, we have a compound that is an exception to the octet rule.

2. There are five groups around the central atom, three bonding pairs and two lone pairs. We again direct the groups toward the vertices of a trigonal bipyramid.

3. With three bonding pairs and two lone pairs, the structural designation is AX₃E₂ with a total of five electron pairs. Because the axial and equatorial positions are not equivalent, we must decide how to arrange the groups to minimize repulsions. If we place both lone pairs in the axial positions, we have six LP–BP repulsions at 90°. If both are in the equatorial positions, we have four LP–BP repulsions at 90°. If one lone pair is axial and the other equatorial, we have one LP–LP repulsion at 90° and three LP–BP repulsions at 90°:



Interactions

90° LP–LP	0	0	1
90° LP–BP	6	4	3

If the lone pairs are axial, the 90 degree LP–LP interactions are 0 and the 90 degree LP–BP interaction is zero. If the lone pairs are equatorial there are zero 90 degree LP–LP interactions and four 90 degree LP–BP interactions. If the lone pairs are axial and equatorial there is one 90 degree LP–LP interaction and three 90 degree LP–BP interaction.

Structure (c) can be eliminated because it has a LP–LP interaction at 90°. Structure (b), with fewer LP–BP repulsions at 90° than (a), is lower in energy. However, we predict a deviation in bond angles because of the presence of the two lone pairs of electrons.

4. The three nuclei in BrF₃ determine its molecular structure, which is described as *T shaped*. This is essentially a trigonal bipyramid that is missing two equatorial vertices. The F_{axial}–Br–F_{axial} angle is 172°, less than 180° because of LP–BP repulsions (Figure 1.3.2.1).

Because lone pairs occupy more space around the central atom than bonding pairs, electrostatic repulsions are more important for lone pairs than for bonding pairs.

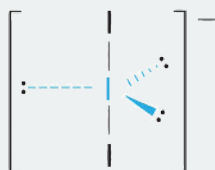
AX₂E₃ Molecules: I₃⁻

1. Each iodine atom contributes seven electrons and the negative charge one, so the Lewis electron structure is



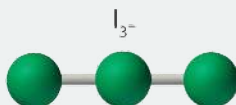
2. There are five electron groups about the central atom in I₃⁻, two bonding pairs and three lone pairs. To minimize repulsions, the groups are directed to the corners of a trigonal bipyramid.

3. With two bonding pairs and three lone pairs, I₃⁻ has a total of five electron pairs and is designated as AX₂E₃. We must now decide how to arrange the lone pairs of electrons in a trigonal bipyramid in a way that minimizes repulsions. Placing them in the axial positions eliminates 90° LP-LP repulsions and minimizes the number of 90° LP-BP repulsions.



The three lone pairs of electrons have equivalent interactions with the three iodine atoms, so we do not expect any deviations in bonding angles.

4. With three nuclei and three lone pairs of electrons, the molecular geometry of I₃⁻ is linear. This can be described as a trigonal bipyramid with three equatorial vertices missing. The ion has an I-I-I angle of 180°, as expected.



Six Electron Groups

Six electron groups form an *octahedron*, a polyhedron made of identical equilateral triangles and six identical vertices (Figure 1.3.2)

AX₆ Molecules: SF₆

1. The central atom, sulfur, contributes six valence electrons, and each fluorine atom has seven valence electrons, so the Lewis electron structure is



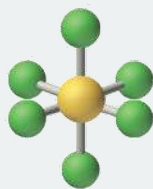
Lewis structure

With an expanded valence, this species is an exception to the octet rule.

2. There are six electron groups around the central atom, each a bonding pair. We see from Figure 1.3.2 that the geometry that minimizes repulsions is *octahedral*.

3. With only bonding pairs, SF₆ is designated as AX₆. All positions are chemically equivalent, so all electronic interactions are equivalent.

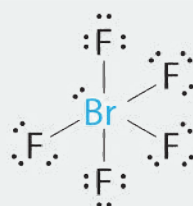
4. There are six nuclei, so the molecular geometry of SF_6 is octahedral.



Molecular geometry
(octahedral)

AX₅E Molecules: BrF_5

1. The central atom, bromine, has seven valence electrons, as does each fluorine, so the Lewis electron structure is

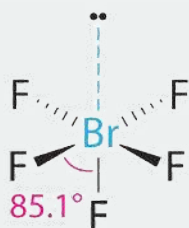


Lewis structure

Five fluorines are bonded to a central bromine. Each fluorine has three lone pairs, Bromine has one lone pair.

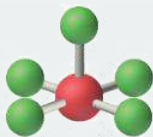
With its expanded valence, this species is an exception to the octet rule.

2. There are six electron groups around the Br, five bonding pairs and one lone pair. Placing five F atoms around Br while minimizing BP–BP and LP–BP repulsions gives the following structure:



3. With five bonding pairs and one lone pair, BrF_5 is designated as AX₅E; it has a total of six electron pairs. The BrF_5 structure has four fluorine atoms in a plane in an equatorial position and one fluorine atom and the lone pair of electrons in the axial positions. We expect all $F_{\text{axial}}\text{--Br--}F_{\text{equatorial}}$ angles to be less than 90° because of the lone pair of electrons, which occupies more space than the bonding electron pairs.

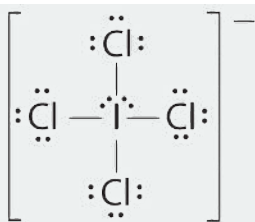
4. With five nuclei surrounding the central atom, the molecular structure is based on an octahedron with a vertex missing. This molecular structure is *square pyramidal*. The $F_{\text{axial}}\text{--Br--}F_{\text{equatorial}}$ angles are 85.1° , less than 90° because of LP–BP repulsions.



Molecular geometry
(square pyramidal)

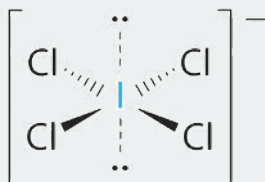
AX₄E₂ Molecules: ICl_4^-

1. The central atom, iodine, contributes seven electrons. Each chlorine contributes seven, and there is a single negative charge. The Lewis electron structure is



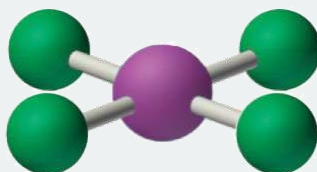
Four chlorines are bonded to a central iodine. Each chlorine has three electron pairs. The iodine has two electron pairs. The molecule is negatively charged.

2. There are six electron groups around the central atom, four bonding pairs and two lone pairs. The structure that minimizes LP-LP, LP-BP, and BP-BP repulsions is



3. ICl_4^- is designated as AX_4E_2 and has a total of six electron pairs. Although there are lone pairs of electrons, with four bonding electron pairs in the equatorial plane and the lone pairs of electrons in the axial positions, all LP-BP repulsions are the same. Therefore, we do not expect any deviation in the Cl-I-Cl bond angles.

4. With five nuclei, the ICl_4^- ion forms a molecular structure that is *square planar*, an octahedron with two opposite vertices missing.



The relationship between the number of electron groups around a central atom, the number of lone pairs of electrons, and the molecular geometry is summarized in Figure 1.3.6.

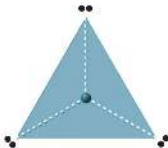
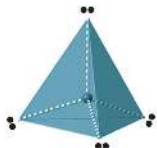
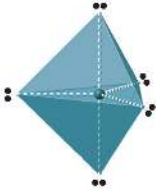
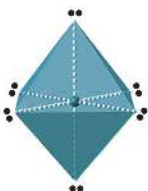
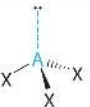
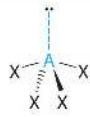
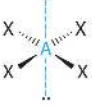
Electron Groups	2	3	4	5	6
Molecular Geometry	 Linear	 Trigonal planar	 Tetrahedral	 Trigonal bipyramidal	 Octahedral
Zero Lone Pairs	 Linear AX_2	 Trigonal planar AX_3	 Tetrahedral AX_4	 Trigonal bipyramidal AX_5	 Octahedral AX_6
One Lone Pair		 Bent (V-shaped) AX_2E	 Trigonal pyramidal AX_3E	 Seesaw AX_5E One axial lone pair	 Square pyramidal AX_6E
Two Lone Pairs			 Bent (V-shaped) AX_2E_2	 T-shaped AX_5E_2 Two axial lone pairs	 Square planar AX_4E_2
Three Lone Pairs				 Linear AX_3E_3 Three axial lone pairs	

Figure 1.3.6: Overview of Molecular Geometries



✓ Example 1.3.1

Using the VSEPR model, predict the molecular geometry of each molecule or ion.

1. PF_5 (phosphorus pentafluoride, a catalyst used in certain organic reactions)
2. H_3O^+ (hydronium ion)

Given: two chemical species

Asked for: molecular geometry

Strategy:

- Draw the Lewis electron structure of the molecule or polyatomic ion.
- Determine the electron group arrangement around the central atom that minimizes repulsions.
- Assign an AX_mE_n designation; then identify the LP–LP, LP–BP, or BP–BP interactions and predict deviations in bond angles.
- Describe the molecular geometry.

Solution:

- A** The central atom, P, has five valence electrons and each fluorine has seven valence electrons, so the Lewis structure of PF_5 is

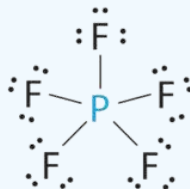
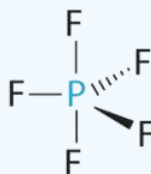


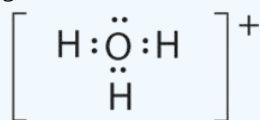
Figure 1.3.6): (CC BY-NC-SA; anonymous)

C All electron groups are bonding pairs, so PF_5 is designated as AX_5 . Notice that this gives a total of five electron pairs. With no lone pair repulsions, we do not expect any bond angles to deviate from the ideal.

D The PF_5 molecule has five nuclei and no lone pairs of electrons, so its molecular geometry is trigonal bipyramidal.



- A** The central atom, O, has six valence electrons, and each H atom contributes one valence electron. Subtracting one electron for the positive charge gives a total of eight valence electrons, so the Lewis electron structure is

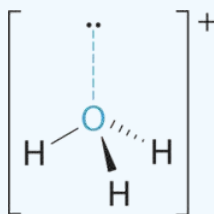


Three hydrogens are bonded to a central oxygen. The oxygen has two lone pairs. The molecule has a charge of plus one.

B There are four electron groups around oxygen, three bonding pairs and one lone pair. Like NH_3 , repulsions are minimized by directing each hydrogen atom and the lone pair to the corners of a tetrahedron.

C With three bonding pairs and one lone pair, the structure is designated as AX_3E and has a total of four electron pairs (three X and one E). We expect the LP–BP interactions to cause the bonding pair angles to deviate significantly from the angles of a perfect tetrahedron.

D There are three nuclei and one lone pair, so the molecular geometry is *trigonal pyramidal*, in essence a tetrahedron missing a vertex. However, the H–O–H bond angles are less than the ideal angle of 109.5° because of LP–BP repulsions:



? Exercise 1.3.1

Using the VSEPR model, predict the molecular geometry of each molecule or ion.

- XeO_3
- PF_6^-
- NO_2^+

Answer a

trigonal pyramidal

Answer b

octahedral

Answer c

linear

✓ Example 1.3.2

Predict the molecular geometry of each molecule.

- XeF_2
- SnCl_2

Given: two chemical compounds

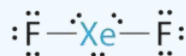
Asked for: molecular geometry

Strategy:

Use the strategy given in Example 1.3.1.

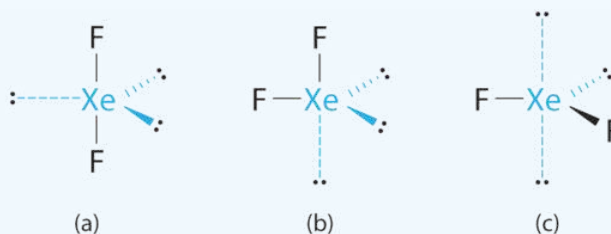
Solution:

- A** Xenon contributes eight electrons and each fluorine seven valence electrons, so the Lewis electron structure is



B There are five electron groups around the central atom, two bonding pairs and three lone pairs. Repulsions are minimized by placing the groups in the corners of a trigonal bipyramid.

C From B, XeF_2 is designated as AX_2E_3 and has a total of five electron pairs (two X and three E). With three lone pairs about the central atom, we can arrange the two F atoms in three possible ways: both F atoms can be axial, one can be axial and one equatorial, or both can be equatorial:



Interactions

90 LP-LP

0

2

2

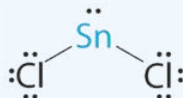
If the two F atoms are axial there are zero 90 LP-LP interactions. If the two F atoms are axial and equatorial or just equatorial, there are 2 90 LP-LP interactions.

The structure with the lowest energy is the one that minimizes LP-LP repulsions. Both (b) and (c) have two 90° LP-LP interactions, whereas structure (a) has none. Thus both F atoms are in the axial positions, like the two iodine atoms around

the central iodine in I_3^- . All LP–BP interactions are equivalent, so we do not expect a deviation from an ideal 180° in the F–Xe–F bond angle.

D With two nuclei about the central atom, the molecular geometry of XeF_2 is linear. It is a trigonal bipyramid with three missing equatorial vertices.

2. **A** The tin atom donates 4 valence electrons and each chlorine atom donates 7 valence electrons. With 18 valence electrons, the Lewis electron structure is



Two chlorines are bonded to a central tin. Each chlorine has three lone pairs. Tin has one lone pair.

B There are three electron groups around the central atom, two bonding groups and one lone pair of electrons. To minimize repulsions the three groups are initially placed at 120° angles from each other.

C From **B** we designate SnCl_2 as AX_2E . It has a total of three electron pairs, two X and one E. Because the lone pair of electrons occupies more space than the bonding pairs, we expect a decrease in the Cl–Sn–Cl bond angle due to increased LP–BP repulsions.

D With two nuclei around the central atom and one lone pair of electrons, the molecular geometry of SnCl_2 is bent, like SO_2 , but with a Cl–Sn–Cl bond angle of 95° . The molecular geometry can be described as a trigonal planar arrangement with one vertex missing.

? Exercise 1.3.2

Predict the molecular geometry of each molecule.

- SO_3
- XeF_4

Answer a

trigonal planar

Answer b

square planar

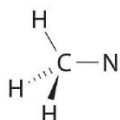


Molecules with No Single Central Atom

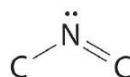
The VSEPR model can be used to predict the structure of somewhat more complex molecules with no single central atom by treating them as linked AX_mE_n fragments. We will demonstrate with methyl isocyanate ($\text{CH}_3\text{–N=C=O}$), a volatile and highly toxic molecule that is used to produce the pesticide Sevin. In 1984, large quantities of Sevin were accidentally released in Bhopal, India,

when water leaked into storage tanks. The resulting highly exothermic reaction caused a rapid increase in pressure that ruptured the tanks, releasing large amounts of methyl isocyanate that killed approximately 3800 people and wholly or partially disabled about 50,000 others. In addition, there was significant damage to livestock and crops.

We can treat methyl isocyanate as linked AX_mE_n fragments beginning with the carbon atom at the left, which is connected to three H atoms and one N atom by single bonds. The four bonds around carbon mean that it must be surrounded by four bonding electron pairs in a configuration similar to AX_4 . We can therefore predict the CH_3-N portion of the molecule to be roughly tetrahedral, similar to methane:



The nitrogen atom is connected to one carbon by a single bond and to the other carbon by a double bond, producing a total of three bonds, $C-N=C$. For nitrogen to have an octet of electrons, it must also have a lone pair:



One carbon bonded to nitrogen and another carbon double bonded to the nitrogen. The nitrogen has one lone pair.

Because multiple bonds are not shown in the VSEPR model, the nitrogen is effectively surrounded by three electron pairs. Thus according to the VSEPR model, the $C-N=C$ fragment should be bent with an angle less than 120° .

The carbon in the $-N=C=O$ fragment is doubly bonded to both nitrogen and oxygen, which in the VSEPR model gives carbon a total of two electron pairs. The $N=C=O$ angle should therefore be 180° , or linear. The three fragments combine to give the following structure:

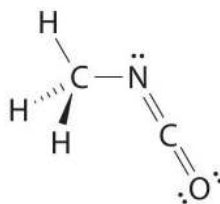


Figure 1.3.7).

Three hydrogens are bonded to a carbon. The carbon is also bonded to a nitrogen. The nitrogen is double bonded to another carbon. The second carbon is double bonded to an oxygen. The nitrogen has one lone pair. The oxygen has two lone pairs.

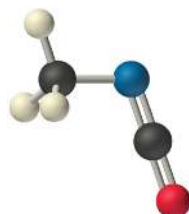


Figure 1.3.7: The Experimentally Determined Structure of Methyl Isocyanate

Certain patterns are seen in the structures of moderately complex molecules. For example, carbon atoms with four bonds (such as the carbon on the left in methyl isocyanate) are generally tetrahedral. Similarly, the carbon atom on the right has two double bonds that are similar to those in CO_2 , so its geometry, like that of CO_2 , is linear. Recognizing similarities to simpler molecules will help you predict the molecular geometries of more complex molecules.

✓ Example 1.3.3

Use the VSEPR model to predict the molecular geometry of propyne ($H_3C-C\equiv CH$), a gas with some anesthetic properties.

Given: chemical compound

Asked for: molecular geometry

Strategy:

Count the number of electron groups around each carbon, recognizing that in the VSEPR model, a multiple bond counts as a single group. Use Figure 1.3.3 to determine the molecular geometry around each carbon atom and then deduce the structure of the molecule as a whole.

Solution:

Because the carbon atom on the left is bonded to four other atoms, we know that it is approximately tetrahedral. The next two carbon atoms share a triple bond, and each has an additional single bond. Because a multiple bond is counted as a single bond in the VSEPR model, each carbon atom behaves as if it had two electron groups. This means that both of these carbons are linear, with $\text{C}-\text{C}\equiv\text{C}$ and $\text{C}\equiv\text{C}-\text{H}$ angles of 180° .

? Exercise 1.3.3

Predict the geometry of allene ($\text{H}_2\text{C}=\text{C}=\text{CH}_2$), a compound with narcotic properties that is used to make more complex organic molecules.

Answer

The terminal carbon atoms are trigonal planar, the central carbon is linear, and the $\text{C}-\text{C}-\text{C}$ angle is 180° .

Molecular Dipole Moments

You previously learned how to calculate the **dipole moments** of simple diatomic molecules. In more complex molecules with polar covalent bonds, the three-dimensional geometry and the compound's symmetry determine whether there is a net dipole moment. Mathematically, dipole moments are *vectors*; they possess both a *magnitude* and a *direction*. The dipole moment of a molecule is therefore the *vector sum* of the dipole moments of the individual bonds in the molecule. If the individual bond dipole moments cancel one another, there is no net dipole moment. Such is the case for CO_2 , a linear molecule (Figure 1.3.8a). Each $\text{C}-\text{O}$ bond in CO_2 is polar, yet experiments show that the CO_2 molecule has no dipole moment. Because the two $\text{C}-\text{O}$ bond dipoles in CO_2 are equal in magnitude and oriented at 180° to each other, they cancel. As a result, the CO_2 molecule has no *net* dipole moment even though it has a substantial separation of charge. In contrast, the H_2O molecule is not linear (Figure 1.3.8b); it is bent in three-dimensional space, so the dipole moments do not cancel each other. Thus a molecule such as H_2O has a net dipole moment. We expect the concentration of negative charge to be on the oxygen, the more electronegative atom, and positive charge on the two hydrogens. This charge polarization allows H_2O to hydrogen-bond to other polarized or charged species, including other water molecules.

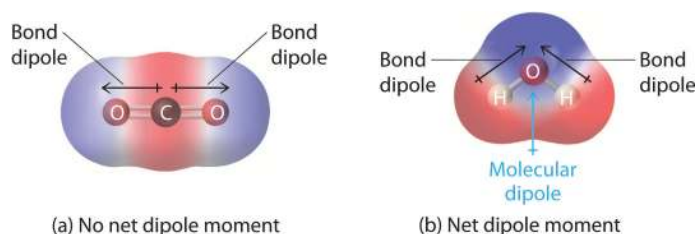


Figure 1.3.8: How Individual Bond Dipole Moments Are Added Together to Give an Overall Molecular Dipole Moment for Two Triatomic Molecules with Different Structures. (a) In CO_2 , the $\text{C}-\text{O}$ bond dipoles are equal in magnitude but oriented in opposite directions (at 180°). Their vector sum is zero, so CO_2 therefore has no net dipole. (b) In H_2O , the $\text{O}-\text{H}$ bond dipoles are also equal in magnitude, but they are oriented at 104.5° to each other. Hence the vector sum is not zero, and H_2O has a net dipole moment.

Other examples of molecules with polar bonds are shown in Figure 1.3.9. In molecular geometries that are highly symmetrical (most notably tetrahedral and square planar, trigonal bipyramidal, and octahedral), individual bond dipole moments completely cancel, and there is no net dipole moment. Although a molecule like CHCl_3 is best described as tetrahedral, the atoms bonded to carbon are not identical. Consequently, the bond dipole moments cannot cancel one another, and the molecule has a dipole moment. Due to the arrangement of the bonds in molecules that have V-shaped, trigonal pyramidal, seesaw, T-shaped, and square pyramidal geometries, the bond dipole moments cannot cancel one another. Consequently, molecules with these geometries always have a nonzero dipole moment. Molecules with asymmetrical charge distributions have a net dipole moment.

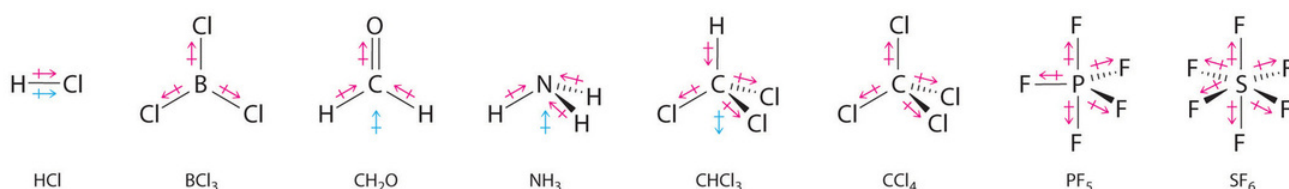


Figure 1.3.9: Molecules with Polar Bonds. Individual bond dipole moments are indicated in red. Due to their different three-dimensional structures, some molecules with polar bonds have a net dipole moment (HCl, CH₂O, NH₃, and CHCl₃), indicated in blue, whereas others do not because the bond dipole moments cancel (BCl₃, CCl₄, PF₅, and SF₆).



✓ Example 1.3.4

Which molecule(s) has a net dipole moment?

- H₂S
- NHF₂
- BF₃

Given: three chemical compounds

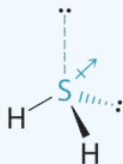
Asked for: net dipole moment

Strategy:

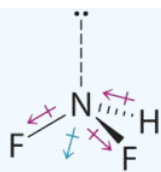
For each three-dimensional molecular geometry, predict whether the bond dipoles cancel. If they do not, then the molecule has a net dipole moment.

Solution:

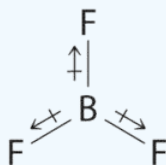
- The total number of electrons around the central atom, S, is eight, which gives four electron pairs. Two of these electron pairs are bonding pairs and two are lone pairs, so the molecular geometry of H₂S is bent (Figure 1.3.6). The bond dipoles cannot cancel one another, so the molecule has a net dipole moment.



- Diffuoroamine has a trigonal pyramidal molecular geometry. Because there is one hydrogen and two fluorines, and because of the lone pair of electrons on nitrogen, the molecule is not symmetrical, and the bond dipoles of NHF₂ cannot cancel one another. This means that NHF₂ has a net dipole moment. We expect polarization from the two fluorine atoms, the most electronegative atoms in the periodic table, to have a greater affect on the net dipole moment than polarization from the lone pair of electrons on nitrogen.



3. The molecular geometry of BF_3 is trigonal planar. Because all the B–F bonds are equal and the molecule is highly symmetrical, the dipoles cancel one another in three-dimensional space. Thus BF_3 has a net dipole moment of zero:



? Exercise 1.3.4

Which molecule(s) has a net dipole moment?

- CH_3Cl
- SO_3
- XeO_3

Answer

CH_3Cl and XeO_3

Summary

Lewis electron structures give no information about **molecular geometry**, the arrangement of bonded atoms in a molecule or polyatomic ion, which is crucial to understanding the chemistry of a molecule. The **valence-shell electron-pair repulsion (VSEPR) model** allows us to predict which of the possible structures is actually observed in most cases. It is based on the assumption that pairs of electrons occupy space, and the lowest-energy structure is the one that minimizes electron pair–electron pair repulsions. In the VSEPR model, the molecule or polyatomic ion is given an AX_mE_n designation, where A is the central atom, X is a bonded atom, E is a nonbonding valence electron group (usually a lone pair of electrons), and m and n are integers. Each group around the central atom is designated as a bonding pair (BP) or lone (nonbonding) pair (LP). From the BP and LP interactions we can predict both the relative positions of the atoms and the angles between the bonds, called the **bond angles**. From this we can describe the **molecular geometry**. The VSEPR model can be used to predict the shapes of many molecules and polyatomic ions, but it gives no information about bond lengths and the presence of multiple bonds. A combination of VSEPR and a bonding model, such as Lewis electron structures, is necessary to understand the presence of multiple bonds.

Molecules with polar covalent bonds can have a *dipole moment*, an asymmetrical distribution of charge that results in a tendency for molecules to align themselves in an applied electric field. Any diatomic molecule with a polar covalent bond has a dipole moment, but in polyatomic molecules, the presence or absence of a net dipole moment depends on the structure. For some highly symmetrical structures, the individual bond dipole moments cancel one another, giving a dipole moment of zero.

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CHAPTER OVERVIEW

2: Atomic Structure

- [2.1: The Bohr Model - Atoms with Orbits](#)
- [2.2: The Wave-Particle Duality of Matter and Energy](#)
- [2.3: Quantum Numbers for Electrons](#)
- [2.4: Atomic Orbitals](#)

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2.1: The Bohr Model - Atoms with Orbits

Learning Objectives

- Define an energy level in terms of the Bohr model.
- Discuss how the Bohr model can be used to explain atomic spectra.

Electric light bulbs contain a very thin wire in them that emits light when heated. The wire is called a filament. The particular wire used in light bulbs is made of tungsten. A wire made of any metal would emit light under these circumstances, but tungsten was chosen because the light it emits contains virtually every frequency and therefore, the light emitted by tungsten appears white. A wire made of some other element would emit light of some color that was not convenient for our uses. Every element emits light when energized by heating or passing electric current through it. Elements in solid form begin to glow when they are heated sufficiently, and elements in gaseous form emit light when electricity passes through them. This is the source of light emitted by neon signs and is also the source of light in a fire.



Figure 2.1.1: Human/Need/Desire. Neon sculpture by Bruce Nauman (1983), who has been characterized as a conceptual artist.

Each Element Has a Unique Spectrum

The light frequencies emitted by atoms are mixed together by our eyes so that we see a blended color. Several physicists, including Angstrom in 1868 and Balmer in 1875, passed the light from energized atoms through glass prisms in such a way that the light was spread out so they could see the individual frequencies that made up the light. The **emission spectrum** (or **atomic spectrum**) of a chemical element is the unique pattern of light obtained when the element is subjected to heat or electricity.



Figure 2.1.2: Atomic Emission Spectrum of Hydrogen.

When hydrogen gas is placed into a tube and electric current passed through it, the color of emitted light is pink. But when the color is spread out, we see that the hydrogen spectrum is composed of four individual frequencies. The pink color of the tube is the result of our eyes blending the four colors. Every atom has its own characteristic spectrum; no two atomic spectra are alike. The image below shows the emission spectrum of iron. Because each element has a unique emission spectrum, elements can be defined using them.

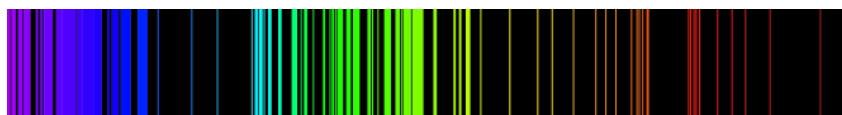


Figure 2.1.3: Atomic Emission Spectrum of Iron.

You may have heard or read about scientists discussing what elements are present in the sun or some more distant star, and after hearing that, wondered how scientists could know what elements were present in a place no one has ever been. Scientists determine what elements are present in distant stars by analyzing the light that comes from stars and finding the atomic spectrum of elements in that light. If the exact four lines that compose hydrogen's atomic spectrum are present in the light emitted from the star, that element contains hydrogen.

Bohr's Model of the Atom

By 1913, the concept of the atom had evolved from Dalton's indivisible spheres idea, to J. J. Thomson's plum pudding model, and then to Rutherford's nuclear atom theory. Rutherford, in addition to carrying out the brilliant experiment that demonstrated the presence of the atomic nucleus, also proposed that the electrons circled the nucleus in a planetary type motion. The solar system or planetary model of the atom was attractive to scientists because it was similar to something with which they were already familiar, namely the solar system.



Figure 2.1.3: Niels Bohr with Albert Einstein at Paul Ehrenfest's home in Leiden (December 1925).

Unfortunately, there was a serious flaw in the planetary model. It was already known that when a charged particle (such as an electron) moves in a curved path, it gives off some form of light and loses energy in doing so. This is, after all, how we produce TV signals. If the electron circling the nucleus in an atom loses energy, it would necessarily have to move closer to the nucleus as it loses energy, and would eventually crash into the nucleus. Furthermore, Rutherford's model was unable to describe how electrons give off light forming each element's unique atomic spectrum. These difficulties cast a shadow on the planetary model and indicated that, eventually, it would have to be replaced.

In 1913, the Danish physicist Niels Bohr proposed a model of the electron cloud of an atom in which electrons orbit the nucleus and were able to produce atomic spectra. Understanding Bohr's model requires some knowledge of electromagnetic radiation (or light).

Energy Levels

Bohr's key idea in his model of the atom is that electrons occupy definite orbitals that require the electron to have a specific amount of energy. In order for an electron to be in the electron cloud of an atom, it must be in one of the allowable orbitals and it must have the precise energy required for that orbit. Orbits closer to the nucleus would require smaller amounts of energy for an electron, and orbits farther from the nucleus would require the electron to have a greater amount of energy. The possible orbits are known as **energy levels**. One of the weaknesses of Bohr's model was that he could not offer a reason why only certain energy levels or orbits were allowed.

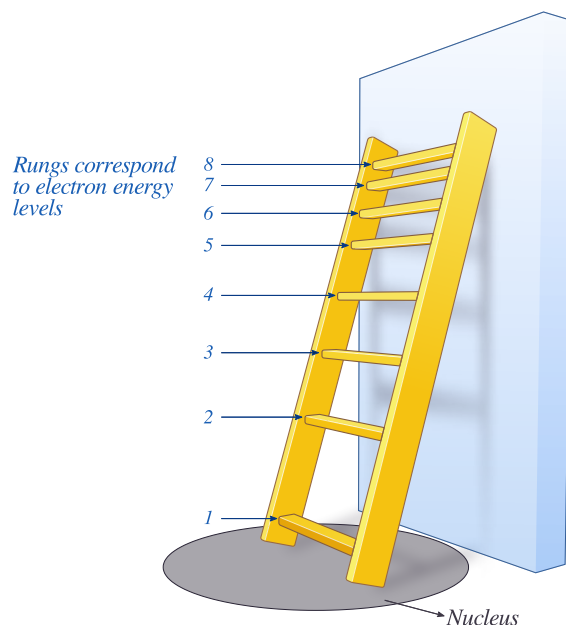


Figure 2.1.4: The energy levels of the electrons can be viewed as rungs on a ladder. Note that the spacing between rungs gets smaller at higher energies (CC BY-NC; Ümit Kaya)

Bohr hypothesized that the only way electrons could gain or lose energy would be to move from one energy level to another, thus gaining or losing precise amounts of energy. The energy levels are **quantized**, meaning that only specific amounts are possible. It would be like a ladder that had rungs only at certain heights. The only way you can be on that ladder is to be on one of the rungs, and the only way you could move up or down would be to move to one of the other rungs. Suppose we had such a ladder with 10 rungs. Other rules for the ladder are that only one person can be on a rung in the normal state, and the ladder occupants must be on the lowest rung available. If the ladder had five people on it, they would be on the lowest five rungs. In this situation, no person could move down because all of the lower rungs are full. Bohr worked out rules for the maximum number of electrons that could be in each energy level in his model, and required that an atom in its normal state (ground state) had all electrons in the lowest energy levels available. Under these circumstances, no electron could lose energy because no electron could move down to a lower energy level. In this way, Bohr's model explained why electrons circling the nucleus did not emit energy and spiral into the nucleus.

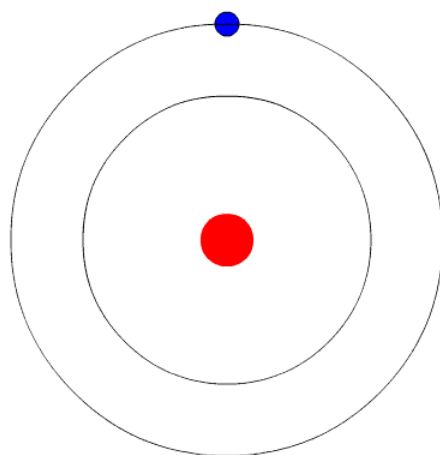


Figure 2.1.5: In Bohr's Model of the atom, electrons absorb energy to move to a higher level and release energy to move to lower levels. (CC BY-SA 3.0; Kurzon).

Bohr's Model and Atomic Spectra

The evidence used to support Bohr's model came from the atomic spectra. He suggested that an atomic spectrum is made by the electrons in an atom moving energy levels. The electrons typically have the lowest energy possible, called the **ground state**. If the electrons are given energy (through heat, electricity, light, etc.) the electrons in an atom could absorb energy by jumping to a higher energy level, or **excited state**. The electrons then give off the energy in the form of a piece of light—called a **photon**—that they had absorbed, to fall back to a lower energy level. The energy emitted by electrons dropping back to lower energy levels will always be precise amounts of energy, because the differences in energy levels are precise. This explains why you see specific lines of light when looking at an atomic spectrum—each line of light matches a specific "step down" that an electron can take in that atom. This also explains why each element produces a different atomic spectrum. Because each element has different acceptable energy levels for its electrons, the possible steps each element's electrons can take differ from all other elements.

Summary

- Bohr's model suggests each atom has a set of unchangeable energy levels, and electrons in the electron cloud of that atom must be in one of those energy levels.
- Bohr's model suggests that the atomic spectra of atoms is produced by electrons gaining energy from some source, jumping up to a higher energy level, then immediately dropping back to a lower energy level and emitting the energy difference between the two energy levels.
- The existence of the atomic spectra is support for Bohr's model of the atom.
- Bohr's model was only successful in calculating energy levels for the hydrogen atom.

Vocabulary

- **Emission spectrum (or atomic spectrum)** - The unique pattern of light given off by an element when it is given energy.
- **Energy levels** - Possible orbits that an electron can have in the electron cloud of an atom.
- **Ground state** - To be in the lowest energy level possible.
- **Excited state** - To be in a higher energy level.
- **Photon** - A piece of electromagnetic radiation, or light, with a specific amount of energy.
- **Quantized** - To have a specific amount.

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2.2: The Wave-Particle Duality of Matter and Energy

Learning Objectives

- To understand the wave–particle duality of matter.

Einstein's photons of light were individual packets of energy having many of the characteristics of particles. Recall that the collision of an electron (a particle) with a sufficiently energetic photon can eject a *photoelectron* from the surface of a metal. Any excess energy is transferred to the electron and is converted to the kinetic energy of the ejected electron. Einstein's hypothesis that energy is concentrated in localized bundles, however, was in sharp contrast to the classical notion that energy is spread out uniformly in a wave. We now describe Einstein's theory of the relationship between energy and mass, a theory that others built on to develop our current model of the atom.

The Wave Character of Matter

Einstein initially assumed that photons had zero mass, which made them a peculiar sort of particle indeed. In 1905, however, he published his special theory of relativity, which related energy and mass according to the famous equation:

$$E = hu = h \frac{c}{\lambda} = mc^2 \quad (2.2.1)$$

According to this theory, a photon of wavelength λ and frequency u has a nonzero mass, which is given as follows:

$$m = \frac{E}{c^2} = \frac{hu}{c^2} = \frac{h}{\lambda c} \quad (2.2.2)$$

That is, light, which had always been regarded as a wave, also has properties typical of particles, a condition known as wave–particle duality (a principle that matter and energy have properties typical of both waves and particles). Depending on conditions, light could be viewed as either a wave or a particle.

In 1922, the American physicist Arthur Compton (1892–1962) reported the results of experiments involving the collision of x-rays and electrons that supported the particle nature of light. At about the same time, a young French physics student, Louis de Broglie (1892–1972), began to wonder whether the converse was true: Could particles exhibit the properties of waves? In his PhD dissertation submitted to the Sorbonne in 1924, de Broglie proposed that a particle such as an electron could be described by a wave whose wavelength is given by

$$\lambda = \frac{h}{mv} \quad (2.2.3)$$

where

- h is Planck's constant,
- m is the mass of the particle, and
- v is the velocity of the particle.

This revolutionary idea was quickly confirmed by American physicists Clinton Davisson (1881–1958) and Lester Germer (1896–1971), who showed that beams of electrons, regarded as particles, were diffracted by a sodium chloride crystal in the same manner as x-rays, which were regarded as waves. It was proven experimentally that electrons do exhibit the properties of waves. For his work, de Broglie received the Nobel Prize in Physics in 1929.

If particles exhibit the properties of waves, why had no one observed them before? The answer lies in the numerator of de Broglie's equation, which is an extremely small number. As you will calculate in Example 2.2.1, Planck's constant (6.63×10^{-34} J•s) is so small that the wavelength of a particle with a large mass is too short (less than the diameter of an atomic nucleus) to be noticeable.



The de Broglie Equation: [The de Broglie Equation, YouTube\(opens in new window\)](#) [youtu.be]

✓ Example 2.2.1: Wavelength of a Baseball in Motion

Calculate the wavelength of a baseball, which has a mass of 149 g and a speed of 100 mi/h.

Given: mass and speed of object

Asked for: wavelength

Strategy:

- Convert the speed of the baseball to the appropriate SI units: meters per second.
- Substitute values into Equation 2.2.3 and solve for the wavelength.

Solution:

The wavelength of a particle is given by $\lambda = h/mv$. We know that $m = 0.149$ kg, so all we need to find is the speed of the baseball:

$$v = \left(\frac{100 \cancel{\text{mi}}}{\cancel{\text{h}}} \right) \left(\frac{1 \cancel{\text{h}}}{60 \cancel{\text{min}}} \right) \left(\frac{1.609 \cancel{\text{km}}}{\cancel{\text{mi}}} \right) \left(\frac{1000 \cancel{\text{m}}}{\cancel{\text{km}}} \right)$$

B Recall that the joule is a derived unit, whose units are $(\text{kg} \cdot \text{m}^2)/\text{s}^2$. Thus the wavelength of the baseball is

$$\lambda = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{(0.149 \text{ kg})(44.69 \text{ m} \cdot \text{s})} = \frac{6.626 \times 10^{-34} \cancel{\text{kg}} \cdot \cancel{\text{m}}^2 \cdot \cancel{\text{s}}^{-2} \cdot \cancel{\text{s}}}{(0.149 \cancel{\text{kg}})(44.69 \cancel{\text{m}} \cdot \cancel{\text{s}}^{-1})} = 9.95 \times 10^{-35} \text{ m}$$

(You should verify that the units cancel to give the wavelength in meters.) Given that the diameter of the nucleus of an atom is approximately 10^{-14} m, the wavelength of the baseball is almost unimaginably small.

? Exercise 2.2.1: Wavelength of a Neutron in Motion

Calculate the wavelength of a neutron that is moving at 3.00×10^3 m/s.

Answer

1.32 Å, or 132 pm

As you calculated in Example 2.2.1, objects such as a baseball or a neutron have such short wavelengths that they are best regarded primarily as particles. In contrast, objects with very small masses (such as photons) have large wavelengths and can be viewed primarily as waves. Objects with intermediate masses, however, such as electrons, exhibit the properties of both particles *and* waves. Although we still usually think of electrons as particles, the wave nature of electrons is employed in an *electron microscope*, which has revealed most of what we know about the microscopic structure of living organisms and materials. Because the

wavelength of an electron beam is much shorter than the wavelength of a beam of visible light, this instrument can resolve smaller details than a light microscope can (Figure 2.2.1).

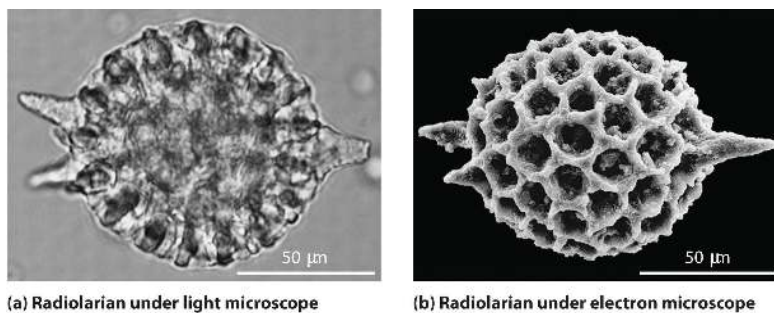


Figure 2.2.1: A Comparison of Images Obtained Using a Light Microscope and an Electron Microscope. Because of their shorter wavelength, high-energy electrons have a higher resolving power than visible light. Consequently, an electron microscope (b) is able to resolve finer details than a light microscope (a). (Radiolaria, which are shown here, are unicellular planktonic organisms.)

An Important Wave Property: Phase And Interference

A wave is a disturbance that travels in space. The magnitude of the wave at any point in space and time varies sinusoidally. While the absolute value of the magnitude of one wave at any point is not very important, the *relative* displacement of two waves, called the phase difference, is vitally important because it determines whether the waves reinforce or interfere with each other. Figure 2.2.2A shows an arbitrary phase difference between two wave and Figure 2.2.2B shows what happens when the two waves are 180 degrees out of phase. The green line is their sum. Figure 2.2.2C shows what happens when the two lines are in phase, exactly superimposed on each other. Again, the green line is the sum of the intensities. A pattern of constructive and destructive interference is obtained when two (or more) diffracting waves interact with each other. This principle of diffraction and interference was used to prove the wave properties of electrons and is the basis for how electron microscopes work.

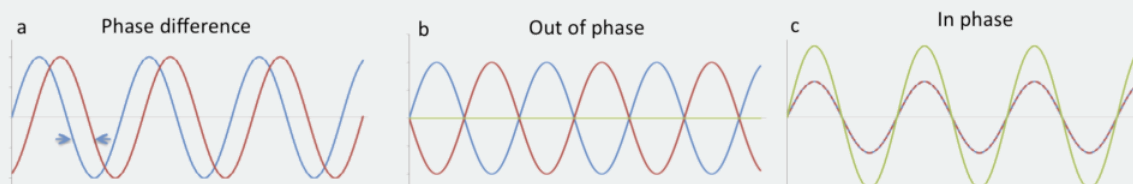
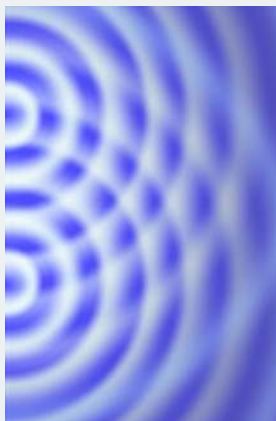


Figure 2.2.2: Phase. Two waves traveling together are displaced by a phase difference. If the phase difference is 0° then they lay on top of each other and reinforce. If the phase difference is 180° they completely cancel each other out.

A shows two waves with a phase difference where the peaks are slightly misaligned. B shows two waves out of phase, the two waves are opposite of each other. C shows two waves in phase, the two waves peak at the same time.



The waves are the white circles that start from the left side. The waves intersect at multiple points.

Photograph of an interference pattern produced by circular water waves in a ripple tank.

For a mathematical analysis of phase aspects in sinusoids, check the math Libretexts library.

Standing Waves

De Broglie also investigated why only certain orbits were allowed in Bohr's model of the hydrogen atom. He hypothesized that the electron behaves like a **standing wave** (a wave that does not travel in space). An example of a standing wave is the motion of a string of a violin or guitar. When the string is plucked, it vibrates at certain fixed frequencies because it is fastened at both ends (Figure 2.2.3). If the length of the string is L , then the lowest-energy vibration (the fundamental) has wavelength

$$\begin{aligned}\frac{\lambda}{2} &= L \\ \lambda &= 2L\end{aligned}\tag{2.2.4}$$

Higher-energy vibrations are called *overtone*s (the vibration of a standing wave that is higher in energy than the fundamental vibration) and are produced when the string is plucked more strongly; they have wavelengths given by

$$\lambda = \frac{2L}{n}\tag{2.2.5}$$

where n has any integral value. When plucked, all other frequencies die out immediately. Only the resonant frequencies survive and are heard. Thus, we can think of the resonant frequencies of the string as being quantized. Notice in Figure 2.2.3 that all overtones have one or more nodes, points where the string does not move. The amplitude of the wave at a node is zero.

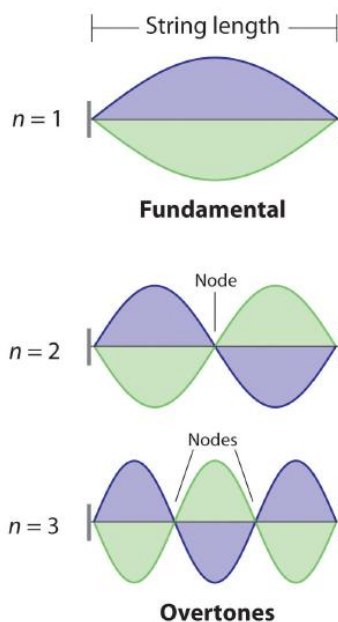


Figure 2.2.3: Standing Waves on a Vibrating String. The vibration with $(n = 1)$ is the fundamental and contains no nodes. Vibrations with higher values of n are called overtones; they contain $(n - 1)$ nodes.

Quantized vibrations and overtones containing nodes are not restricted to one-dimensional systems, such as strings. A two-dimensional surface, such as a drumhead, also has quantized vibrations. Similarly, when the ends of a string are joined to form a circle, the only allowed vibrations are those with wavelength

$$2\pi r = n\lambda\tag{2.2.6}$$

where r is the radius of the circle. De Broglie argued that Bohr's allowed orbits could be understood if the electron behaved like a *standing circular wave* (Figure 2.2.4). The standing wave could exist only if the circumference of the circle was an integral multiple of the wavelength such that the propagated waves were all in phase, thereby increasing the net amplitudes and causing *constructive interference*. Otherwise, the propagated waves would be out of phase, resulting in a net decrease in amplitude and causing *destructive interference*. The nonresonant waves interfere with themselves! De Broglie's idea explained Bohr's allowed orbits and energy levels nicely: in the lowest energy level, corresponding to $n = 1$ in Equation 2.2.6, one complete wavelength would close the circle. Higher energy levels would have successively higher values of n with a corresponding number of nodes.

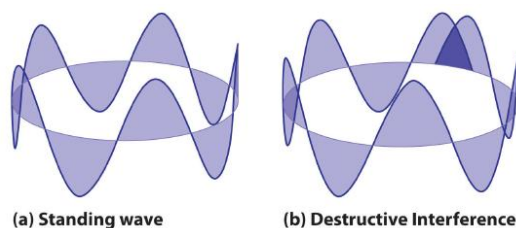


Figure 2.2.4: Standing Circular Wave and Destructive Interference. (a) In a standing circular wave with $(n = 5)$, the circumference of the circle corresponds to exactly five wavelengths, which results in constructive interference of the wave with itself when overlapping occurs. (b) If the circumference of the circle is not equal to an integral multiple of wavelengths, then the wave does not overlap exactly with itself, and the resulting destructive interference will result in cancellation of the wave. Consequently, a standing wave cannot exist under these conditions.

Like all analogies, although the standing wave model helps us understand much about why Bohr's theory worked, it also, if pushed too far, can mislead. As you will see, some of de Broglie's ideas are retained in the modern theory of the electronic structure of the atom: the wave behavior of the electron and the presence of nodes that increase in number as the energy level increases. Unfortunately, his (and Bohr's) explanation also contains one major feature that we now know to be incorrect: in the currently accepted model, the electron in a given orbit is *not* always at the same distance from the nucleus.

The Heisenberg Uncertainty Principle

Because a wave is a disturbance that travels in space, it has no fixed position. One might therefore expect that it would also be hard to specify the exact position of a *particle* that exhibits wavelike behavior. A characteristic of light is that it can be bent or spread out by passing through a narrow slit. You can literally see this by half closing your eyes and looking through your eye lashes. This reduces the brightness of what you are seeing and somewhat fuzzes out the image, but the light bends around your lashes to provide a complete image rather than a bunch of bars across the image. This is called diffraction.

This behavior of waves is captured in [Maxwell's equations](#) (1870 or so) for electromagnetic waves and was and is well understood. An "uncertainty principle" for light is, if you will, merely a conclusion about the nature of electromagnetic waves and nothing new. De Broglie's idea of wave-particle duality means that particles such as electrons which exhibit wavelike characteristics will also undergo diffraction from slits whose size is on the order of the electron wavelength.

This situation was described mathematically by the German physicist Werner Heisenberg (1901–1976; Nobel Prize in Physics, 1932), who related the position of a particle to its momentum. Referring to the electron, Heisenberg stated that “at every moment the electron has only an inaccurate position and an inaccurate velocity, and between these two inaccuracies there is this uncertainty relation.” Mathematically, the **Heisenberg uncertainty principle** states that the uncertainty in the position of a particle (Δx) multiplied by the uncertainty in its momentum [$\Delta(mv)$] is greater than or equal to Planck's constant divided by 4π :

$$(\Delta x)(\Delta[mv]) \geq \frac{h}{4\pi} \quad (2.2.7)$$

Because Planck's constant is a very small number, the Heisenberg uncertainty principle is important only for particles such as electrons that have very low masses. These are the same particles predicted by de Broglie's equation to have measurable wavelengths.

If the precise position x of a particle is known absolutely ($\Delta x = 0$), then the uncertainty in its momentum must be infinite:

$$(\Delta[mv]) = \frac{h}{4\pi(\Delta x)} = \frac{h}{4\pi(0)} = \infty \quad (2.2.8)$$

Because the mass of the electron at rest (m) is both constant and accurately known, the uncertainty in $\Delta(mv)$ must be due to the Δv term, which would have to be infinitely large for $\Delta(mv)$ to equal infinity. That is, according to Equation 2.2.8, the more accurately we know the exact position of the electron (as $\Delta x \rightarrow 0$), the less accurately we know the speed and the kinetic energy of the electron ($1/2 mv^2$) because $\Delta(mv) \rightarrow \infty$. Conversely, the more accurately we know the precise momentum (and the energy) of the electron [as $\Delta(mv) \rightarrow 0$], then $\Delta x \rightarrow \infty$ and we have no idea where the electron is.

Bohr's model of the hydrogen atom violated the Heisenberg uncertainty principle by trying to specify *simultaneously* both the position (an orbit of a particular radius) and the energy (a quantity related to the momentum) of the electron. Moreover, given its mass and wavelike nature, the electron in the hydrogen atom could not possibly orbit the nucleus in a well-defined circular path as

predicted by Bohr. You will see, however, that the *most probable radius* of the electron in the hydrogen atom is exactly the one predicted by Bohr's model.

✓ Example 2.2.1: Quantum Nature of Baseballs

Calculate the minimum uncertainty in the position of the pitched baseball from Example 2.2.1 that has a mass of exactly 149 g and a speed of 100 ± 1 mi/h.

Given: mass and speed of object

Asked for: minimum uncertainty in its position

Strategy:

- Rearrange the inequality that describes the Heisenberg uncertainty principle (Equation 2.2.7) to solve for the minimum uncertainty in the position of an object (Δx).
- Find Δv by converting the velocity of the baseball to the appropriate SI units: meters per second.
- Substitute the appropriate values into the expression for the inequality and solve for Δx .

Solution:

A The Heisenberg uncertainty principle (Equation 2.2.7) tells us that

$$(\Delta x)(\Delta(mv)) = h/4\pi$$

. Rearranging the inequality gives

$$\Delta x \geq \left(\frac{h}{4\pi} \right) \left(\frac{1}{\Delta(mv)} \right)$$

B We know that $h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$ and $m = 0.149 \text{ kg}$. Because there is no uncertainty in the mass of the baseball, $\Delta(mv) = m\Delta v$ and $\Delta v = \pm 1 \text{ mi/h}$. We have

$$\Delta x = \left(\frac{1 \cancel{\text{mi}}}{\cancel{h}} \right) \left(\frac{1 \cancel{h}}{60 \cancel{\text{min}}} \right) \left(\frac{1 \cancel{\text{min}}}{60 \cancel{s}} \right) \left(\frac{1.609 \cancel{\text{km}}}{\cancel{\text{mi}}} \right) \left(\frac{1000 \cancel{m}}{\cancel{\text{km}}} \right) = 0.4469 \text{ m/s}$$

C Therefore,

$$\Delta x \geq \left(\frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{4 (3.1416)} \right) \left(\frac{1}{(0.149 \text{ kg}) (0.4469 \text{ m}\cdot\text{s}^{-1})} \right)$$

Inserting the definition of a joule ($1 \text{ J} = 1 \text{ kg}\cdot\text{m}^2/\text{s}^2$) gives

$$\Delta x \geq \left(\frac{6.626 \times 10^{-34} \cancel{\text{kg}}\cdot\cancel{\text{m}}^2\cdot\cancel{s}}{4 (3.1416) (\cancel{s}^2)} \right) \left(\frac{1 \cancel{s}}{(0.149 \cancel{\text{kg}}) (0.4469 \cancel{\text{m}})} \right)$$

$$\Delta x \geq 7.92 \pm \times 10^{-34} \text{ m}$$

This is equal to 3.12×10^{-32} inches. We can safely say that if a batter misjudges the speed of a fastball by 1 mi/h (about 1%), he will not be able to blame Heisenberg's uncertainty principle for striking out.

? Exercise 2.2.2

Calculate the minimum uncertainty in the position of an electron traveling at one-third the speed of light, if the uncertainty in its speed is $\pm 0.1\%$. Assume its mass to be equal to its mass at rest.

Answer

$6 \times 10^{-10} \text{ m}$, or 0.6 nm (about the diameter of a benzene molecule)

Summary

An electron possesses both particle and wave properties. The modern model for the electronic structure of the atom is based on recognizing that an electron possesses particle and wave properties, the so-called **wave-particle duality**. Louis de Broglie showed that the wavelength of a particle is equal to Planck's constant divided by the mass times the velocity of the particle.

$$\lambda = \frac{h}{mv}$$

The electron in Bohr's circular orbits could thus be described as a **standing wave**, one that does not move through space. Standing waves are familiar from music: the lowest-energy standing wave is the **fundamental** vibration, and higher-energy vibrations are **overtones** and have successively more **nodes**, points where the amplitude of the wave is always zero. Werner Heisenberg's **uncertainty principle** states that it is impossible to precisely describe both the location and the speed of particles that exhibit wavelike behavior.

$$(\Delta x)(\Delta[mv]) \geq \frac{h}{4\pi}$$

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2.3: Quantum Numbers for Electrons

Learning Objectives

- Explain what spectra are.
- Learn the quantum numbers that are assigned to electrons.

There are two fundamental ways of generating light: either heat an object up to be so hot that it glows, or pass an electrical current through a sample of matter (usually a gas). Incandescent lights and fluorescent lights generate light via these two methods, respectively.

A hot object gives off a continuum of light. We notice this when the visible portion of the electromagnetic spectrum is passed through a prism: the prism separates light into its constituent colors, and all colors are present in a continuous rainbow (Figure 2.3.1a- Prisms and Light). This image is known as a **continuous spectrum**. However, when electricity is passed through a gas and light is emitted and this light is passed through a prism, we see only certain lines of light in the image (Figure 2.3.1b). This image is called a line spectrum. It turns out that every element has its own unique, characteristic line spectrum.

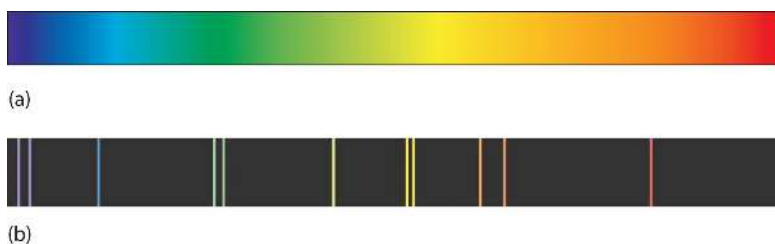


Figure 2.3.1: Prisms and Light. (a) A glowing object gives off a full rainbow of colors, which are noticed only when light is passed through a prism to make a continuous spectrum. (b) However, when electricity is passed through a gas, only certain colors of light are emitted. Here are the colors of light in the line spectrum of Hg.

Why does the light emitted from an electrically excited gas have only certain colors, while light given off by hot objects has a continuous spectrum? For a long time, it was not well explained. Particularly simple was the spectrum of hydrogen gas, which could be described easily by an equation; no other element has a spectrum that is so predictable (Figure 2.3.2 - Hydrogen Spectrum). Late nineteenth century scientists found that the positions of the lines obeyed a pattern given by the equation

$$\frac{1}{\lambda} = (109,700\text{cm}^{-1}) \left(\frac{1}{4} - \frac{1}{n^2} \right)$$

where $n = 3, 4, 5, 6$, etc. However, they could not explain why this was so.



Figure 2.3.2: Hydrogen Spectrum. The spectrum of hydrogen was particularly simple and could be predicted by a simple mathematical expression.

In 1913, the Danish scientist Niels Bohr suggested a reason why the hydrogen atom spectrum looked this way. He suggested that the electron in a hydrogen atom could not have any random energy, having *only* certain fixed values of energy that were indexed by the number n (the same n in the equation above and now called a **quantum number**). Quantities that have certain specific values are **quantized** values. Bohr suggested that the energy of the electron in hydrogen was quantized because it was in a specific orbit. Because the energies of the electron can have only certain values, the changes in energies can have only certain values (somewhat similar to a staircase—not only are the stair steps set at specific heights, but the height between steps is fixed). Finally, Bohr suggested that the energy of light emitted from electrified hydrogen gas was equal to the energy difference of the electron's energy states:

$$E_{\text{light}} = h\nu = \Delta E_{\text{electron}}$$

This means that only certain frequencies (and thus, certain wavelengths) of light are emitted. Figure 2.3.3 - Bohr's Model of the Hydrogen Atom, shows a model of the hydrogen atom based on Bohr's ideas.

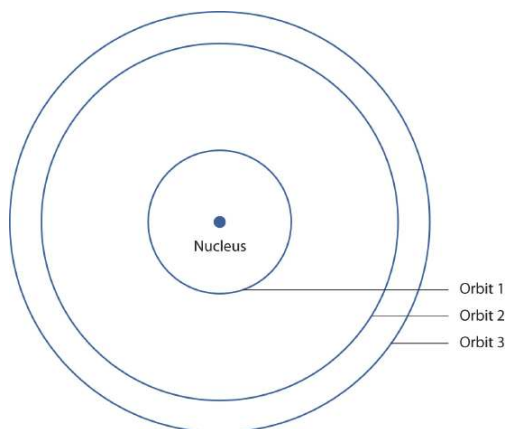


Figure 2.3.3: Bohr's Model of the Hydrogen Atom. Bohr's description of the hydrogen atom had specific orbits for the electron, which had quantized energies.

Bohr's ideas were useful, but were applicable only to the hydrogen atom. However, later researchers generalized Bohr's ideas into a new theory called **quantum mechanics**, which explains the behavior of electrons as if they were acting as a wave, not as particles. Quantum mechanics predicts two major things: quantized energies for electrons of all atoms (not just hydrogen) and an organization of electrons within atoms. Electrons are no longer thought of as being randomly distributed around a nucleus or restricted to certain orbits (in that regard, Bohr was wrong). Instead, electrons are collected into groups and subgroups that explain much about the chemical behavior of the atom.

In the quantum-mechanical model of an atom, the state of an electron is described by four quantum numbers, not just the one predicted by Bohr. The first quantum number is called the **principal quantum number (n)**. The principal quantum number largely determines the energy of an electron. Electrons in the same atom that have the same principal quantum number are said to occupy an electron **shell** of the atom. The principal quantum number can be any nonzero positive integer: 1, 2, 3, 4, ...

Within a shell, there may be multiple possible values of the next quantum number, the **angular momentum quantum number (ℓ)**. The ℓ quantum number has a minor effect on the energy of the electron but also affects the spatial distribution of the electron in three-dimensional space—that is, the shape of an electron's distribution in space. The value of the ℓ quantum number can be any integer between 0 and $n - 1$: $\ell = 0, 1, 2, \dots, n - 1$.

Thus, for a given value of n , there are different possible values of ℓ :

Table with two columns and four rows. The first (left) column is labeled "If n equals" and the second (right) column is labeled " ℓ can be". Underneath the columns in the rows are different values. All of the rows have numerical values.

If n equals	ℓ can be
1	0
2	0 or 1
3	0, 1, or 2
4	0, 1, 2, or 3

and so forth. Electrons within a shell that have the same value of ℓ are said to occupy a **subshell** in the atom. Commonly, instead of referring to the numerical value of ℓ , a letter represents the value of ℓ (to help distinguish it from the principal quantum number):

Table with two columns and four rows. The first (left) column is labeled "If ℓ equals" and the second (right) column is labeled "The letter is". The rows underneath the left column are numbers and the rows underneath the right column are letters.

If ℓ equals	The letter is
0	s
1	p

If ℓ equals	The letter is
2	<i>d</i>
3	<i>f</i>

The next quantum number is called the **magnetic quantum number (m_ℓ)**. For any value of ℓ , there are $2\ell + 1$ possible values of m_ℓ , ranging from $-\ell$ to ℓ :

$$-\ell < m_\ell < \ell$$

or

$$|m_\ell| < \ell$$

The following explicitly lists the possible values of m_ℓ for the possible values of ℓ :

Table with two columns and four rows. The first (left) column is labeled "If ℓ equals" and the second (right) column is labeled "The m_ℓ values can be". The rows underneath the left column are positive numbers and the rows underneath the right column are negative numbers.

If ℓ equals	The m_ℓ values can be
0	0
1	-1, 0, or 1
2	-2, -1, 0, 1, or 2
3	-3, -2, -1, 0, 1, 2, or 3

The particular value of m_ℓ dictates the orientation of an electron's distribution in space. When ℓ is zero, m_ℓ can be only zero, so there is only one possible orientation. When ℓ is 1, there are three possible orientations for an electron's distribution. When ℓ is 2, there are five possible orientations of electron distribution. This goes on and on for other values of ℓ , but we need not consider any higher values of ℓ here. Each value of m_ℓ designates a certain orbital. Thus, there is only one orbital when ℓ is zero, three orbitals when ℓ is 1, five orbitals when ℓ is 2, and so forth. The m_ℓ quantum number has no effect on the energy of an electron unless the electrons are subjected to a magnetic field—hence its name.

The ℓ quantum number dictates the general shape of electron distribution in space (Figure 2.3.4 - Electron Orbitals). Any s orbital is spherically symmetric (Figure 2.3.4a - Electron Orbitals), and there is only one orbital in any s subshell. Any p orbital has a two-lobed, dumbbell-like shape (Figure 2.3.4b - Electron Orbitals); because there are three of them, we normally represent them as pointing along the x-, y-, and z-axes of Cartesian space. The d orbitals are four-lobed rosettes (Figure 2.3.4c - Electron Orbitals) and they are oriented differently in space (the one labeled *d_{xy}* and a torus instead of four lobes, but it is equivalent to the other orbitals). When there is more than one possible value of m_ℓ , each orbital is labeled with one of the possible values. It should be noted that the diagrams in Figure 2.3.4 are estimates of the electron distribution in space, not surfaces electrons are fixed on.

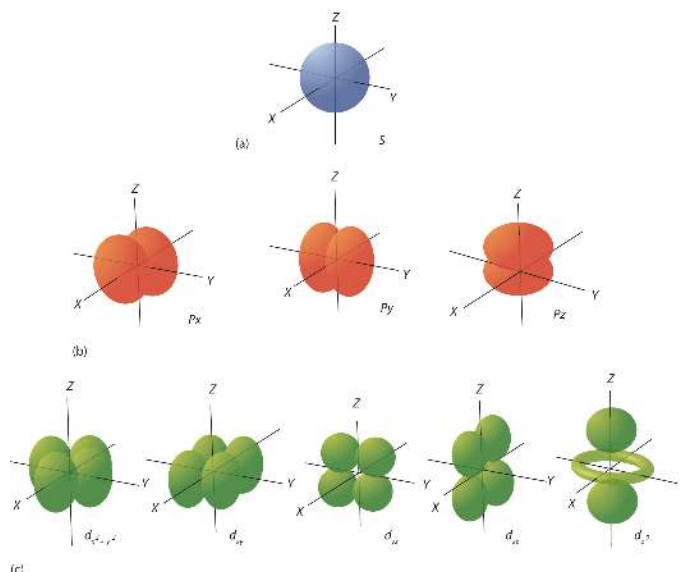


Figure 2.3.4: Electron Orbitals. (a) The lone s orbital is spherical in distribution. (b) The three p orbitals are shaped like dumbbells, and each one points in a different direction. (c) The five d orbitals are rosette in shape, except for the d_{z²} orbital, which is a "dumbbell + torus" combination. They are all oriented in different directions.

The final quantum number is the **spin quantum number** (m_s). Electrons and other subatomic particles behave as if they are spinning (we cannot tell if they really are, but they behave as if they are). Electrons themselves have two possible spin states, and because of mathematics, they are assigned the quantum numbers $+1/2$ and $-1/2$. These are the only two possible choices for the spin quantum number of an electron.

✓ Example 2.3.1

Of the set of quantum numbers $\{n, \ell, m_\ell, m_s\}$, which are possible and which are not allowed?

- $\{3, 2, 1, +1/2\}$
- $\{2, 2, 0, -1/2\}$
- $\{3, -1, 0, +1/2\}$

Solution

- The principal quantum number n must be an integer, as it is here. The quantum number ℓ must be less than n , which it is. The m_ℓ quantum number must be between $-\ell$ and ℓ , which it is. The spin quantum number is $+1/2$, which is allowed. Because this set of quantum numbers follows all restrictions, it is possible.
- The quantum number n is an integer, but the quantum number ℓ must be less than n , which it is not. Thus, this is not an allowed set of quantum numbers.
- The principal quantum number n is an integer, but ℓ is not allowed to be negative. Therefore, this is not an allowed set of quantum numbers.

? Exercise 2.3.1

Of the set of quantum numbers $\{n, \ell, m_\ell, m_s\}$, which are possible and which are not allowed?

- $\{4, 2, -2, 1\}$
- $\{3, 1, 0, -1/2\}$

Answers

- Spin must be either $+1/2$ or $-1/2$, so this set of quantum number is not allowed.
- allowed

✓ Chemistry is Everywhere: Neon Lights

A neon light is basically an electrified tube with a small amount of gas in it. Electricity excites electrons in the gas atoms, which then give off light as the electrons go back into a lower energy state. However, many so-called "neon" lights do not contain neon!

Although we know now that a gas discharge gives off only certain colors of light, without a prism or other component to separate the individual light colors, we see a composite of all the colors emitted. It is not unusual for a certain color to predominate. True neon lights, with neon gas in them, have a reddish-orange light due to the large amount of red-, orange-, and yellow-colored light emitted. However, if krypton is used instead of neon, a whitish light is emitted, while using argon yields a blue-purple light. A light filled with nitrogen gas glows purple, as does a helium lamp. Other gases—and mixtures of gases—emit other colors of light. Ironically, despite its importance in the development of modern electronic theory, hydrogen lamps emit little visible light and are rarely used for illumination purposes.



The Human/Need/Desire statue consists of purple "NEED", orange "HUMAN", green "HUMAN", pink "DESIRE", red "HOPE", and blue "DREAM".

Neon lights. The different colors of these "neon" lights are caused by gases other than neon in the discharge tubes. *Human/Need/Desire.* Neon sculpture by Bruce Nauman (1983), who has been characterized as a conceptual artist. (CC BY-SA 3.0; eschipul).

Key Takeaways

Electrons in atoms have quantized energies. The state of electrons in atoms is described by four quantum numbers.

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2.4: Atomic Orbitals

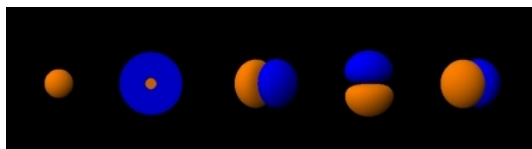
Skills to Develop

- Illustrate the general shape of atomic orbitals
- Identify the relationship between quantum numbers

The "old quantum mechanics" introduced the idea of quantization, and it was good for describing the position of spectroscopic lines of single electron atoms. But it couldn't predict how strong the lines were. The "new quantum mechanics" of Schrodinger and Heisenberg took the wave-particle duality to its logical conclusion. While Bohr's model was still "classical" in that there was a defined orbit or trajectory (a path that could be calculated) for the electron, Schrodinger and Heisenberg changed that. Basically, where is a wave? If a particle behaves as a wave, you can't point to the exact spot where it is. Also, if light energy is quantized, it turns out that you can't measure the path taken by an electron without changing the path. In microscopy, which is using microscopes to look at small things, you can't separate things that are closer together than the wavelength used. This is why we use X-ray diffraction and electron microscopes with very short wavelengths to look at atoms and molecules. So if you want to measure the electron's path with light, and measure it precisely on an atomic scale, you have to use a short wavelength of light. But if you use a short wavelength then it has a lot of energy ($E = h\nu$), enough to change the electron's direction. This is the basis of the Uncertainty Principle.

The result of this (and also of Schrodinger's 3-D, space-filling wavefunction) is that we no longer describe electrons using orbits, or defined paths. Instead we talk about **orbitals**, which are defined by wavefunctions $\Psi(x,y,z)$ like the one calculated in the previous section. It turns out (although I think Schrodinger didn't exactly intend this at first) that $\Psi(x,y,z)^2$ is the probability of finding the "particle" at position (x,y,z) .

Schrodinger found the standing waves or $\Psi(x,y,z)$ for the electron in a hydrogen atom. These are much more complicated than the wavefunction we found because they are in 3-D and also have a potential energy to worry about. (But they aren't that complicated: you can look at them [here](#).) There are an infinite number of functions that solve the equation, just like in the simple example. In the 1-D example, we used 1 **quantum number** n to determine the energies. As n increased, so did the energy, and so did the number of nodes (places where the amplitude is zero). In 3-D, the standing waves are specified by 3 quantum numbers. (Actually, Bohr and others were using 3 quantum numbers before Schrodinger published this, because it makes sense in 3-D.) The principal quantum number n corresponds roughly to the radius of the orbit in the Bohr model, or to the "most probable distance from the nucleus" in the orbital model. This also corresponds to the energy: the electron is lower energy when it is close to the nucleus, because of the Coulomb attraction. The second quantum number ℓ gives the shape. In the Bohr model this meant ellipse or circle. In Schrodinger's model the shapes are 3-D. You can look at them in detail on [Wikipedia](#) (scroll down to the table of images) or with an animated applet like this. This is also a good time to check out the "orbitals" tab on [Ptable](#). Pick an element, then move over the arrows to see a picture of each orbital.



The first 5 hydrogen orbitals, from Wikimedia Commons

Finally, the third quantum number tells the orientation. In the Bohr model this meant what plane the orbit was in. In the figure, you can see that the last 3 orbitals have the same shape but point along different directions (x , y and z).

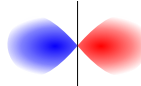
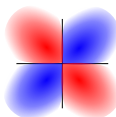
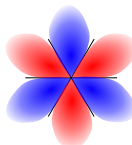
Notice that standard pictures of orbitals show most of them with 2 colors. This represents the phase of the orbital (whether Ψ is + or - at that point). This doesn't effect the energy or the probability of finding the particle there, but it is very important when atoms interact with each other, like forming bonds, which is what chemistry is all about! When waves interact with each other, it matters a lot whether the peak (high point) overlaps with the trough (low point) or not. This is true of water waves, sound waves, light waves and electron waves.

There are lots of ways of showing orbitals, but usually they just draw a surface so that you have 50% or 90% or whatever chance of finding the electron inside the surface. (Always, the probability of finding the electron becomes 0 as you get far enough from the nucleus.) The second orbital in the picture is shown as a slice, so you can see that the inside near the nucleus has the opposite phase as the outside. Wherever the color changes, there must be a node (Ψ passes through 0 as it goes from + or -). Thus the first orbital

has no node, which makes sense because more nodes mean higher energy. The second has 1 spherical node. The next three have a planar (flat) node. If you look at more orbitals, you'll notice that the nodes keep increasing.

Here's the pattern of orbital shapes and quantum numbers.

- The principal quantum number n tells you how big the orbital is and what the energy is. It also tells you how many spherical nodes the orbital has. The values go from $n = 1, 2, 3, 4, 5, 6, 7, \dots$ they could keep going but we haven't found elements that need that many orbitals yet! The number of spherical nodes in the orbital is $n - \ell - 1$.
- The angular momentum quantum number ℓ tells you the shape. If $\ell = 0$, the orbital has spherical symmetry (it's round), and we say it is an "s orbital". If $\ell = 1$, the orbital has one planar node, and it's called a "p orbital". See the figure below for d and f orbitals, with 2 and 3 planar nodes each. The possible values of ℓ are 0, 1, ... $n - 1$.
- The magnetic quantum number m_ℓ tells the orientation of the orbital. The possible values are $-\ell, -\ell + 1, \dots, 0, 1, \ell - 1, \ell$. For instance, for the p orbitals, it can be -1, 0, 1. You can remember the number of orientations using the table below.

ℓ		
0	s	
1	p	
2	d	
3	f	

Shapes of orbitals can be easily predicted by knowing the number of planar nodes, shown as black lines. The nucleus is at the center of each orbital. (Note that there are other possible positions of the nodes for d and f orbitals, but don't worry about this now. Also note that shapes shown here are approximate, not calculated.)

1s 0 0	nℓ ℓ m _ℓ	
2s 0 0	2p 1 1	
2p 1 -1	2p 1 0	
3s 0 0	3p 1 1	3d 2 2
3p 1 -1	3p 1 0	3d 2 1
3d 2 -2	3d 2 -1	3d 2 0

A geometric pattern for remembering the number of each type of orbitals and the possible values of the quantum numbers.

Outside Links

- [Atomic Orbitals Explained](#), by DCaulf (15 min)

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- [Emily V Eames](#) (City College of San Francisco)

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CHAPTER OVERVIEW

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3.1: Electronic Structure of Atoms (Electron Configurations)

Learning Objectives

- Derive the predicted ground-state electron configurations of atoms
- Identify and explain exceptions to predicted electron configurations for atoms and ions
- Relate electron configurations to element classifications in the periodic table

Having introduced the basics of atomic structure and quantum mechanics, we can use our understanding of quantum numbers to determine how atomic orbitals relate to one another. This allows us to determine which orbitals are occupied by electrons in each atom. The specific arrangement of electrons in orbitals of an atom determines many of the chemical properties of that atom.

3.1.1: Orbital Energies and Atomic Structure

The energy of atomic orbitals increases as the principal quantum number, n , increases. In any atom with two or more electrons, the repulsion between the electrons makes energies of subshells with different values of l differ so that the energy of the orbitals increases within a shell in the order $s < p < d < f$. Figure 3.1.1 depicts how these two trends in increasing energy relate. The 1s orbital at the bottom of the diagram is the orbital with electrons of lowest energy. The energy increases as we move up to the 2s and then 2p, 3s, and 3p orbitals, showing that the increasing n value has more influence on energy than the increasing l value for small atoms. However, this pattern does not hold for larger atoms. The 3d orbital is higher in energy than the 4s orbital. Such overlaps continue to occur frequently as we move up the chart.

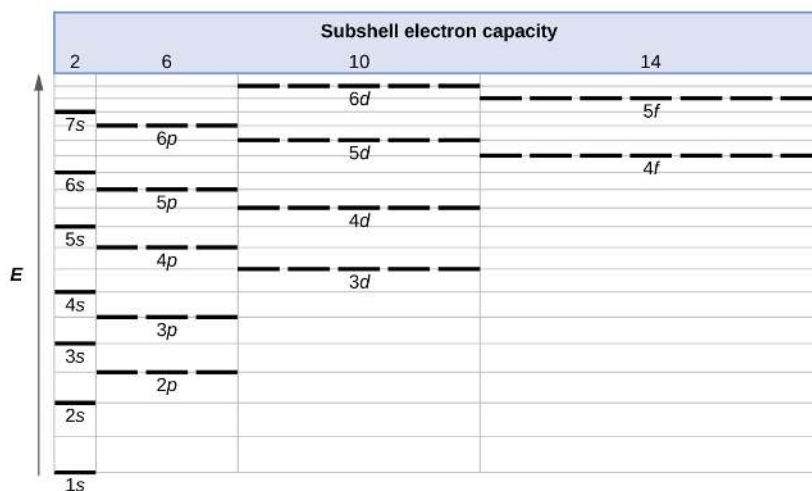


Figure 3.1.1: Generalized energy-level diagram for atomic orbitals in an atom with two or more electrons (not to scale).

Electrons in successive atoms on the periodic table tend to fill low-energy orbitals first. Thus, many students find it confusing that, for example, the 5p orbitals fill immediately after the 4d, and immediately before the 6s. The filling order is based on observed experimental results, and has been confirmed by theoretical calculations. As the principal quantum number, n , increases, the size of the orbital increases and the electrons spend more time farther from the nucleus. Thus, the attraction to the nucleus is weaker and the energy associated with the orbital is higher (less stabilized). But this is not the only effect we have to take into account. Within each shell, as the value of l increases, the electrons are less penetrating (meaning there is less electron density found close to the nucleus), in the order $s > p > d > f$. Electrons that are closer to the nucleus slightly repel electrons that are farther out, offsetting the more dominant electron–nucleus attractions slightly (recall that all electrons have -1 charges, but nuclei have $+Z$ charges). This phenomenon is called shielding and will be discussed in more detail in the next section. Electrons in orbitals that experience more shielding are less stabilized and thus higher in energy. For small orbitals (1s through 3p), the increase in energy due to n is more significant than the increase due to l ; however, for larger orbitals the two trends are comparable and cannot be simply predicted. We will discuss methods for remembering the observed order.

The arrangement of electrons in the orbitals of an atom is called the electron configuration of the atom. We describe an electron configuration with a symbol that contains three pieces of information (Figure 3.1.2):

1. The number of the principal quantum shell, n ,

2. The letter that designates the orbital type (the subshell, l), and
3. A superscript number that designates the number of electrons in that particular subshell.

For example, the notation $2p^4$ (read "two-p-four") indicates four electrons in a p subshell ($l = 1$) with a principal quantum number (n) of 2. The notation $3d^8$ (read "three-d-eight") indicates eight electrons in the d subshell (i.e., $l = 2$) of the principal shell for which $n = 3$.

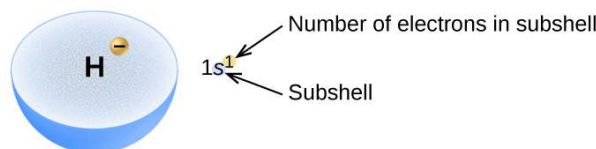


Figure 3.1.2: The diagram of an electron configuration specifies the subshell (n and l value, with letter symbol) and superscript number of electrons.

3.1.2: The Aufbau Principle

To determine the electron configuration for any particular atom, we can "build" the structures in the order of atomic numbers. Beginning with hydrogen, and continuing across the periods of the periodic table, we add one proton at a time to the nucleus and one electron to the proper subshell until we have described the electron configurations of all the elements. This procedure is called the Aufbau principle, from the German word *Aufbau* ("to build up"). Each added electron occupies the subshell of lowest energy available (in the order shown in Figure 3.1.3), subject to the limitations imposed by the allowed quantum numbers according to the Pauli exclusion principle. Electrons enter higher-energy subshells only after lower-energy subshells have been filled to capacity. Figure 3.1.3 illustrates the traditional way to remember the filling order for atomic orbitals.

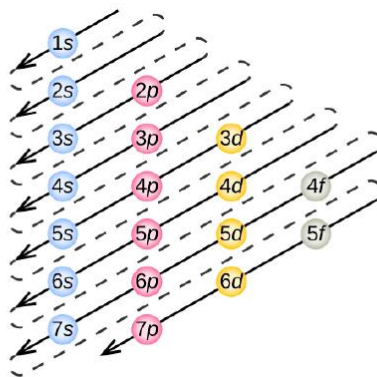
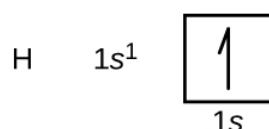


Figure 3.1.3: The arrow leads through each subshell in the appropriate filling order for electron configurations. This chart is straightforward to construct. Simply make a column for all the s orbitals with each n shell on a separate row. Repeat for p , d , and f . Be sure to only include orbitals allowed by the quantum numbers (no $1p$ or $2d$, and so forth). Finally, draw diagonal lines from top to bottom as shown.

Since the arrangement of the periodic table is based on the electron configurations, Figure 3.1.4 provides an alternative method for determining the electron configuration. The filling order simply begins at hydrogen and includes each subshell as you proceed in increasing Z order. For example, after filling the $3p$ block up to Ar, we see the orbital will be $4s$ (K, Ca), followed by the $3d$ orbitals.

We will now construct the ground-state electron configuration and orbital diagram for a selection of atoms in the first and second periods of the periodic table. Orbital diagrams are pictorial representations of the electron configuration, showing the individual orbitals and the pairing arrangement of electrons. We start with a single hydrogen atom (atomic number 1), which consists of one proton and one electron. Referring to either Figure 3.1.3 or 3.1.4, we would expect to find the electron in the 1s orbital. By convention, the $m_s = +\frac{1}{2}$ value is usually filled first. The electron configuration and the orbital diagram are:

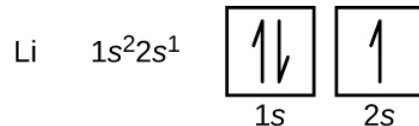


He $1s^2$

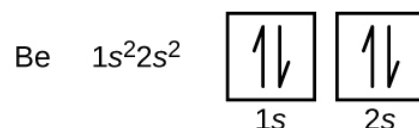
↑↓
 $1s$

The $n = 1$ shell is completely filled in a helium atom.

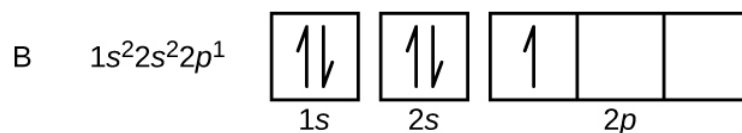
The next atom is the alkali metal lithium with an atomic number of 3. The first two electrons in lithium fill the 1s orbital and have the same sets of four quantum numbers as the two electrons in helium. The remaining electron must occupy the orbital of next lowest energy, the 2s orbital (Figure 3.1.3 or 3.1.4). Thus, the electron configuration and orbital diagram of lithium are:



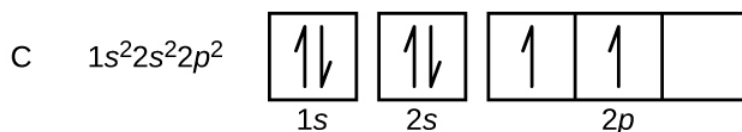
An atom of the alkaline earth metal beryllium, with an atomic number of 4, contains four protons in the nucleus and four electrons surrounding the nucleus. The fourth electron fills the remaining space in the 2s orbital.



An atom of boron (atomic number 5) contains five electrons. The $n = 1$ shell is filled with two electrons and three electrons will occupy the $n = 2$ shell. Because any s subshell can contain only two electrons, the fifth electron must occupy the next energy level, which will be a 2p orbital. There are three degenerate 2p orbitals ($m_l = -1, 0, +1$) and the electron can occupy any one of these p orbitals. When drawing orbital diagrams, we include empty boxes to depict any empty orbitals in the same subshell that we are filling.



Carbon (atomic number 6) has six electrons. Four of them fill the 1s and 2s orbitals. The remaining two electrons occupy the 2p subshell. We now have a choice of filling one of the 2p orbitals and pairing the electrons or of leaving the electrons unpaired in two different, but degenerate, p orbitals. The orbitals are filled as described by Hund's rule: the lowest-energy configuration for an atom with electrons within a set of degenerate orbitals is that having the maximum number of unpaired electrons. Thus, the two electrons in the carbon 2p orbitals have identical n , l , and m_s quantum numbers and differ in their m_l quantum number (in accord with the Pauli exclusion principle). The electron configuration and orbital diagram for carbon are:



Nitrogen (atomic number 7) fills the 1s and 2s subshells and has one electron in each of the three 2p orbitals, in accordance with Hund's rule. These three electrons have unpaired spins. Oxygen (atomic number 8) has a pair of electrons in any one of the 2p orbitals (the electrons have opposite spins) and a single electron in each of the other two. Fluorine (atomic number 9) has only one 2p orbital containing an unpaired electron. All of the electrons in the noble gas neon (atomic number 10) are paired, and all of the orbitals in the $n = 1$ and the $n = 2$ shells are filled. The electron configurations and orbital diagrams of these four elements are:

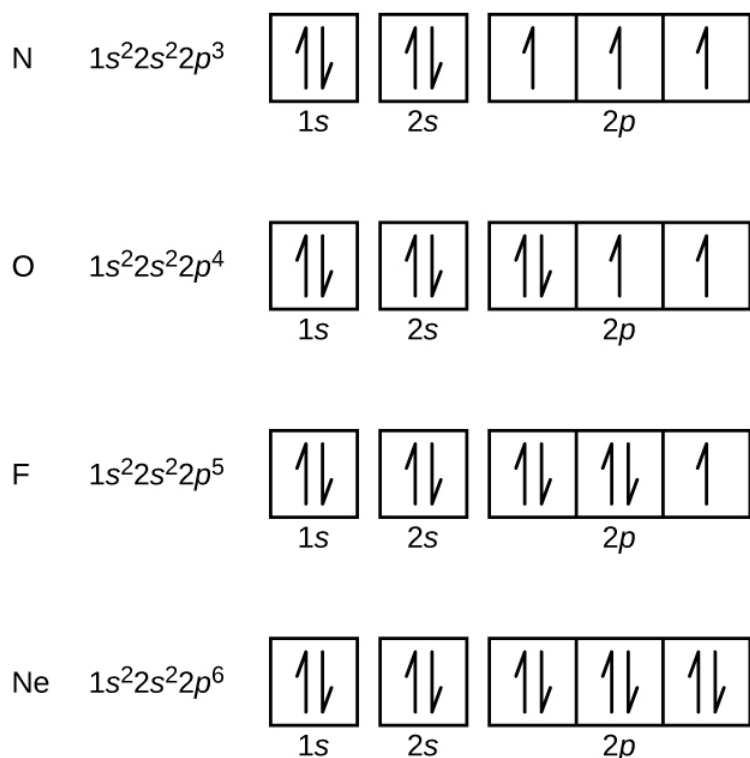


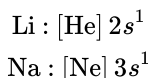
Figure 3.1.5: Since the core electron shells correspond to noble gas electron configurations, we can abbreviate electron configurations by writing the noble gas that matches the core electron configuration, along with the valence electrons in a condensed format. For our sodium example, the symbol [Ne] represents core electrons, ($1s^2 2s^2 2p^6$) and our abbreviated or condensed configuration is [Ne] $3s^1$.

The alkali metal sodium (atomic number 11) has one more electron than the neon atom. This electron must go into the lowest-energy subshell available, the 3s orbital, giving a $1s^2 2s^2 2p^6 3s^1$ configuration. The electrons occupying the outermost shell orbital(s) (highest value of n) are called valence electrons, and those occupying the inner shell orbitals are called core electrons (Figure \PageIndex5\PageIndex5). Since the core electron shells correspond to noble gas electron configurations, we can abbreviate electron configurations by writing the noble gas that matches the core electron configuration, along with the valence electrons in a condensed format. For our sodium example, the symbol [Ne] represents core electrons, ($1s^2 2s^2 2p^6$) and our abbreviated or condensed configuration is [Ne] $3s^1$.



Figure 3.1.5: A core-abbreviated electron configuration (right) replaces the core electrons with the noble gas symbol whose configuration matches the core electron configuration of the other element.

Similarly, the abbreviated configuration of lithium can be represented as [He] $2s^1$, where [He] represents the configuration of the helium atom, which is identical to that of the filled inner shell of lithium. Writing the configurations in this way emphasizes the similarity of the configurations of lithium and sodium. Both atoms, which are in the alkali metal family, have only one electron in a valence s subshell outside a filled set of inner shells.



The alkaline earth metal magnesium (atomic number 12), with its 12 electrons in a [Ne] $3s^2$ configuration, is analogous to its family member beryllium, [He] $2s^2$. Both atoms have a filled s subshell outside their filled inner shells. Aluminum (atomic number 13), with 13 electrons and the electron configuration [Ne] $3s^2 3p^1$, is analogous to its family member boron, [He] $2s^2 2p^1$.

The electron configurations of silicon (14 electrons), phosphorus (15 electrons), sulfur (16 electrons), chlorine (17 electrons), and argon (18 electrons) are analogous in the electron configurations of their outer shells to their corresponding family members carbon, nitrogen, oxygen, fluorine, and neon, respectively, except that the principal quantum number of the outer shell of the heavier elements has increased by one to $n = 3$. Figure 3.1.6 shows the lowest energy, or ground-state, electron configuration for these elements as well as that for atoms of each of the known elements.

Electron Configuration Table

Figure 3.1.6 shows a periodic table where each element's box contains its atomic number, symbol, name, and ground-state electron configuration. The configurations follow the periodic law, showing similar patterns within groups. For example, Group 1 elements have configurations ending in ns^1 , and Group 18 elements have configurations ending in $ns^2 np^6$. The lanthanide and actinide series are shown separately at the bottom, with their configurations starting from $4f$ and $5f$ respectively.

Figure 3.1.6: This version of the periodic table shows the outer-shell electron configuration of each element. Note that down each group, the configuration is often similar.

When we come to the next element in the periodic table, the alkali metal potassium (atomic number 19), we might expect that we would begin to add electrons to the $3d$ subshell. However, all available chemical and physical evidence indicates that potassium is like lithium and sodium, and that the next electron is not added to the $3d$ level but is, instead, added to the $4s$ level (Figure 3.1.3 or 3.1.4). As discussed previously, the $3d$ orbital with no radial nodes is higher in energy because it is less penetrating and more shielded from the nucleus than the $4s$, which has three radial nodes. Thus, potassium has an electron configuration of $[\text{Ar}]4s^1$. Hence, potassium corresponds to Li and Na in its valence shell configuration. The next electron is added to complete the $4s$ subshell and calcium has an electron configuration of $[\text{Ar}]4s^2$. This gives calcium an outer-shell electron configuration corresponding to that of beryllium and magnesium.

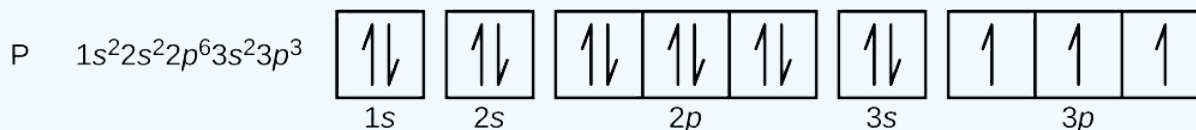
Beginning with the transition metal scandium (atomic number 21), additional electrons are added successively to the $3d$ subshell. This subshell is filled to its capacity with 10 electrons (remember that for $l = 2$ [d orbitals], there are $2l + 1 = 5$ values of m_l , meaning that there are five d orbitals that have a combined capacity of 10 electrons). The $4p$ subshell fills next. Note that for three series of elements, scandium (Sc) through copper (Cu), yttrium (Y) through silver (Ag), and lutetium (Lu) through gold (Au), a total of 10 d electrons are successively added to the $(n - 1)$ shell next to the n shell to bring that $(n - 1)$ shell from 8 to 18 electrons. For two series, lanthanum (La) through lutetium (Lu) and actinium (Ac) through lawrencium (Lr), 14 f electrons ($l = 3$, $2l + 1 = 7$ m_l values; thus, seven orbitals with a combined capacity of 14 electrons) are successively added to the $(n - 2)$ shell to bring that shell from 18 electrons to a total of 32 electrons.

✓ Example 3.1.1: Quantum Numbers and Electron Configurations

What is the electron configuration and orbital diagram for a phosphorus atom? What are the four quantum numbers for the last electron added?

Solution

The atomic number of phosphorus is 15. Thus, a phosphorus atom contains 15 electrons. The order of filling of the energy levels is $1s$, $2s$, $2p$, $3s$, $3p$, $4s$, . . . The 15 electrons of the phosphorus atom will fill up to the $3p$ orbital, which will contain three electrons:



The last electron added is a $3p$ electron. Therefore, $n = 3$ and, for a p -type orbital, $l = 1$. The m_l value could be -1 , 0 , or $+1$. The three p orbitals are degenerate, so any of these m_l values is correct. For unpaired electrons, convention assigns the value of $+\frac{1}{2}$ for the spin quantum number; thus, $m_s = +\frac{1}{2}$.

? Exercise 3.1.1

Identify the atoms from the electron configurations given:

- $[\text{Ar}]4s^2 3d^5$
- $[\text{Kr}]5s^2 4d^{10} 5p^6$

Answer a

Mn

Answer b

Xe

The periodic table can be a powerful tool in predicting the electron configuration of an element. However, we do find exceptions to the order of filling of orbitals that are shown in Figure 3.1.3 or 3.1.4. For instance, the electron configurations of the transition metals chromium (Cr; atomic number 24) and copper (Cu; atomic number 29), among others, are not those we would expect. In general, such exceptions involve subshells with very similar energy, and small effects can lead to changes in the order of filling.

In the case of Cr and Cu, we find that half-filled and completely filled subshells apparently represent conditions of preferred stability. This stability is such that an electron shifts from the $4s$ into the $3d$ orbital to gain the extra stability of a half-filled $3d$ subshell (in Cr) or a filled $3d$ subshell (in Cu). Other exceptions also occur. For example, niobium (Nb, atomic number 41) is predicted to have the electron configuration $[\text{Kr}]5s^2 4d^3$. Experimentally, we observe that its ground-state electron configuration is actually $[\text{Kr}]5s^1 4d^4$. We can rationalize this observation by saying that the electron–electron repulsions experienced by pairing the electrons in the $5s$ orbital are larger than the gap in energy between the $5s$ and $4d$ orbitals. There is no simple method to predict the exceptions for atoms where the magnitude of the repulsions between electrons is greater than the small differences in energy between subshells.

3.1.3: Electron Configurations and the Periodic Table

As described earlier, the periodic table arranges atoms based on increasing atomic number so that elements with the same chemical properties recur periodically. When their electron configurations are added to the table (Figure 3.1.6), we also see a periodic recurrence of similar electron configurations in the outer shells of these elements. Because they are in the outer shells of an atom, valence electrons play the most important role in chemical reactions. The outer electrons have the highest energy of the electrons in

an atom and are more easily lost or shared than the core electrons. Valence electrons are also the determining factor in some physical properties of the elements.

Elements in any one group (or column) have the same number of valence electrons; the alkali metals lithium and sodium each have only one valence electron, the alkaline earth metals beryllium and magnesium each have two, and the halogens fluorine and chlorine each have seven valence electrons. The similarity in chemical properties among elements of the same group occurs because they have the same number of valence electrons. It is the loss, gain, or sharing of valence electrons that defines how elements react.

It is important to remember that the periodic table was developed on the basis of the chemical behavior of the elements, well before any idea of their atomic structure was available. Now we can understand why the periodic table has the arrangement it has—the arrangement puts elements whose atoms have the same number of valence electrons in the same group. This arrangement is emphasized in Figure 3.1.6, which shows in periodic-table form the electron configuration of the last subshell to be filled by the Aufbau principle. The colored sections of Figure 3.1.6 show the three categories of elements classified by the orbitals being filled: main group, transition, and inner transition elements. These classifications determine which orbitals are counted in the valence shell, or highest energy level orbitals of an atom.

1. **Main group elements** (sometimes called **representative elements**) are those in which the last electron added enters an s or a p orbital in the outermost shell, shown in blue and red in Figure 3.1.6. This category includes all the nonmetallic elements, as well as many metals and the intermediate semimetallic elements. The valence electrons for main group elements are those with the highest n level. For example, gallium (Ga, atomic number 31) has the electron configuration $[\text{Ar}]4s^23d^{10}4p^1$, which contains three valence electrons (underlined). The completely filled d orbitals count as core, not valence, electrons.
2. **Transition elements or transition metals.** These are metallic elements in which the last electron added enters a d orbital. The valence electrons (those added after the last noble gas configuration) in these elements include the ns and $(n - 1)d$ electrons. The official IUPAC definition of transition elements specifies those with partially filled d orbitals. Thus, the elements with completely filled orbitals (Zn, Cd, Hg, as well as Cu, Ag, and Au in Figure 3.1.6) are not technically transition elements. However, the term is frequently used to refer to the entire d block (colored yellow in Figure 3.1.6), and we will adopt this usage in this textbook.
3. **Inner transition elements** are metallic elements in which the last electron added occupies an f orbital. They are shown in green in Figure 3.1.6. The valence shells of the inner transition elements consist of the $(n - 2)f$, the $(n - 1)d$, and the ns subshells. There are two inner transition series:
 1. The lanthanide series: lanthanide (La) through lutetium (Lu)
 2. The actinide series: actinide (Ac) through lawrencium (Lr)

Lanthanum and actinium, because of their similarities to the other members of the series, are included and used to name the series, even though they are transition metals with no f electrons.

3.1.4: Electron Configurations of Ions

We have seen that ions are formed when atoms gain or lose electrons. A cation (positively charged ion) forms when one or more electrons are removed from a parent atom. For main group elements, the electrons that were added last are the first electrons removed. For transition metals and inner transition metals, however, electrons in the s orbital are easier to remove than the d or f electrons, and so the highest ns electrons are lost, and then the $(n - 1)d$ or $(n - 2)f$ electrons are removed. An anion (negatively charged ion) forms when one or more electrons are added to a parent atom. The added electrons fill in the order predicted by the Aufbau principle.

✓ Example 3.1.2: Predicting Electron Configurations of Ions

What is the electron configuration and orbital diagram of:

- a. Na^+
- b. P^{3-}
- c. Al^{2+}
- d. Fe^{2+}
- e. Sm^{3+}

Solution

First, write out the electron configuration for each parent atom. We have chosen to show the full, unabbreviated configurations to provide more practice for students who want it, but listing the core-abbreviated electron configurations is also acceptable.

Next, determine whether an electron is gained or lost. Remember electrons are negatively charged, so ions with a positive charge have *lost* an electron. For main group elements, the last orbital gains or loses the electron. For transition metals, the last *s* orbital loses an electron before the *d* orbitals.

- Na: $1s^2 2s^2 2p^6 3s^1$. Sodium cation loses one electron, so Na^+ : $1s^2 2s^2 2p^6 3s^1 = \text{Na}^+$: $1s^2 2s^2 2p^6$.
- P: $1s^2 2s^2 2p^6 3s^2 3p^3$. Phosphorus trianion gains three electrons, so P^{3-} : $1s^2 2s^2 2p^6 3s^2 3p^6$.
- Al: $1s^2 2s^2 2p^6 3s^2 3p^1$. Aluminum dication loses two electrons Al^{2+} : $1s^2 2s^2 2p^6 3s^2 3p^1 = \text{Al}^{2+}$: $1s^2 2s^2 2p^6 3s^1$.
- Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$. Iron(II) loses two electrons and, since it is a transition metal, they are removed from the 4s orbital Fe^{2+} : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6 = 1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$.
- Sm: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^6$. Samarium trication loses three electrons. The first two will be lost from the 6s orbital, and the final one is removed from the 4f orbital. Sm^{3+} : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^6 = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 4f^5$.

? Exercise 3.1.2

- Which ion with a +2 charge has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^5$?
- Which ion with a +3 charge has this configuration?

Answer a

Tc^{2+}

Answer b

Ru^{3+}

Summary

The relative energy of the subshells determine the order in which atomic orbitals are filled (1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, and so on). Electron configurations and orbital diagrams can be determined by applying the Pauli exclusion principle (no two electrons can have the same set of four quantum numbers) and Hund's rule (whenever possible, electrons retain unpaired spins in degenerate orbitals).

Electrons in the outermost orbitals, called valence electrons, are responsible for most of the chemical behavior of elements. In the periodic table, elements with analogous valence electron configurations usually occur within the same group. There are some exceptions to the predicted filling order, particularly when half-filled or completely filled orbitals can be formed. The periodic table can be divided into three categories based on the orbital in which the last electron to be added is placed: main group elements (s and p orbitals), transition elements (d orbitals), and inner transition elements (f orbitals).

Glossary

Aufbau principle

procedure in which the electron configuration of the elements is determined by "building" them in order of atomic numbers, adding one proton to the nucleus and one electron to the proper subshell at a time

core electron

electron in an atom that occupies the orbitals of the inner shells

electron configuration

electronic structure of an atom in its ground state given as a listing of the orbitals occupied by the electrons

Hund's rule

every orbital in a subshell is singly occupied with one electron before any one orbital is doubly occupied, and all electrons in singly occupied orbitals have the same spin

orbital diagram

pictorial representation of the electron configuration showing each orbital as a box and each electron as an arrow

valence electrons

electrons in the outermost or valence shell (highest value of n) of a ground-state atom; determine how an element reacts

valence shell

outermost shell of electrons in a ground-state atom; for main group elements, the orbitals with the highest n level (s and p subshells) are in the valence shell, while for transition metals, the highest energy s and d subshells make up the valence shell and for inner transition elements, the highest s , d , and f subshells are included

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3.2: Electron Configurations According to Bohr and Pauli

Skills to Develop

- Describe the Pauli Exclusion Principle

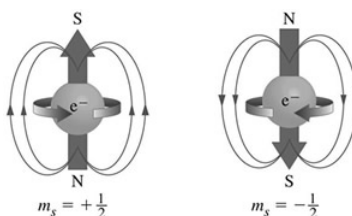
Many-electron Atoms

If there are multiple electrons, which orbits do they occupy? In atoms larger than hydrogen, the larger nuclear charge means that the orbits should be closer to the nucleus. If all the electrons are in the lowest energy orbit, even if repulsion expands the orbit a little, then the size of elements would get smaller as they get heavier. Also, it would get harder and harder to pull electrons off heavier elements, because they would be bound much more tightly to the more charged nuclei. Both of these are the opposite of the facts: sizes of elements increase a little as you go down the periodic table, and it is hardest to remove electrons from the lightest elements. Thus, it was clear that only some electrons could be in the lowest orbit.

Pauli was a theoretician "so good that experimental apparatus broke when he walked through the lab door." (It's a joke that theorists, who usually just think, can't handle lab equipment.) He suggested that theory and data would fit well if each orbit (defined by 3 quantum numbers) could hold exactly 2 electrons. Thus as soon as each orbit was full, with 2, the next electron would have to go in the next higher orbit. Using this rule, Bohr and others determined the electron configurations (which electrons were in which state or orbit) of most of the elements, and found that the order matched the periodic table nicely! The movement to the next principal quantum number started a new period, so the theory fit all the data on valence and other properties.

Electron Spin

Pauli didn't know at the time why each orbital holds 2 electrons, but later it was found that a fourth quantum number was needed, because strong magnetic fields split the energy of the 2 electrons in one orbital into 2 different levels. (This is the basis of many important experimental techniques, especially NMR, used by chemists, and MRI, used in medical imaging.) A proposed explanation for this is that the electrons can "spin" in either direction, just like the earth spinning to give us day and night. This isn't exactly what happens, but the word **spin** is still used to describe this effect. The **spin quantum number** has values of $+1/2$ or $-1/2$. Thus, Pauli's idea is now called the Pauli Exclusion Principle, and it says that no 2 electrons in one atom can have exactly the same quantum numbers. Two electrons can occupy one orbital, but they must have opposite spins.



An illustration of the different spin quantum numbers.

Electron Configurations

Bohr figured out the number of electrons in each **shell**, where a shell is all the electrons with the same principal quantum number. The pattern he used, which you can verify with the periodic table, was 2, 8, 8, 18, 18, 32, 32.

Based on Bohr's model, you can find the number of **valence electrons** or electrons in the highest shell by looking at the periodic table. (For now, let's not worry about transition metals, and lanthanoides.) Alkalis have 1 valence electron, because we have just started a new shell. Alkaline earths have 2, B has 3, C has 4, N has 5. Chalcogens have 6, halogens have 7, noble gases have 8. (You can see that this is kind of close to the **valence** we mentioned earlier.

Outside Link

- [CrashCourse Chemistry: The Electron](#)

Contributors and Attributions

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3.3: Atomic Structure - Electron Configurations

Objective

After completing this section, you should be able to write the ground-state electron configuration for each of the elements up to and including atomic number 36.

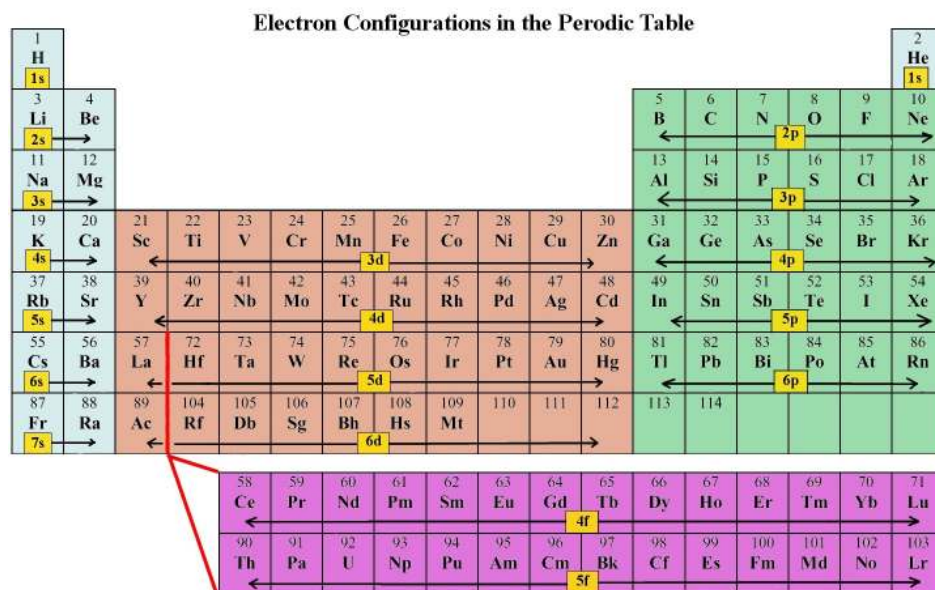
Key Terms

Make certain that you can define, and use in context, the key terms below.

- ground-state electronic configuration
- Hund's rule
- Pauli exclusion principle
- aufbau principle

The electron configuration of an atom is the representation of the arrangement of electrons distributed among the orbital shells and subshells. Commonly, the electron configuration is used to describe the orbitals of an atom in its ground state, but it can also be used to represent an atom that has ionized into a cation or anion by compensating with the loss of or gain of electrons in their subsequent orbitals. Many of the physical and chemical properties of elements can be correlated to their unique electron configurations. The valence electrons, electrons in the outermost shell, are the determining factor for the unique chemistry of the element.

Electron Configurations in the Periodic Table



1 H 1s																	2 He 1s
3 Li 2s	4 Be 2s											5 B 2p	6 C 2p	7 N 2p	8 O 2p	9 F 2p	10 Ne 2p
11 Na 3s	12 Mg 3s											13 Al 3p	14 Si 3p	15 P 3p	16 S 3p	17 Cl 3p	18 Ar 3p
19 K 4s	20 Ca 4s	21 Sc 3d	22 Ti 3d	23 V 3d	24 Cr 3d	25 Mn 3d	26 Fe 3d	27 Co 3d	28 Ni 3d	29 Cu 3d	30 Zn 3d	31 Ga 4p	32 Ge 4p	33 As 4p	34 Se 4p	35 Br 4p	36 Kr 4p
37 Rb 5s	38 Sr 5s	39 Y 4d	40 Zr 4d	41 Nb 4d	42 Mo 4d	43 Tc 4d	44 Ru 4d	45 Rh 4d	46 Pd 4d	47 Ag 4d	48 Cd 4d	49 In 5p	50 Sn 5p	51 Sb 5p	52 Te 5p	53 I 5p	54 Xe 5p
55 Cs 6s	56 Ba 6s	57 La 5d	58 Ce 5d	59 Pr 5d	60 Nd 5d	61 Pm 5d	62 Sm 5d	63 Eu 5d	64 Gd 5d	65 Tb 5d	66 Dy 5d	67 Ho 5d	68 Er 5d	69 Tm 5d	70 Yb 5d	71 Lu 5d	
87 Fr 7s	88 Ra 7s	89 Ac 6d	90 Th 6d	91 Pa 6d	92 U 6d	93 Np 6d	94 Pu 6d	95 Am 6d	96 Cm 6d	97 Bk 6d	98 Cf 6d	99 Es 6d	100 Fm 6d	101 Md 6d	102 No 6d	103 Lr 6d	

Figure 3.3.1: The Periodic Table. (CC BY-SA-NC; Sarah Faizi via LibreTexts)

Electron Configurations

The electron configuration of an **atom** is the representation of the arrangement of electrons distributed among the orbital shells and subshells. Commonly, the electron configuration is used to describe the orbitals of an atom in its ground state, but it can also be used to represent an atom that has **ionized** into a cation or anion by compensating with the loss of or gain of electrons in their subsequent orbitals. Many of the physical and chemical properties of **elements** can be correlated to their unique electron configurations. The valence electrons, electrons in the outermost shell, are the determining factor for the unique chemistry of the element.

Before assigning the electrons of an atom into orbitals, one must become familiar with the basic concepts of electron configurations. Every element on the periodic table consists of atoms, which are composed of protons, neutrons, and electrons. Electrons exhibit a negative charge and are found around the nucleus of the atom in electron orbitals, defined as the volume of

space in which the electron can be found within 95% probability. The four different types of orbitals (s,p,d, and f) have different shapes, and one orbital can hold a maximum of two electrons. The p, d, and f orbitals have different sublevels, thus can hold more electrons.

As stated, the electron configuration of each element is unique to its position on the periodic table. The energy level is determined by the period and the number of electrons is given by the atomic number of the element. Orbitals on different energy levels are similar to each other, but they occupy different areas in space. The 1s orbital and 2s orbital both have the characteristics of an s orbital (radial nodes, spherical volume probabilities, can only hold two electrons, etc.) but, as they are found in different energy levels, they occupy different spaces around the nucleus. Each orbital can be represented by specific blocks on the periodic table. The s-block is the region of the [alkali metals](#) including helium (Groups 1 & 2), the d-block are the [transition metals](#) (Groups 3 to 12), the [p-block](#) are the main group elements from Groups 13 to 18, and the f-block are the [lanthanides](#) and [actinides](#) series.

Using the periodic table to determine the electron configurations of atoms is key, but also keep in mind that there are certain rules to follow when assigning electrons to different orbitals. The periodic table is an incredibly helpful tool in writing electron configurations. For more information on how electron configurations and the periodic table are linked, visit the [Connecting Electrons to the Periodic Table](#) module.

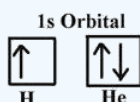
Rules for Assigning Electron Orbitals

Pauli Exclusion Principle

The Pauli exclusion principle states that no two electrons can have the same four quantum numbers. The first three (n , l , and m_l) may be the same, but the fourth quantum number must be different. A single orbital can hold a maximum of two electrons, which **must** have opposing spins; otherwise they would have the same four quantum numbers, which is forbidden. One electron is spin up ($m_s = +1/2$) and the other would spin down ($m_s = -1/2$). This tells us that each subshell has double the electrons per orbital. The s subshell has 1 orbital that can hold up to 2 electrons, the p subshell has 3 orbitals that can hold up to 6 electrons, the d subshell has 5 orbitals that hold up to 10 electrons, and the f subshell has 7 orbitals with 14 electrons.

✓ Example 1: Hydrogen and Helium

The first three quantum numbers of an electron are $n=1$, $l=0$, $m_l=0$. Only two electrons can correspond to these, which would be either $m_s = -1/2$ or $m_s = +1/2$. As we already know from our studies of quantum numbers and electron orbitals, we can conclude that these four quantum numbers refer to the 1s subshell. If only one of the m_s values are given then we would have $1s^1$ (denoting hydrogen) if both are given we would have $1s^2$ (denoting helium). Visually, this is be represented as:



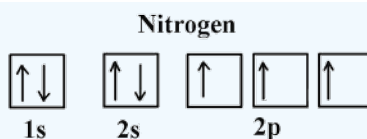
As shown, the 1s subshell can hold only two electrons and, when filled, the electrons have opposite spins.

Hund's Rule

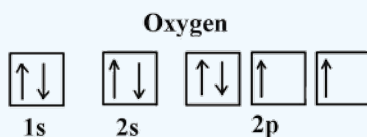
When assigning electrons in orbitals, each electron will first fill all the orbitals with similar energy (also referred to as degenerate) before pairing with another electron in a half-filled orbital. Atoms at ground states tend to have as many unpaired electrons as possible. When visualizing this processes, think about how electrons are exhibiting the same behavior as the same poles on a magnet would if they came into contact; as the negatively charged electrons fill orbitals they first try to get as far as possible from each other before having to pair up.

✓ Example 2: Oxygen and Nitrogen

If we look at the correct electron configuration of the Nitrogen ($Z = 7$) atom, a very important element in the biology of plants: $1s^2 2s^2 2p^3$



We can clearly see that p orbitals are half-filled as there are three electrons and three p orbitals. This is because Hund's Rule states that the three electrons in the 2p subshell will fill all the empty orbitals first before filling orbitals with electrons in them. If we look at the element after nitrogen in the same period, oxygen ($Z = 8$) its electron configuration is: $1s^2 2s^2 2p^4$ (for an atom).



Oxygen has one more electron than nitrogen and as the orbitals are all half filled the electron must pair up.

Occupation of Orbitals

Electrons fill orbitals in a way to minimize the energy of the atom. Therefore, the electrons in an atom fill the principal energy levels in order of increasing energy (the electrons are getting farther from the nucleus). The relative energy of the orbitals is shown in Figure 3.3.2

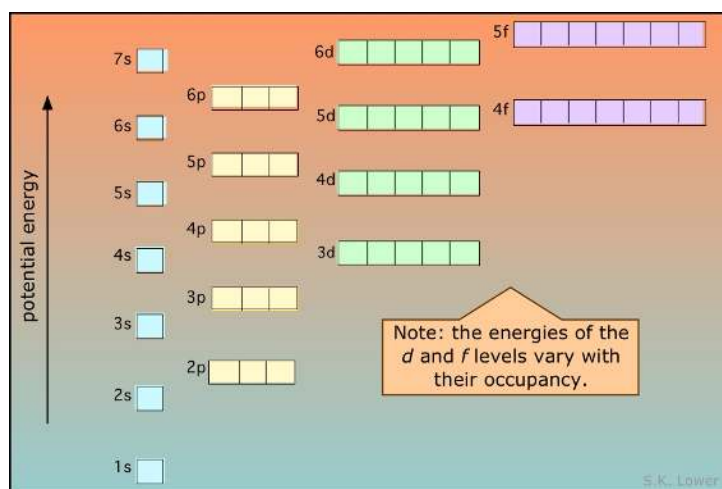


Figure 3.3.2: The relative potential energy of atomic orbitals. (CC BY-NC; Stephen Lower)

The order of levels filled is then:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, and 7p

The general order in which orbitals are filled is depicted in Figure 3.3.3. Subshells corresponding to each value of n are written from left to right on successive horizontal lines, where each row represents a row in the periodic table. The order in which the orbitals are filled is indicated by the diagonal lines running from the upper right to the lower left. Accordingly, the 4s orbital is filled prior to the 3d orbital because of shielding and penetration effects. Consequently, the electron configuration of potassium, which begins the fourth period, is $[\text{Ar}]4s^1$, and the configuration of calcium is $[\text{Ar}]4s^2$. Five 3d orbitals are filled by the next 10 elements, the transition metals, followed by three 4p orbitals. Notice that the last member of this row is the noble gas krypton ($Z = 36$), $[\text{Ar}]4s^2 3d^{10} 4p^6 = [\text{Kr}]$, which has filled 4s, 3d, and 4p orbitals. The fifth row of the periodic table is essentially the same as the fourth, except that the 5s, 4d, and 5p orbitals are filled sequentially.

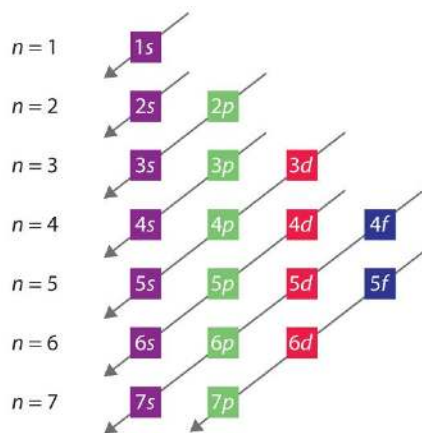


Figure 3.3.3: Predicting the Order in Which Orbitals Are Filled in Multielectron Atoms. If you write the subshells for each value of the principal quantum number on successive lines, the observed order in which they are filled is indicated by a series of diagonal lines running from the upper right to the lower left.

The Aufbau Process

Aufbau comes from the German word "aufbauen" meaning "to build." When writing electron configurations, orbitals are built up from atom to atom. When writing the electron configuration for an atom, orbitals are filled in order of increasing atomic number. However, there are some exceptions to this rule.

✓ Example 3: 3rd row elements

Following the pattern across a period from B (Z=5) to Ne (Z=10), the number of electrons increases and the subshells are filled. This example focuses on the p subshell, which fills from boron to neon.

- B (Z=5) configuration: $1s^2 2s^2 2p^1$
- C (Z=6) configuration: $1s^2 2s^2 2p^2$
- N (Z=7) configuration: $1s^2 2s^2 2p^3$
- O (Z=8) configuration: $1s^2 2s^2 2p^4$
- F (Z=9) configuration: $1s^2 2s^2 2p^5$
- Ne (Z=10) configuration: $1s^2 2s^2 2p^6$

The Number of Valence Electrons

The number of valence electrons of an element can be determined by the periodic table group (vertical column) in which the element is categorized. With the exception of groups 3–12 (the [transition metals](#)), the units digit of the group number identifies how many valence electrons are associated with a neutral atom of an element listed under that particular column. For example in group 16, the units digit is 6 and elements in this group have 6 valence electrons.

Table 3.3.1: Valence electrons derived from periodic table group

Periodic table group	Valence electrons
Group 1: alkali metals	1
Group 2: alkaline earth metals	2
Groups 3-12: transition metals	2* (The 4s shell is complete and cannot hold any more electrons)
Group 13: boron group	3
Group 14: carbon group	4
Group 15: pnictogens	5
Group 16: chalcogens	6
Group 17: halogens	7

Periodic table group	Valence electrons
Group 18: noble gases	8**

* The general method for counting valence electrons is generally not useful for transition metals. Instead the modified **d electron count method** is used.

** Except for **helium**, which has only two valence electrons.

The electron configuration of an element is the arrangement of its electrons in its atomic orbitals. By knowing the electron configuration of an element, we can predict and explain a great deal of its chemistry.

✓ Example 1.3.1

Draw an orbital diagram and use it to derive the electron configuration of phosphorus, $Z = 15$. What is its valence electron configuration?

Given: atomic number

Asked for: orbital diagram and valence electron configuration for phosphorus

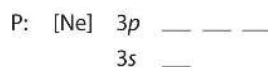
Strategy:

- Locate the nearest noble gas preceding phosphorus in the periodic table. Then subtract its number of electrons from those in phosphorus to obtain the number of valence electrons in phosphorus.
- Referring to Figure 1.3.1, draw an orbital diagram to represent those valence orbitals. Following Hund's rule, place the valence electrons in the available orbitals, beginning with the orbital that is lowest in energy. Write the electron configuration from your orbital diagram.
- Ignore the inner orbitals (those that correspond to the electron configuration of the nearest noble gas) and write the valence electron configuration for phosphorus.

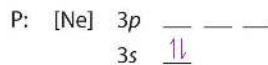
Solution:

A Because phosphorus is in the third row of the periodic table, we know that it has a [Ne] closed shell with 10 electrons. We begin by subtracting 10 electrons from the 15 in phosphorus.

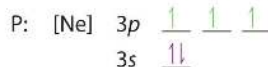
B The additional five electrons are placed in the next available orbitals, which Figure 1.2.5 tells us are the 3s and 3p orbitals:



Because the 3s orbital is lower in energy than the 3p orbitals, we fill it first:



Hund's rule tells us that the remaining three electrons will occupy the degenerate 3p orbitals separately but with their spins aligned:



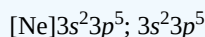
The electron configuration is $[\text{Ne}]3s^23p^3$.

C We obtain the valence electron configuration by ignoring the inner orbitals, which for phosphorus means that we ignore the [Ne] closed shell. This gives a valence-electron configuration of $3s^23p^3$.

? Exercise 1.3.1

Draw an orbital diagram and use it to derive the electron configuration of chlorine, $Z = 17$. What is its valence electron configuration?

Answer



The sixth row of the periodic table will be different from the preceding two because the $4f$ orbitals, which can hold 14 electrons, are filled between the $6s$ and the $5d$ orbitals. The elements that contain $4f$ orbitals in their valence shell are the lanthanides. When the $6p$ orbitals are finally filled, we have reached the next (and last known) noble gas, radon ($Z = 86$), $[\text{Xe}]6s^24f^{14}5d^{10}6p^6 = [\text{Rn}]$. In the last row, the $5f$ orbitals are filled between the $7s$ and the $6d$ orbitals, which gives the 14 actinide elements. Because the large number of protons makes their nuclei unstable, all the actinides are radioactive.

✓ Example 1.3.2

Write the electron configuration of mercury ($Z = 80$), showing all the inner orbitals.

Given: atomic number

Asked for: complete electron configuration

Strategy:

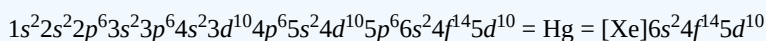
Using the orbital diagram in Figure 3.3.3 and the periodic table as a guide, fill the orbitals until all 80 electrons have been placed.

Solution:

By placing the electrons in orbitals following the order shown in Figure 3.3.3 and using the periodic table as a guide, we obtain

$1s^2$	row 1	2 electrons
$2s^22p^6$	row 2	8 electrons
$3s^23p^6$	row 3	8 electrons
$4s^23d^{10}4p^6$	row 4	18 electrons
$5s^24d^{10}5p^6$	row 5	18 electrons
	row 1–5	54 electrons

After filling the first five rows, we still have $80 - 54 = 26$ more electrons to accommodate. According to Figure 1.3.1, we need to fill the $6s$ (2 electrons), $4f$ (14 electrons), and $5d$ (10 electrons) orbitals. The result is mercury's electron configuration:



with a filled $5d$ subshell, a $6s^24f^{14}5d^{10}$ valence shell configuration, and a total of 80 electrons. (You should always check to be sure that the total number of electrons equals the atomic number.)

Summary

Based on the Pauli principle and a knowledge of orbital energies obtained using hydrogen-like orbitals, it is possible to construct the periodic table by filling up the available orbitals beginning with the lowest-energy orbitals (the **aufbau principle**), which gives rise to a particular arrangement of electrons for each element (its **electron configuration**). **Hund's rule** says that the lowest-energy arrangement of electrons is the one that places them in degenerate orbitals with their spins parallel. For chemical purposes, the most important electrons are those in the outermost principal shell, the **valence electrons**.

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SECTION OVERVIEW

3.4: Periodic Trends

Periodic trends are specific patterns that are present in the periodic table that illustrate different aspects of a certain element, including its size and its electronic properties. Major periodic trends include: [electronegativity](#), [ionization energy](#), [electron affinity](#), [atomic radius](#), melting point, and [metallic character](#). Periodic trends, arising from the arrangement of the periodic table, provide chemists with an invaluable tool to quickly predict an element's properties. These trends exist because of the similar atomic structure of the elements within their respective group families or periods, and because of the periodic nature of the elements.

3.4.1: Characteristics of Metals

3.4.2: Characteristics of Nonmetals

3.4.3: Effective Nuclear Charge

3.4.4: Electron Affinity

3.4.5: Ionization Energy

3.4.6: Sizes of Atoms and Ions

3.4.7: Slater's Rules for Effective Nuclear Charge

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3.4.1: Characteristics of Metals

Skills to Develop

- List and explain the properties of metals

Remember that metals are on the left and bottom of the periodic table. Based on the periodic trends in the last 3 sections, this means that they are usually bigger, more likely to lose electrons, and less likely to gain electrons, than the non-metals.

Elemental Properties

In the elemental form, metals are usually shiny, can be bent or stretched, and conduct heat and electricity. This is because metals hold their valence electrons kind of loosely, because of the low IE. It's a general pattern that the closer an atom is to the noble gas electron configuration, the fewer bonds it makes. Metals are far from the noble gas configuration, so they usually make bonds to many neighbors. Thus, they have structures in which each atom touches many neighbors (sometimes 6, usually 8 or 12). Because they don't have very many electrons, the valence electrons are shared by many atoms in a "delocalized ocean" of electrons that aren't really attached to particular atoms. These "free floating" electrons allow the metal to conduct heat and electricity. Also, because the bonds in a metal aren't pointed directly from atom to atom, they don't break easily. This means the metals can be bent and stretched. The technical words are malleable (can be pounded into foil) and ductile (can be stretched into wire). The sea of valence electrons allows the nuclei to be pushed around without separating. I don't think there's a simple explanation for why metals are shiny, though.

Reaction Patterns

Metals can mix with each other to form alloys that are similar to elemental metals. When they react with non-metals, they usually lose electrons to form cations. The cations are then attracted to the anions, so the result are ionic or sort of ionic compounds. The easier it is for a metal to lose electrons, the more reactive it is. If you haven't already, watch this video about the reactivity of the alkali metals. The metals on the right that have bigger ionization energies form more covalent compounds with non-metals, with more electron sharing and less pure electrostatic attraction. These metals are also more flexible about what ionic charge they have. See why by going to [Ptable](#) and watching the purple move right as you go from IE_1 to IE_4 or higher. The transition metals stay green: they don't take a sudden jump to much higher IE.

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3.4.2: Characteristics of Nonmetals

Skills to Develop

- List some characteristics of nonmetals
- Contrast metals and nonmetals

Remember that non-metals are on the right and top of the periodic table. Based on the periodic trends in the last 4 sections, this means that they are usually smaller, more likely to gain electrons, and less likely to lose electrons, than the metals.

Elemental Properties

In the elemental form, non-metals can be gas, liquid or solid. They aren't shiny (lustrous) and they don't conduct heat or electricity well. Usually their melting points are lower than for metals, although there are exceptions. The solids usually break easily, and can't bend like metals. It's a general pattern that the closer an atom is to the noble gas electron configuration, the fewer bonds it makes. Non-metals are close to the noble gas configuration, so they usually make a few bonds to a few neighbors. The noble gases make no bonds, and are monatomic (single atoms); halogens make 1 bond to 1 other atom, etc. This means that they don't usually form extended structures (except diamond and graphite). Instead, they form separate molecules. These molecules aren't held together tightly, so solids can easily melt or break. The electrons are held tightly by just 1 - 2 atoms, so they can't conduct electricity.

Reaction Patterns

Non-metals can react with each other to form compounds in which electrons are shared. These compounds have some of the same characteristics as the elemental forms: usually they melt or boil at relatively low temperature and don't conduct heat or electricity. When non-metals react with metals, they usually gain electrons to form anions. The cations are then attracted to the anions, so the result are ionic or sort of ionic compounds. The more a non-metal wants to gain electrons, the more reactive it is. Thus, the halogens are all reactive, but iodine is pretty safe, while bromine, chlorine and especially fluorine are really nasty and dangerous! Oxygen only seems safe and friendly to us because we are adapted to it. When oxygen first appeared in the atmosphere due to photosynthesis, most of the early life forms probably died from it; we descended from the survivors.

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3.4.3: Effective Nuclear Charge

Skills to Develop

- Explain the difference between nuclear charge and effective nuclear charge

The reason electrons are attached to atoms is the Coulomb's law attraction between the positively charged nucleus and the negatively charged electrons. Without the **nuclear charge** holding on to the electrons, they would have no reason to stay in orbitals near nuclei. So it makes sense that energy of the orbitals and their size depend on the nuclear charge. For instance, equivalent orbitals get lower in energy and smaller (more density closer to the nucleus) when nuclear charge increases. (If you want to see where nuclear charge is in the orbital equations, follow [this](#) link and click on an orbital; then scroll down to see the equation. Z_{eff} is the effective nuclear charge.)

There are 2 reasons an electron might not spend that much time actually right next to the nucleus, even though there is an attraction. One is **angular momentum**. Remember from physics that angular momentum is basically the momentum in the "around the center" direction multiplied by r , the distance from the center. Thus, if the electron is "in" the nucleus, $r = 0$, and angular momentum is 0. Remember also the second quantum number is the angular momentum quantum number ℓ , which corresponds to s, p, d and f orbitals. For s orbitals, $\ell = 0$, and angular momentum is zero, so the electron can hang out at the nucleus. For the other shapes (p,d,f) angular momentum is not zero, and there is a node at the nucleus. So only s orbitals can hang out right at the nucleus.

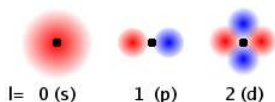


Figure 3.4.3.1: A basic illustration of orbital shapes with varying angular momentum and the nucleus being the black dot in the center.

The other reason an electron might not be able to get that close to the nucleus is because of the other electrons. Electrons repel each other, and because of the exclusion principle there can only be 2 electrons in each orbital. So think about lithium, element 3. Its first 2 electrons are in 1s. The third electron is in 2s. Because the principal quantum number is bigger, the 2s electron is usually farther from the nucleus than the 1s electrons. That means that often the 1s electrons are between the 2s electron and the nucleus. This means that the total Coulomb attraction felt by the 2s electron is smaller than you would calculate using just nuclear charge and distance, because there is also the electron-electron repulsion. This is the basis of the **effective nuclear charge**. Because of the electron-electron repulsions, the outer electrons in a many-electron atom feel less attraction toward the nucleus, so they feel like the nuclear charge is smaller than it actually is. So effective nuclear charge is always smaller than actual nuclear charge.

Effective nuclear charge depends on the type of electron. Electrons in s orbitals, even 4s or 5s, still spend some time right at the nucleus, and when they are there, they feel the full nuclear charge, so on average the s electrons feel a nuclear charge closer to the actual nuclear charge. Electrons in d or f orbitals really don't get very close to the nucleus, so they really get blocked, or **shielded** by inner electrons. They feel a smaller effective nuclear charge than s electrons. And electrons in p orbitals are in between.

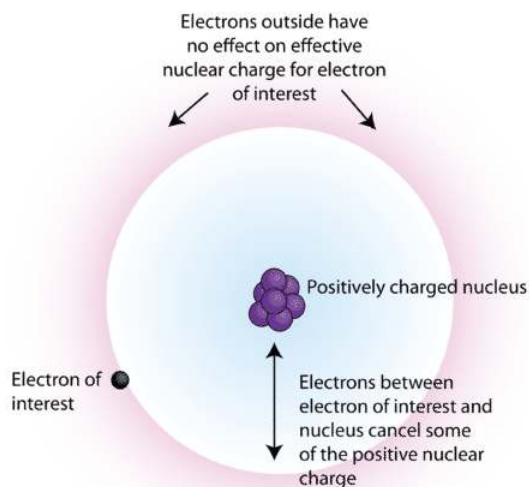


Figure 3.4.3.1: An illustration of the effects of electron shielding on outer electrons. (CC BY-NC; CK-12)

Usually if you do any calculation of orbitals for many-electron atoms, you will use effective nuclear charge instead of actual nuclear charge. The size and energy of the orbitals will depend on effective nuclear charge, not on actual nuclear charge. Size and energy of orbitals determines some very important chemical properties, including the size of the element (as an atom, ion, or in a molecule) and how easily it loses or gains electrons. Electrons take up most of the space in an atom, so orbital size tells you size. Losing electrons requires the energy by which they are bound, which is the roughly same as the orbital energy. Adding electrons only works if the orbital where they will go is lower energy than where they came from.

Outside Link

- [Effective Nuclear Charge](#) (10 min)

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3.4.4: Electron Affinity

Skills to Develop

- Define electron affinity
- Describe the periodic trend of electron affinity

Electron affinity is a measure of how much an atom wants to gain an electron, becoming an anion. Unfortunately 2 different definitions are used: intro textbooks use 1 definition and everyone else uses the other! I think you should use the standard advanced definition, according to which electron affinity $EA = IE_0$, the energy of this reaction:



The other definition just has the opposite sign, because it's the energy of this process:



Why does Electron Affinity matter?

Like ionization energy, electron affinity tells us how likely an atom is to steal electrons from other atoms, or just convince them to transfer their loyalty partially.

Predicting Relative Electron Affinities

It pretty much follows the same pattern you would expect based on ionization energy. If the new electron goes into an orbital that feels high effective nuclear charge, gaining an electron is good. If it goes into an orbital that is in a higher shell or subshell, or that feels low effective nuclear charge, gaining an electron is bad. The only other thing is that it's easier to add electrons to bigger atoms, because then they can spread out and not have so much electron-electron repulsion. For this reason, chlorine has more favorable EA than fluorine (in the gas phase, fluorine is still much more reactive).

Look at EA for yourself!

Go to [Ptable's](#) electron affinity page. See the general trend (bigger middle and right) with big effects at the end and middle of each block (noble gases, mercury family, alkaline earths, nitrogen, manganese).

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3.4.5: Ionization Energy

Skills to Develop

- Describe the significance and periodic trend of ionization energy

Ionization energy is the energy needed to remove an electron from an atom or ion. Unlike atomic radii, we can and do measure ionization energies in the gas phase, when the atom or ion is not interacting with anything else. The first ionization energy, IE_1 , is the energy of this reaction



The **second ionization energy**, IE_2 , is the energy of



You can also measure third, fourth, etc. All of these assume that the highest energy electron is knocked off. If you are removing core electrons, you would write them like this: IE_{1s} , to show what orbital the electron comes from.

How do you Measure Ionization Energy?

Generally you do this by shining high energy photons on the material you want to study. UV will ionize valence electrons and X-ray can ionize core electrons. You can vary the wavelength of the photons, and also measure the kinetic energy of the electrons that come off, to see what the binding energy (orbital energy) for each electron is. You can also measure the ionization energy of molecules, which is very interesting because it can tell you how the orbital energies change because of bonding.

Why does it matter?

Ionization energy tells us how likely an atom is to form a cation, and if so, what charge. In general, it tells us how tightly the electron is bound, how stable it is. It can tell us the energies of real orbitals, the effects electrons have on each other, and help us predict reactivity and properties of molecules. (We'll talk more about this when we get to bonding!)

Predicting Relative Ionization Energies

Ionization energy depends on orbital energy, which depends on the type of orbital and the effective nuclear charge. Thus, it follows predictable patterns in the periodic table. As you go down, n increases, and the energy of the orbital increases. That means the orbital is less stable, so it's easier to pull off the electron, so ionization energy decreases. (Stable, bound electrons have negative energies; electrons that aren't in an atom have 0 energy.) As you go across the periodic table, usually the type of orbital is the same, and the effective nuclear charge increases, making the orbital more stable, so ionization energy increases. But when you change subshells, the ionization energy might increase less, because the new subshell is less stable. Also, remember Hund's rule: electrons are more stable when they don't share the same orbital. So if you have to put a new electron into an occupied orbital, that also makes the ionization energy increase less.

You can predict any relative IE just by thinking about how big the Coulomb forces are. Bigger n , means bigger distance, weaker force. Removing an electron from a neutral atom is easier than removing an electron from a cation, because of the charge. Also consider effective nuclear charge and electron-electron repulsions (especially in the same orbital). In summary, mostly IE increases up and to the right, because of low shells and high effective nuclear charge.

Look at IE for yourself!

Go to [Table's](#) ionization energy page. You can look at first, second, third, etc. See the general trend (bigger up and right), and also notice some exceptions as you change blocks (s-block or d-block to p-block).

Outside Links

- [Khan Academy: Periodic Table Trends - Ionization Energy](#) (12 min)
- [CrashCourse Chemistry: The Electron](#) (13 min)

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3.4.6: Sizes of Atoms and Ions

Skills to Develop

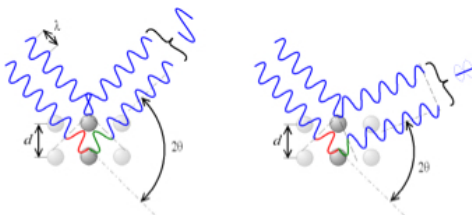
- Describe the significance of and periodic trend for atomic radii

What are Atomic Radii?

Atomic radii are the radii of atoms, a measure of how big the atoms are. That seems kind of simple. It's a useful idea because if we know the radii, we can predict how big molecules are, whether different parts will touch each other, etc. This is good for designing molecules for particular purposes, or interpreting data, and other things.

How do you Measure Atomic Radii?

This is where the trouble starts! Atoms are more like clouds than metal balls. It's easy to measure the diameter of a metal ball, because it doesn't change; the ball is hard. But how do you measure the size of a single cloud that is touching many other clouds? Remember from the nuclear model of the atom that the nucleus is very tiny. Almost all the space in an atom is taken by the electrons in their orbitals, and the orbitals, like clouds, don't have obvious edges; also, they can change size and shape when other atoms are nearby because of Coulomb forces from other nuclei and electrons. We usually measure the size of atoms using **X-ray crystallography**. Basically we shine X-rays on a **crystal** (like a salt crystal or a diamond, a crystal is an orderly arrangement of atoms with sharp, straight edges). The X-rays interact with the electrons in the crystal, and the picture we get from the X-rays can tell us the electron density at each point in the crystal. Most atoms have lots of electron density because they have 6 or more electrons. We can see how far apart these electron density peaks are, and that tells us where the atoms are. Then we guess their size based on how far away they are from each other. I say "guess" because the distance between atoms depends on whether they are bonding or not bonding, etc. So the size depends on the type of environment we look at. We can't look at all types of atoms in the same environment because they have different bonding properties, but by looking at lots of different situations we can see some general trends.



An illustration of x-ray crystallography with constructive, left, and destructive, right, wave interference.

Predicting Relative Sizes

Because electrons are what take up space in atoms, the result is that the size of the biggest filled orbital determines the size of the atom or ion. Sizes of orbitals depend on the quantum numbers ($n = 1, n = 3$, etc.) and also on the effective nuclear charge. An orbital of any type will get smaller as the effective nuclear charge gets bigger, because the attraction to the nucleus is greater. As you go down the periodic table, usually atoms get bigger because n gets bigger (there are electrons in higher shells). Effective nuclear charge does get bigger too going down the periodic table, but this effect is smaller than the change in shell. As you go left across the periodic table, the effective nuclear charge increases. The number of electrons also increases, but they are usually in the same shell or subshell, so the effective nuclear charge increase is more important, and the atoms or ions get smaller going left. There are many exceptions, but for now bigger to the right and down is what you should remember.



A simple illustration of the trend for atomic radii across the periodic table.

The sizes of ions follow a simple pattern. When you remove electrons, making cations, there are less electrons and less electron-electron repulsions, so the cation is smaller than the atom. The more electrons you take off, the smaller it gets. Anions are the opposite. When you add electrons, they repel each other, and there are more of them, so anions are bigger than atoms, and get bigger as you add electrons. You can combine these patterns with the general pattern for atoms to predict relative size of ions.

In general, to predict relative sizes, ask: How many electrons? What shell? What effective nuclear charge? Find the differences between the particles you are comparing, and see what effect the differences should have.

Check out the Atomic Radii for yourself!

Go to [Ptable's](#) radius page, and look at the radii. Try selecting different types of radii, like calculated, empirical, covalent, and Van der Waals. Notice that some types of radii only have data for some elements, and that the patterns change a little depending on how you measure.

Outside Link

- [Ionization Energy and Atomic Radii](#) (10 min)

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3.4.7: Slater's Rules for Effective Nuclear Charge

Skills to Develop

- Describe how to calculate the shielding constant using Slater's rules
- Identify a periodic trend for effective nuclear charge
- Calculate effective nuclear charge

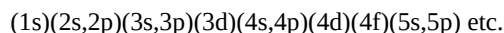
Effective nuclear charge is really important, because it determines the size and energy of orbitals, which determine most properties of atoms. So it's useful to be able to predict effective nuclear charge! Slater's rules give a simple approximation of effective nuclear charge that works pretty well.

Based on the last section, we can expect that effective nuclear charge will depend on the number of electrons that might get between, so it depends on the electron we are looking at. For any electron, to find the effective nuclear charge it feels, we need to know how many other electrons might get in the way, and how much time it spends near the nucleus. Based on these, we will calculate a **shielding constant**, S . Then,

$$Z_{\text{eff}} = Z - S \quad (3.4.7.1)$$

where Z is the actual nuclear charge (which is the same as the atomic number) and Z_{eff} is the effective nuclear charge.

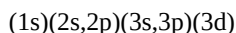
To calculate S , we will write out all the electrons in atom until we get to the group of the electron we want, like this:



1. Each other electron (not counting the one we have picked) in the same group () as the chosen electron, contributes 0.35 to S . (This means electrons in the same group shield each other 35%.)
2. If the chosen electron is d or f, every electron in groups to the left contributes 1.00 to S . (This means that d and f electrons are shielded 100% by electrons with lower n or same n and lower ℓ .)
3. If the chosen electron is s or p, all the electrons in the next lower shell ($n - 1$) contribute 0.85 to S . (This means that s and p electrons are shielded 85% by the electrons one shell lower.) And all the electrons in even lower shells contribute 1.00 to S . (All electrons in shells $n - 2$ or lower shield 100%.)

The outcome of this is that Z_{eff} changes suddenly when going from one period to another. As you go from Li to Be, Z_{eff} (for the new electron) increases, because you add one proton ($Z + 1$) and it is only shielded 35% ($S + 0.35$). When you get to B, you added one proton, and it still shields 35%. So Z_{eff} increases until you go from Ne to Na. Now, suddenly, the (1s) electrons shield 100% instead of 85%, and the (2s,2p) shield 85% instead of 35%! So Z_{eff} goes down suddenly. From Na to Ar, Z_{eff} increases slowly again. From Ar to K, it drops again.

For an example, let's calculate Z_{eff} for a d electron in Zn, atomic number 30. Notice that although 4s is filled, we don't include it because it comes to the right of the d electrons we are looking at.



$$S = 18(1) + 9(0.35) = 21.15 \quad (3.4.7.2)$$

$$Z_{\text{eff}} = 31 - 26 = 5 \quad (3.4.7.3)$$

You can see that just like changing periods (going to a new shell), going from the d-block to the p-block also gives a drop in Z_{eff} (partly because you actually are going to a new shell, as well as subshell).

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