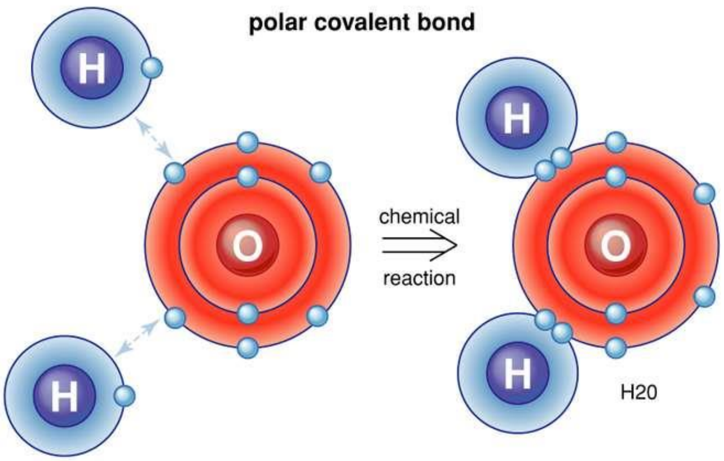
Covalent bond

Covalent bond, in chemistry, the interatomic linkage that results from the sharing of an electron pair between two atoms. The binding arises from the electrostatic attraction of their nuclei for the same electrons. A covalent bond forms when the bonded atoms have a lower total energy than that of widely separated atoms.



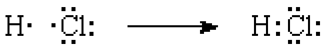
A single line indicates a bond between two atoms (*i.e.*, involving one electron pair), double lines (=) indicate a double bond between two atoms (*i.e.*, involving two electron pairs), and triple lines (≡) represent a triple bond, as found, for example, in carbon monoxide (C≡O). Single bonds consist of one sigma (σ) bond, double bonds have one σ and one pi (π) bond, and triple bonds have one σ and two π bonds.

The idea that two electrons can be shared between two atoms and serve as the link between them was first introduced in 1916 by the American chemist G.N. Lewis, who described the formation of such bonds as resulting from the tendencies of certain atoms to combine with one another in order for both to have the electronic structure of a corresponding noble-gas atom.

Covalent bonds are directional, meaning that atoms so bonded prefer specific orientations relative to one another; this in turn gives molecules definite shapes, as in the angular (bent) structure of the H_2O molecule. Covalent bonds between identical atoms (as in H_2) are nonpolar—*i.e.*, electrically uniform—while those between unlike atoms are polar—*i.e.*, one atom is slightly negatively charged and the other is slightly positively charged. This partial ionic character of covalent bonds increases with the difference in the electronegativities of the two atoms.

Lewis formulation of a covalent bond

In Lewis terms a covalent bond is a shared electron pair. The bond between a hydrogen atom and a chlorine atom in hydrogen chloride is formulated as follows:

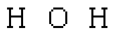


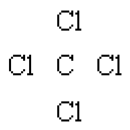
In a Lewis structure of a covalent compound, the shared electron pair between the hydrogen and chlorine ions is represented by a line. The electron pair is called a bonding pair; the three other pairs of electrons on the chlorine atom are called lone pairs and play no direct role in holding the two atoms together.

Each atom in the hydrogen chloride molecule attains a closed-shell octet of electrons by sharing and hence achieves a maximum lowering of energy. In general, an incomplete shell means that some attracting power of a nucleus may be wasted, and adding electrons beyond a closed shell would entail the energetic disadvantage of beginning the next shell of the atom concerned. Lewis's octet rule is again applicable and is seen to represent the extreme means of achieving lower energy rather than being a goal in itself.

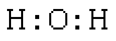
A covalent bond forms if the bonded atoms have a lower total energy than the widely separated atoms. The simplest interpretation of the decrease in energy that occurs when electrons are shared is that both electrons lie between two attracting centres (the nuclei of the two atoms linked by the bond) and hence lie lower in energy than when they experience the attraction of a single centre. This explanation, however, requires considerable modification to capture the full truth about bonding, and it will be discussed further below when bonding is considered in terms of quantum mechanics.

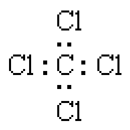
Lewis structures of more complex molecules can be constructed quite simply by extending the process that has been described for hydrogen chloride. First, the valence electrons that are available for bonding are counted (2 × 1 + 6 = 8 in H_2O, for example, and 4 + 4 × 7 = 32 in carbon tetrachloride, CCl_4), and the chemical symbols for the elements





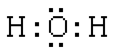
are placed in the arrangement that reflects which are neighbours:

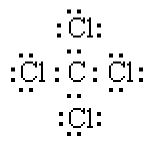




Next, one bonding pair is added between each linked pair of atoms:

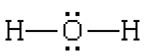
The remaining electrons are then added to the atoms in such a way that each atom has a share in an octet of electrons

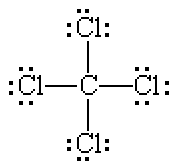




(this is the octet-rule part of the procedure):

Finally, each bonding pair is represented by a dash:





(Note that Lewis structures do not necessarily show the actual shape of the molecule, only the topological pattern of their bonds.)

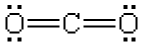
In some older formulations of Lewis structures, a distinction was made between bonds formed by electrons that have been supplied by both atoms (as in H—Cl, where one shared electron can be regarded as supplied by the hydrogen atom and the other by the chlorine atom) and covalent bonds formed when both electrons can be regarded as supplied by one atom, as in the formation of OH^- from O^{2-} and H^+. Such a bond was called a coordinate covalent bond or a dative bond and symbolized $O \rightarrow H^-$. However, the difficulties encountered in the attempt to keep track of the origin of bonding electrons and the suggestion that a coordinate covalent bond differs somehow from a covalent bond (it does not) have led to this usage falling into disfavour.

Advanced aspects of Lewis structures

The Lewis structures illustrated so far have been selected for their simplicity. A number of elaborations are given below.

Multiple bonds

First, an atom may complete its octet by sharing more than one pair of electrons with a bonded neighbour. Two shared pairs of electrons, represented by a double dash (=), form a double bond. Double bonds are found in numerous compounds, including carbon dioxide:

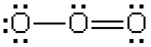


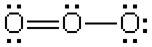
Three shared pairs of electrons are represented by a triple dash (≡) and form a triple bond. Triple bonds are found in, for example, carbon monoxide, nitrogen molecules, and acetylene, shown respectively as:

A double bond is stronger than a single bond, and a triple bond is stronger than a double bond. However, a double bond is not necessarily twice as strong as a single bond, nor is a triple bond necessarily three times as strong. Quadruple bonds, which contain four shared pairs of electrons, are rare but have been identified in some compounds in which two metal atoms are bonded directly together.

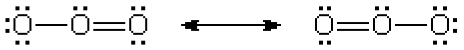
Resonance

There is sometimes an ambiguity in the location of double bonds. This ambiguity is illustrated by the Lewis structure for ozone (O_3). The following are two possible structures:





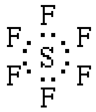
In such cases, the actual Lewis structure is regarded as a blend of these contributions and is written:



The blending together of these structures is actually a quantum mechanical phenomenon called resonance, which will be considered in more detail below. At this stage, resonance can be regarded as a blending process that spreads double-bond character evenly over the atoms that participate in it. In ozone, for instance, each oxygen-oxygen bond is rendered equivalent by resonance, and each one has a mixture of single-bond and double-bond character (as indicated by its length and strength).

Hypervalence

Lewis structures and the octet rule jointly offer a succinct indication of the type of bonding that occurs in molecules and show the pattern of single and multiple bonds between the atoms. There are many compounds, however, that do not conform to the octet rule. The most common exceptions to the octet rule are the so-called hypervalent compounds. These are species in which there are more atoms attached to a central atom than can be accommodated by an octet of electrons. An example is sulfur hexafluoride, SF_6, for which writing a Lewis structure with six S—F bonds requires that at least 12 electrons be present around the sulfur atom:



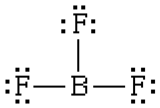
(Only the bonding electrons are shown here.) In Lewis terms, hypervalence requires the expansion of the octet to 10, 12, and even in some cases 16 electrons. Hypervalent compounds are very common and in general are no less stable than compounds that conform to the octet rule.

The existence of hypervalent compounds would appear to deal a severe blow to the validity of the octet rule and Lewis's approach to covalent bonding if the expansion of the octet could not be rationalized or its occurrence predicted. Fortunately, it can be rationalized, and the occurrence of hypervalence can be anticipated. In simple terms, experience has shown that hypervalence is rare in periods 1 and 2 of the periodic table (through neon) but is common in and after period 3. Thus, the octet rule can be used with confidence for carbon, nitrogen, oxygen, and fluorine, but hypervalence must be anticipated thereafter. The conventional explanation of this distinction takes note of the fact that, in period-3 elements, the valence shell has $n = 3$, and this is the first shell in which *d* orbitals are available. (As noted above, these orbitals are occupied after the 4*s* orbitals have been filled and account for the occurrence of the transition metals in period 4.) It is therefore argued that atoms of this and subsequent periods can utilize the empty *d* orbitals to accommodate electrons beyond an octet and hence permit the formation of hypervalent species.

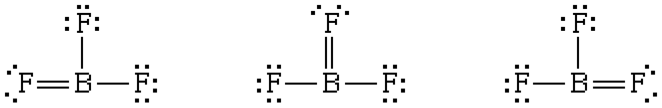
In chemistry, however, it is important not to allow mere correlations to masquerade as explanations. Although it is true that *d* orbitals are energetically accessible in elements that display hypervalence, it does not follow that they are responsible for it. Indeed, quantum mechanical theories of the chemical bond do not need to invoke *d*-orbital involvement. These theories suggest that hypervalence is probably no more than a consequence of the greater radii of the atoms of period-3 elements compared with those of period 2, with the result that a central atom can pack more atoms around itself. Thus, hypervalence is more a steric (geometric) problem than an outcome of *d*-orbital availability. How six atoms can be bonded to a central atom by fewer than six pairs of electrons is discussed below.

Incomplete-octet compounds

Less common than hypervalent compounds, but by no means rare, are species in which an atom does not achieve an octet of electrons. Such compounds are called incomplete-octet compounds. An example is the compound boron trifluoride, BF_3, which is used as an industrial catalyst. The boron (B) atom supplies three valence electrons, and a representation of the compound's structure is:



The boron atom has a share in only six valence electrons. It is possible to write Lewis structures that do satisfy the octet rule.



However, whereas in the incomplete octet structure the fluorine atoms have three lone pairs, in these resonance structures one fluorine atom has only two lone pairs, so it has partly surrendered an electron to the boron atom. This is energetically disadvantageous for such an electronegative element as fluorine (which is in fact the most electronegative element), and the three octet structures turn out to have a higher energy than the incomplete-octet structure. The latter is therefore a better representation of the actual structure of the molecule. Indeed, it is exactly because the BF_3 molecule has an incomplete-octet structure that it is so widely employed as a catalyst, for it can use the vacancies in the valence shell of the boron atom to form bonds to other atoms and thereby facilitate certain chemical reactions.

Electron-deficient compounds

Another type of exception to the Lewis approach to bonding is the existence of compounds that possess too few electrons for a Lewis structure to be written. Such compounds are called electron-deficient compounds. A prime example of an electron-deficient compound is diborane, B_2H_6. This compound requires at least seven bonds to link its eight atoms together, but it has only $2 \times 3 + 6 \times 1 = 12$ valence electrons, which is enough to form only six covalent bonds. Once again, it appears that, as in hypervalent compounds, the existence of electron-deficient compounds signifies that a pair of electrons can bond together more than two atoms. The discussion of the quantum mechanical theory of bonding below shows that this is indeed the case.

A number of exceptions to Lewis's theory of bonding have been catalogued here. It has further deficiencies. For example, the theory is not quantitative and gives no clue to how the strengths of bonds or their lengths can be assessed. In the form in which it has been presented, it also fails to suggest the shapes of molecules. Furthermore, the theory offers no justification for regarding an electron pair as the central feature of a covalent bond. Indeed, there are species that possess bonds that rely on the presence of a single electron. (The one-electron transient species H_2^+ is an example.) Nevertheless, in spite of these difficulties, Lewis's approach to bonding has proved exceptionally useful. It predicts when the octet rule is likely to be valid and when hypervalence can be anticipated, and the occurrence of multiple bonds and the presence of lone pairs of electrons correlate with the chemical properties of a wide variety of species. Lewis's approach is still widely used as a rule of thumb for assessing the structures and properties of covalent species, and modern quantum mechanical theories echo its general content.

The VSEPR Model

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 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.

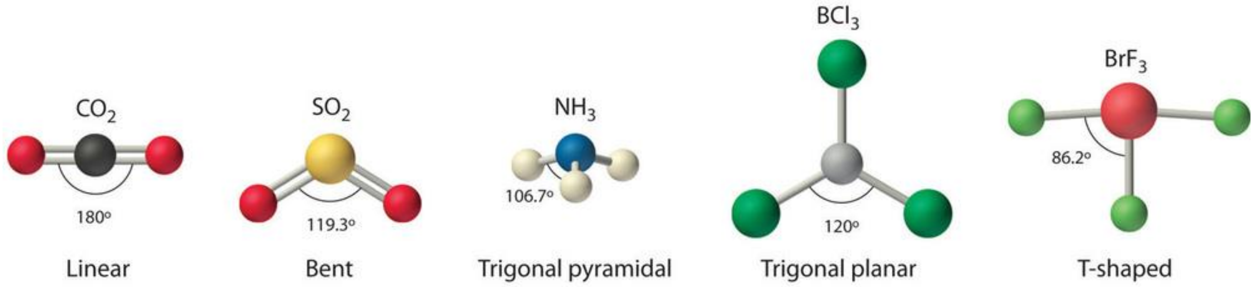
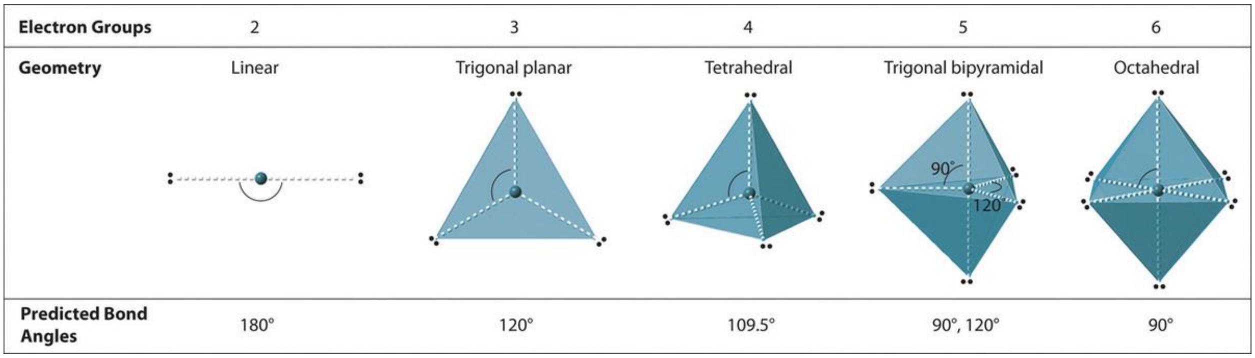


Figure: Common Structures for Molecules and Polyatomic Ions That Consist of a Central Atom Bonded to Two or Three Other Atoms

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



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: 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.

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.

VESPR Produce to predict Molecular geometry

This VESPR procedure is summarized as follows:

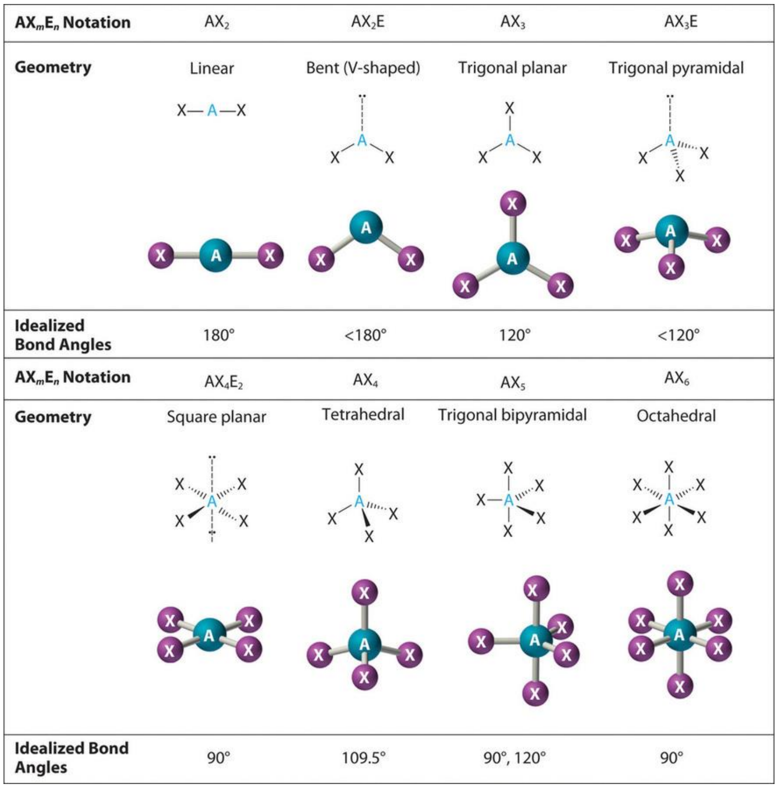
1. Draw the Lewis electron structure of the molecule or polyatomic ion.

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 above and below figures, 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	Bent (V-shaped)	Trigonal planar	Trigonal pyramidal
Idealized Bond Angles	180°	<180°	120°	<120°

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°, 120°	90°

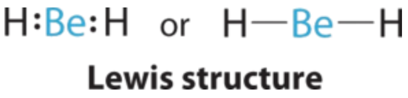
Figure: Common Molecular Geometries for Species with Two to Six Electron Groups. Lone pairs are shown using a dashed line.

Two Electron Groups

Our first example is a molecule with two bonded atoms and no lone pairs of electrons, BeH2BeH2.

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 that the arrangement that minimizes repulsions places the groups 180° apart.

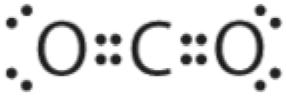


3. Both groups around the central atom are bonding pairs (BP). Thus BeH_2 is designated as AX_2.

4. From Figure we see that with two bonding pairs, the molecular geometry that minimizes repulsions in BeH_2 is *linear.*

AX_2 Molecules: CO_2

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 BeH_2, the arrangement that minimizes repulsions places the groups 180° apart.

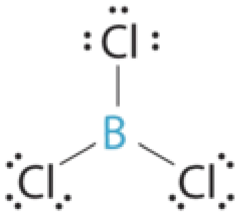
3. Once again, both groups around the central atom are bonding pairs (BP), so CO_2 is designated as AX_2.

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 CO_2 is linear. The structure of CO_2 is shown in Figure.

Three Electron Groups

AX_3 Molecules: BCl_3

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



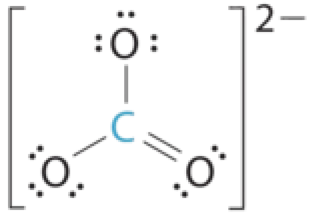
Lewis structure

3. All electron groups are bonding pairs (BP), so the structure is designated as AX_3.

4. From Figure we see that with three bonding pairs around the central atom, the molecular geometry of BCl_3 is *trigonal planar*, as shown in Figure.

AX_3 Molecules: CO_3^{2-}

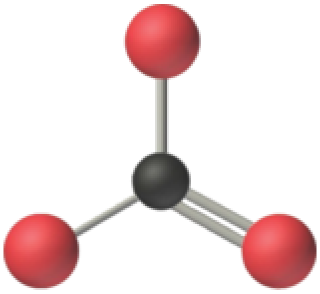
1. The central atom, carbon, has four valence electrons, and each oxygen atom has six valence electrons. As you learned previously, the Lewis electron structure of one of three resonance forms is represented as



Lewis structure

3. All electron groups are bonding pairs (BP). With three bonding groups around the central atom, the structure is designated as AX_3.

4. We see from Figure that the molecular geometry of CO_3^{2-} is trigonal planar with bond angles of 120°.

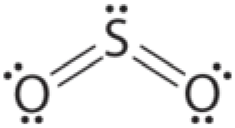


Molecular geometry
(trigonal planar)

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

AX_2E Molecules: SO_2

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.



3. There are two bonding pairs and one lone pair, so the structure is designated as AX_2E. 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. Thus bonding pairs and lone pairs repel each other electrostatically in the order BP–BP < LP–BP < LP–LP. In SO_2, 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. The O-S-O bond angle is expected to be *less than* 120° because of the extra space taken up by the lone pair.

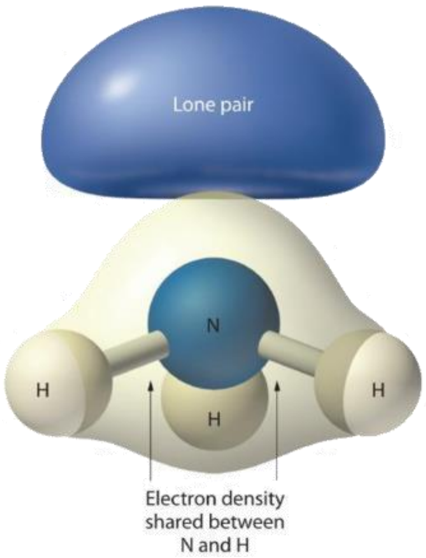
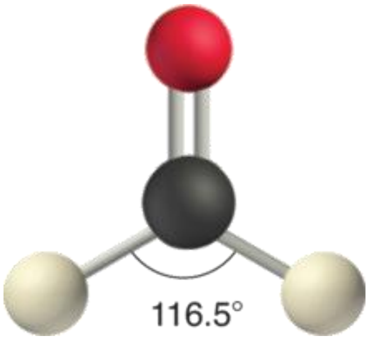


Figure: The Difference in the Space Occupied by a Lone Pair of Electrons and by a Bonding Pair

As with SO_2, 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 CH_2O (AX_3), 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°).

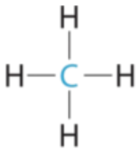


Four Electron Groups

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.

AX_4 Molecules: CH_4

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

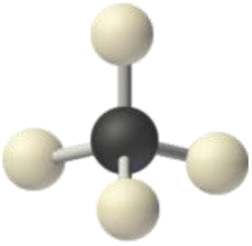


Lewis structure

2. There are four electron groups around the central atom. As shown in Figure, 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 AX_4.

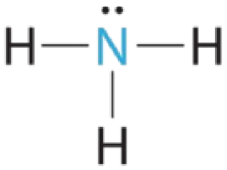
4. With four bonding pairs, the molecular geometry of methane is *tetrahedral*.



Molecular geometry
(tetrahedral)

AX_3E Molecules: NH_3

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

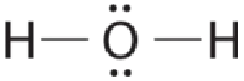
2. There are four electron groups around nitrogen, three bonding pairs and one lone pair. Repulsions are minimized by directing each hydrogen atom and the lone pair to the corners of a tetrahedron.

3. With three bonding pairs and one lone pair, the structure is designated as AX_3E. 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. However, the H–N–H bond angles are less than the ideal angle of 109.5° because of LP–BP repulsions.

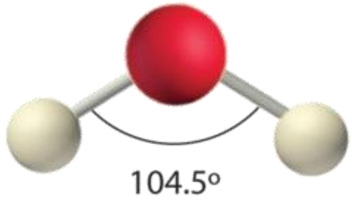
AX_2E_2 Molecules: H_2O

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



2. With two bonding pairs and two lone pairs, the structure is designated as AX_2E_2 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.

3. 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 NH_3, 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.

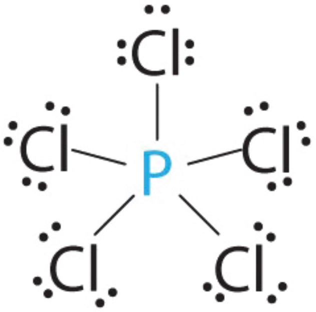


Five Electron Groups

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.

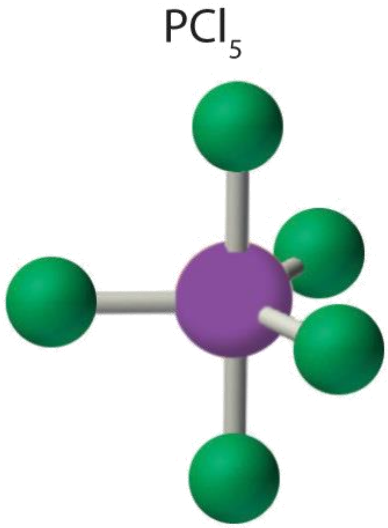
AX_5 Molecules: PCl_5

1. Phosphorus has five valence electrons and each chlorine has seven valence electrons, so the Lewis electron structure of PCl_5 is



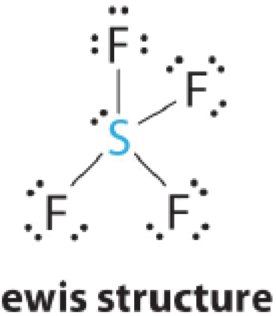
2. All electron groups are bonding pairs, so the structure is designated as AX_5. There are no lone pair interactions.

3. The molecular geometry of PCl_5 is *trigonal bipyramidal*, as shown in Figure. 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.



AX$_4$E Molecules: SF$_4$

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



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.

3. We designate SF$_4$ as AX$_4$E; 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.

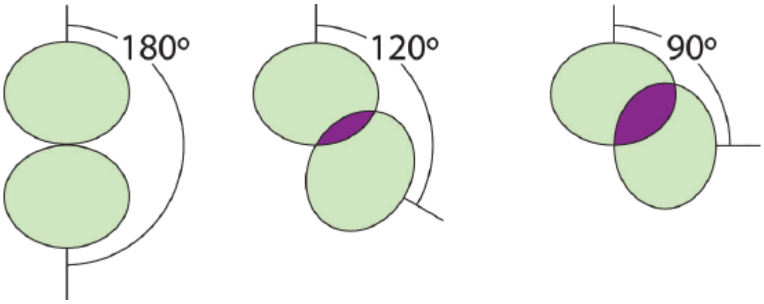
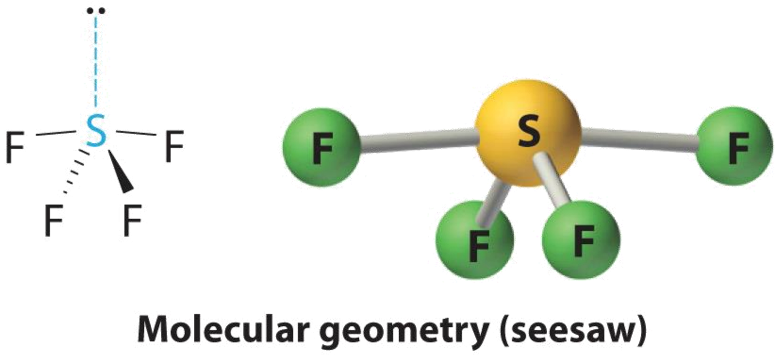


Figure: Illustration of the Area Shared by Two Electron Pairs versus the Angle between Them

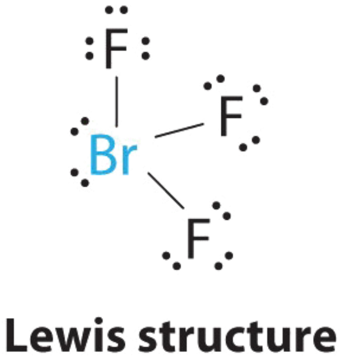
At 90°, the two electron pairs share a relatively large region of space, which leads to strong repulsive electron–electron interactions.

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.



AX_3E_2 Molecules: BrF_3

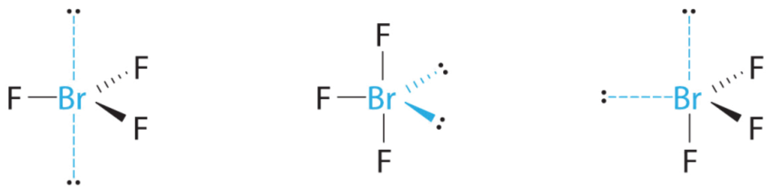
1. The bromine atom has seven valence electrons, and each fluorine has seven valence electrons, so the Lewis electron structure is



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 AX_3E_2 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°:



Lone pairs axial (a) **Lone pairs equatorial** (b) **Lone pairs axial and equatorial** (c)

Interactions			
90° LP–LP	0	0	1
90° LP–BP	6	4	3

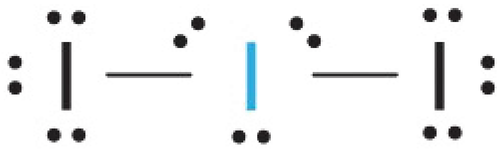
Structure (c) can be eliminated because it has a LP–LP interaction at 90°. Structure (b), with fewer LP–BP repulsions at 90° than (a), is lower in energy. However, we predict a deviation in bond angles because of the presence of the two lone pairs of electrons.

4. The three nuclei in BrF_3 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.

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.

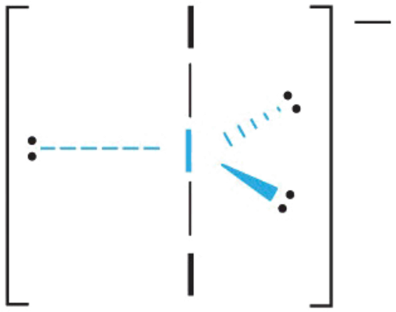
AX_2E_3 Molecules: I_3^-

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



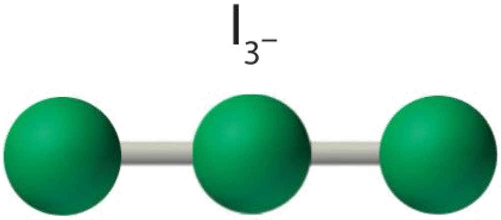
2. There are five electron groups about the central atom in I_3^-, two bonding pairs and three lone pairs. To minimize repulsions, the groups are directed to the corners of a trigonal bipyramid.

3. With two bonding pairs and three lone pairs, I_3^- has a total of five electron pairs and is designated as AX_2E_3. 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 I_3^- 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.

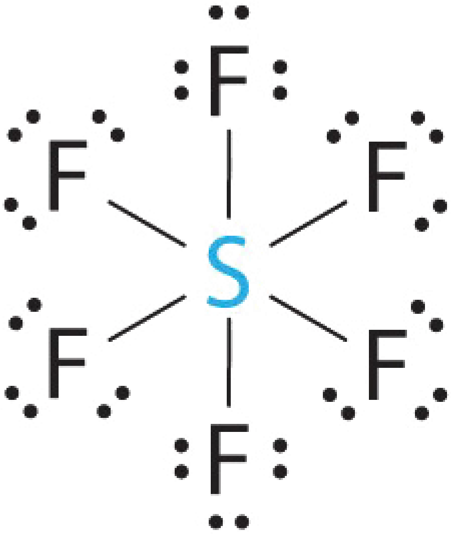


Six Electron Groups

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

AX_6 Molecules: SF_6

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



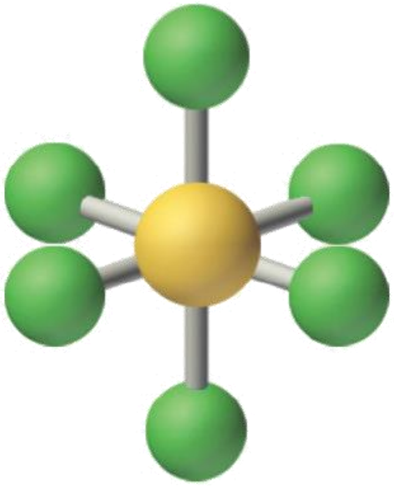
Lewis structure

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 that the geometry that minimizes repulsions is *octahedral*.

3. With only bonding pairs, SF_6 is designated as AX_6. All positions are chemically equivalent, so all electronic interactions are equivalent.

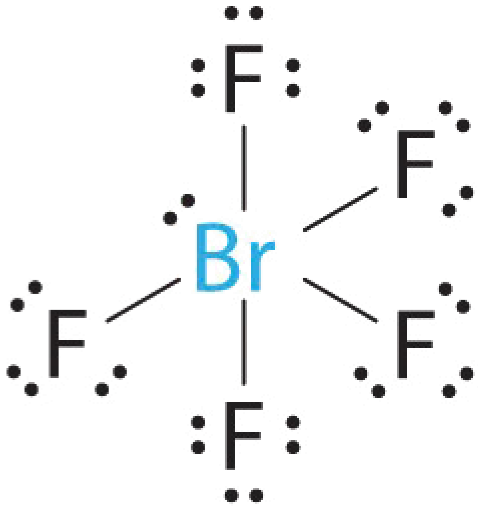
4. There are six nuclei, so the molecular geometry of SF_6 is octahedral.



Molecular geometry (octahedral)

AX_5E Molecules: BrF_5

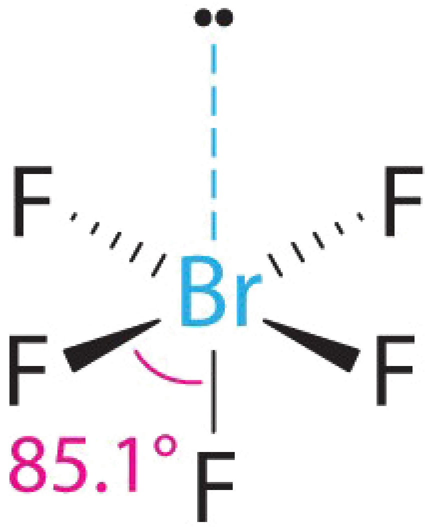
1. The central atom, bromine, has seven valence electrons, as does each fluorine, so the Lewis electron structure is



Lewis structure

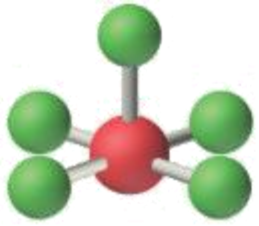
With its expanded valence, this species is an exception to the octet rule.

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 F_{axial}–Br–$F_{equatorial}$ angles to be less than 90° because of the lone pair of electrons, which occupies more space than the bonding electron pairs.

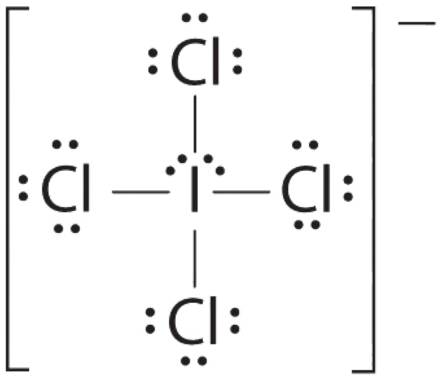
4. With five nuclei surrounding the central atom, the molecular structure is based on an octahedron with a vertex missing. This molecular structure is *square pyramidal*. The F_{axial}–B–$F_{equatorial}$ angles are 85.1°, less than 90° because of LP–BP repulsions.



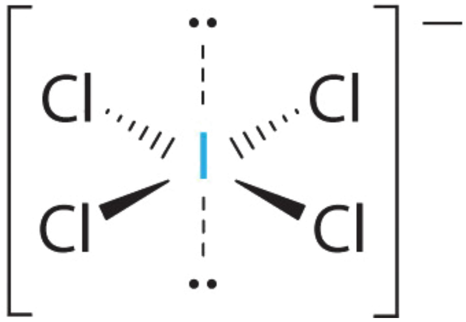
Molecular geometry (square pyramidal)

AX_4E_2 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

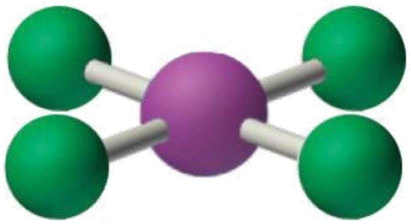


2. There are six electron groups around the central atom, four bonding pairs and two lone pairs. The structure that minimizes LP–LP, LP–BP, and BP–BP repulsions is



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

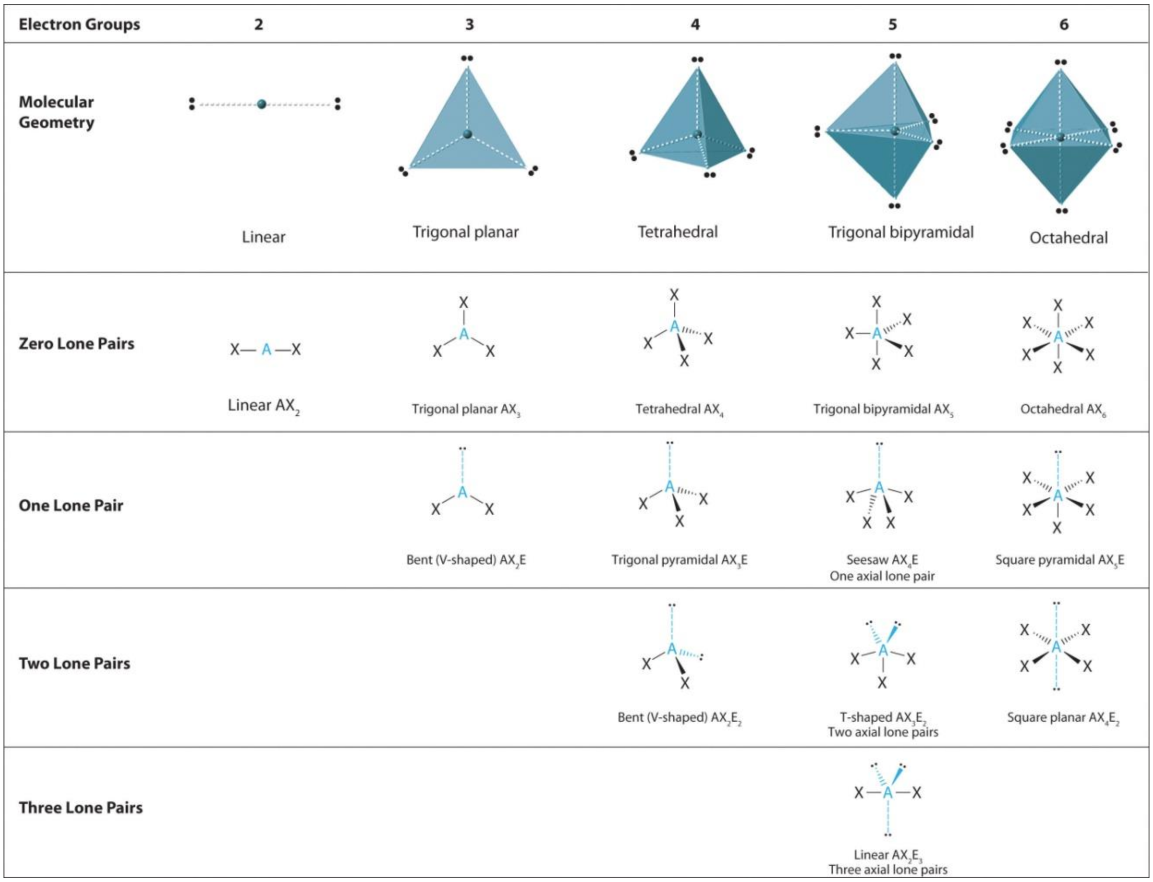


Figure: *Overview of Molecular Geometries*

Example

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

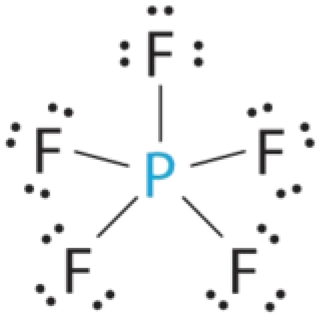
Asked for: molecular geometry

Strategy:

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

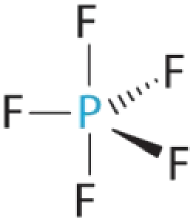
Solution:

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

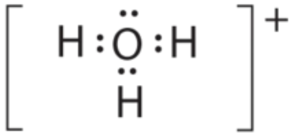


C All electron groups are bonding pairs, so PF_5 is designated as AX_5. Notice that this gives a total of five electron pairs. With no lone pair repulsions, we do not expect any bond angles to deviate from the ideal.

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



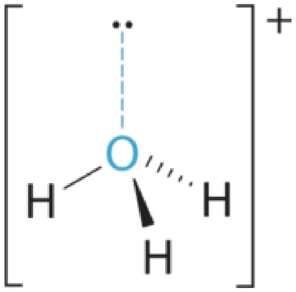
2. **A** The central atom, O, has six valence electrons, and each H atom contributes one valence electron. Subtracting one electron for the positive charge gives a total of eight valence electrons, so the Lewis electron structure is



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:



Limitations of the VSEPR model

The VSEPR theory is simple yet powerful. Nevertheless, like any simplified model, it has its limitations. First, although it predicts that the bond angle in H_2O is less than the tetrahedral angle, it does not make any attempt to predict the magnitude of the decrease. Second, the theory makes no predictions about the lengths of the bonds, which is another aspect of the shape of a molecule. Third, it ascribes the entire criterion of shape to electrostatic repulsions between bonding pairs, when in fact there are numerous contributions to the total energy of a molecule, and electrostatic effects are not necessarily the dominant ones. Fourth, the theory relies on some vague concepts, such as the difference in repelling effects of lone pairs and bonding pairs. There also are some species for which VSEPR theory fails. Nevertheless, despite these limitations and uncertainties, VSEPR theory is a useful rule of thumb and can be used with reasonable confidence for numerous species.

Orbital hybridization

The observation of molecules in the various electronic shapes shown above is, at first blush, in conflict with our picture of atomic orbitals. For an atom such as oxygen, we know that the 2s orbital is spherical, and that the $2p_x$, $2p_y$, and $2p_z$ orbitals are dumbell-shaped and point along the Cartesian axes. The water molecule contains two hydrogen atoms bound to oxygen not at a 90° angle, but at an angle of 104.5°. Given the relative orientations of the atomic orbitals, how do we arrive at angles between electron domains of 104.5°, 120°, and so on? To understand this we will need to learn a little bit about the quantum mechanics of electrons in atoms and molecules.

The atomic orbitals ψ represent solutions to the **Schrödinger wave equation**,

$E\psi=H\hat{}\psi(1.3.1)$

Here E is the energy of an electron in the orbital, and H^H^ is the Hamiltonian operator.

Orbital hybridization involves making *linear combinations* of the atomic orbitals that are solutions to the Schrödinger equation. Mathematically, this is justified by recognizing that the Schrödinger equation is a *linear* differential equation. As such, any sum of solutions to the Schrödinger equation is also a valid solution. However, we still impose the constraint that our hybrid orbitals must be **orthogonal** and **normalized**.

Rules for orbital hybridization:

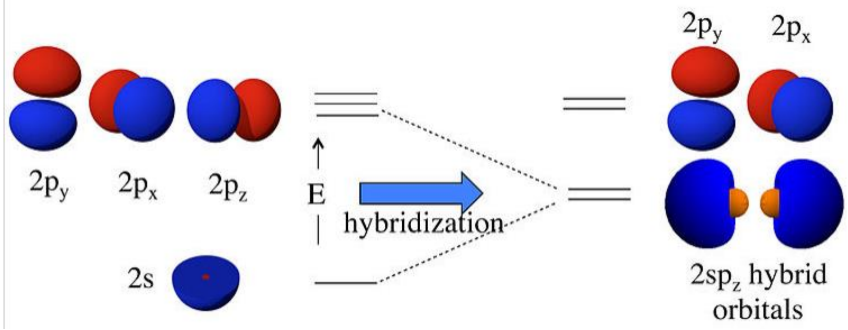
- Add and subtract atomic orbitals to get hybrid orbitals.
- We get the same number of orbitals out as we put in.
- The energy of a hybrid orbital is the weighted average of the atomic orbitals that make it up.
- The coefficients are determined by the constraints that the hybrid orbitals must be orthogonal and normalized.

For **sp hybridization**, as in the BeF_2 or CO_2 molecule, we make two linear combinations of the 2s and $2p_z$ orbitals (assigning z as the axis of the Be-F bond):

$$\psi_1=1/\sqrt{2}(2s)+1/\sqrt{2}(2p_z)$$

$$\psi_2=1/\sqrt{2}(2s)-1/\sqrt{2}(2p_z)$$

What this means physically is explained in the figure below. By combining the 2s and $2p_z$ orbitals we have created two new orbitals with large lobes (high electron probability) pointing along the z-axis. These two orbitals are degenerate and have an energy that is halfway between the energy of the 2s and $2p_z$ orbitals.



Linear combinations of the 2s and $2p_z$ atomic orbitals make two $2sp_z$ hybrids. The $2p_x$and $2p_y$ orbitals are unchanged.

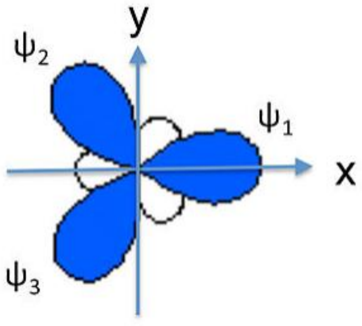
For an isolated Be atom, which has two valence electrons, the lowest energy state would have two electrons spin-paired in the 2s orbital. However, these electrons would not be available for bonding. By **promoting** these electrons to the degenerate $2sp_z$ hybrid orbitals, they become unpaired and are prepared for bonding to the F atoms in BeF_2. This will occur if the **bonding energy** (in the promoted state) exceeds the promotion energy. The **overall bonding energy**, i.e., the energy released by combining a Be atom in its ground state with two F atoms, is the difference between the bonding and promotion energies.

We can similarly construct **sp^2 hybrids** (e.g., for the BF_3 molecule or the NO_3^- anion) from one 2s and two 2p atomic orbitals. Taking the plane of the molecule as the xy plane, we obtain three hybrid orbitals at 120° to each other. The three hybrids are:

$$\psi_1=1/\sqrt{3}(2s)+\sqrt{2}/\sqrt{3}(2p_x)$$

$$\psi_2=1/\sqrt{3}(2s)-1/\sqrt{6}(2p_x)+1/\sqrt{2}(2p_y)$$

$$\psi_3=1/\sqrt{3}(2s)-1/\sqrt{6}(2p_x)-1/\sqrt{2}(2p_y)$$



These orbitals are again degenerate and their energy is the weighted average of the energies of the 2s, $2p_x$, and $2p_y$ atomic orbitals.

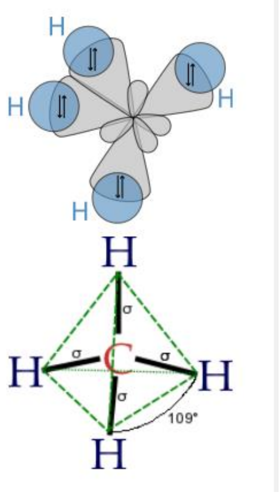
Finally, to make a sp^3 hybrid, as in CH_4, H_2O, etc., we combine all four atomic orbitals to make four degenerate hybrids:

$$\psi_1=1/2(2s+2p_x+2p_y+2p_z)$$

$$\psi_2=1/2(2s-2p_x-2p_y+2p_z)$$

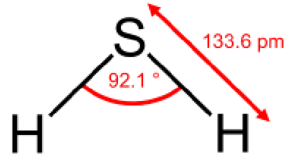
$$\psi_3=1/2(2s+2p_x-2p_y-2p_z)$$

$$\psi_4=1/2(2s-2p_x+2p_y-2p_z)$$



The lobes of the **sp^3 hybrid** orbitals point towards the vertices of a tetrahedron (or alternate corners of a cube), consistent with the tetrahedral bond angle in CH_4 and the nearly tetrahedral angles in NH_3 and H_2O. Similarly, we can show that we can construct the trigonal bipyramidal electronic shape by making sp and sp^2 hybrids, and the octahedral geometry from three sets of sp hybrids. The picture that emerges from this is that the atomic orbitals can hybridize as required by the shape that best minimizes electron pair repulsions.

Interestingly however, the bond angles in PH_3, H_2S and H_2Se are close to 90°, suggesting that P, S, and Se primarily use their p-orbitals in bonding to H in these molecules. This is consistent with the fact that the energy difference between s and p orbitals stays roughly constant going down the periodic table, but the bond energy *decreases* as the valence electrons get farther away from the nucleus. In compounds of elements in the 3rd, 4th, and 5th rows of the periodic table, there thus is a *decreasing tendency to use s-p orbital hybrids in bonding*. For these heavier elements, the bonding energy is not enough to offset the energy needed to promote the s electrons to s-p hybrid orbitals.



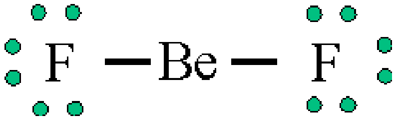
Prediction of Structure using VSEPR theory and Hybridization:

For polyatomic molecules we would like to be able to explain:

- The number of bonds formed
- Their geometries

sp Hybrid Orbitals

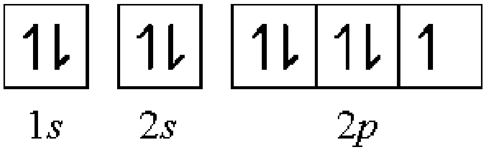
Consider the Lewis structure of gaseous molecules of BeF_2:



- The VSEPR model predicts this structure will be linear
- What would **valence bond theory** predict about the structure?

The fluorine atom electron configuration:

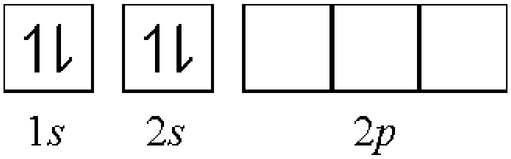
- $1s^2 2s^2 2p^5$



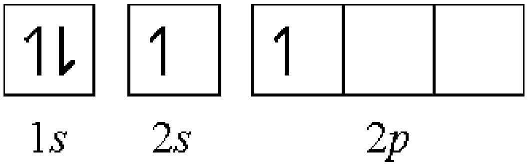
- There is an unpaired electron in a 2p orbital
- This unpaired 2p electron can be paired with an unpaired electron in the Be atom to form a covalent bond

The Be atom electron configuration:

- $1s^2 2s^2$



- In the ground state, there are no unpaired electrons (the Be atom is incapable of forming a covalent bond with a fluorine atom
- However, the Be atom could obtain an unpaired electron by promoting an electron from the 2s orbital to the 2p orbital:

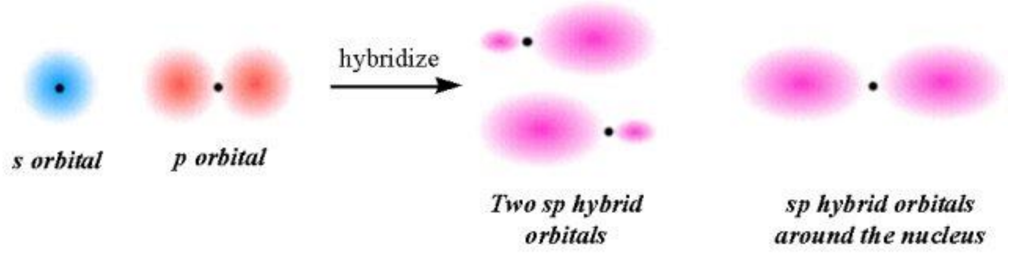


This would actually result in <u>two</u> unpaired electrons, one in a 2s orbital and another in a 2p orbital

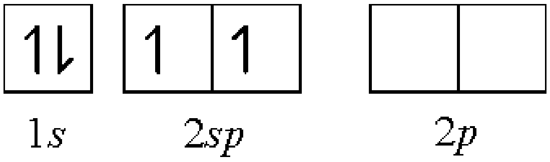
- The Be atom can now form two covalent bonds with fluorine atoms
- We would <u>not</u> expect these bonds to be identical (one is with a 2s electron orbital, the other is with a 2p electron orbital)

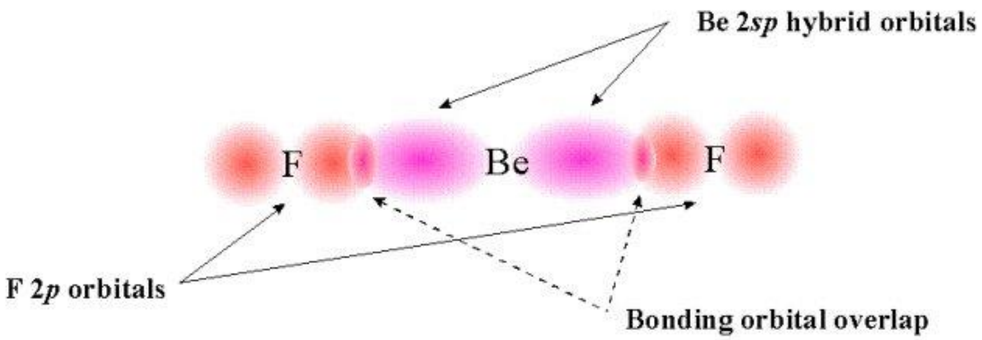
However, the structure of BeF_2 is linear and the bond lengths are identical

- We can combine wavefunctions for the 2s and 2p electrons to produce a "hybrid" orbital for both electrons
- This hybrid orbital is an "sp" hybrid orbital



- The orbital diagram for this hybridization would be represented as:





Note:

- The Be 2sp orbitals are identical and oriented 180° from one another (i.e. bond lengths will be identical and the molecule linear)
- The promotion of a Be 2s electron to a 2p orbital to allow sp hybrid orbital formation **requires energy**.
    - The elongated sp hybrid orbitals have one large lobe which can overlap (bond) with another atom more effectively
    - This produces a stronger bond (higher bond energy) which offsets the energy required to promote the 2s electron

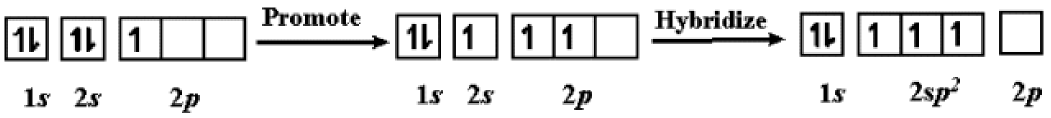
sp^2 and sp^3 Hybrid Orbitals

Whenever orbitals are mixed (hybridized):

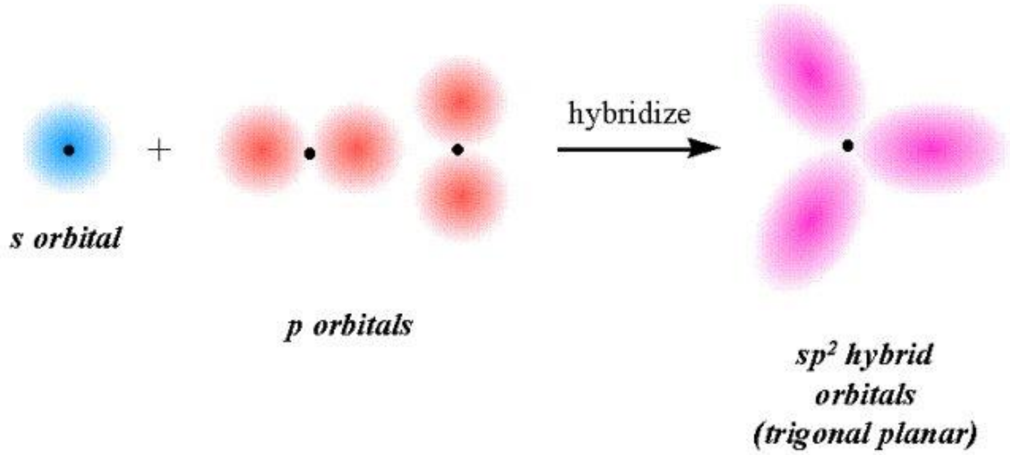
- The number of hybrid orbitals produced **is equal to the sum of the orbitals being hybridized**
- Each hybrid orbital is identical **except that they are oriented in different directions**

BF$_3$

Boron electron configuration:



- The three sp^2 hybrid orbitals have a trigonal planar arrangement to minimize electron repulsion

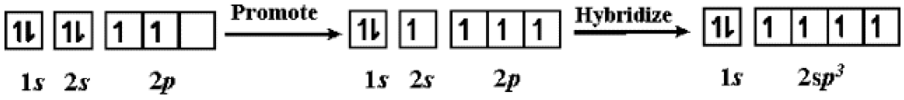


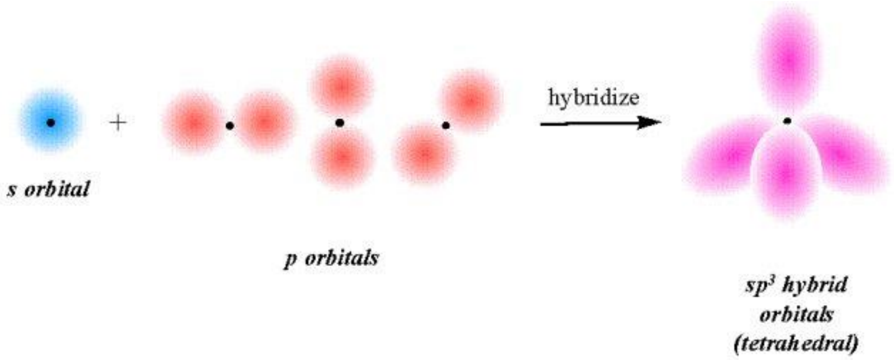
Note:

sp^2 refers to a hybrid orbital being constructed from one s orbital and two p orbitals. Although it looks like an electron configuration notation, the superscript '2' DOES NOT refer to the number of electrons in an orbital.

- An s orbital can also mix with all 3 p orbitals in the same subshell

CH_4





- Thus, using **valence bond theory**, we would describe the bonds in methane as follows: each of the carbon sp^3 hybrid orbitals can overlap with the 1s orbitals of a hydrogen atom to form a bonding pair of electrons

Note:

sp^3 refers to a hybrid orbital being constructed from one s orbital and three p orbitals. Although it looks like an electron configuration notation, the superscript '3' DOES NOT refer to the number of electrons in an orbital.

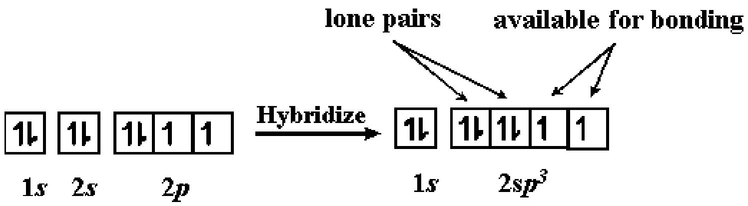
The two steps often observed when constructing hybrid orbitals is to

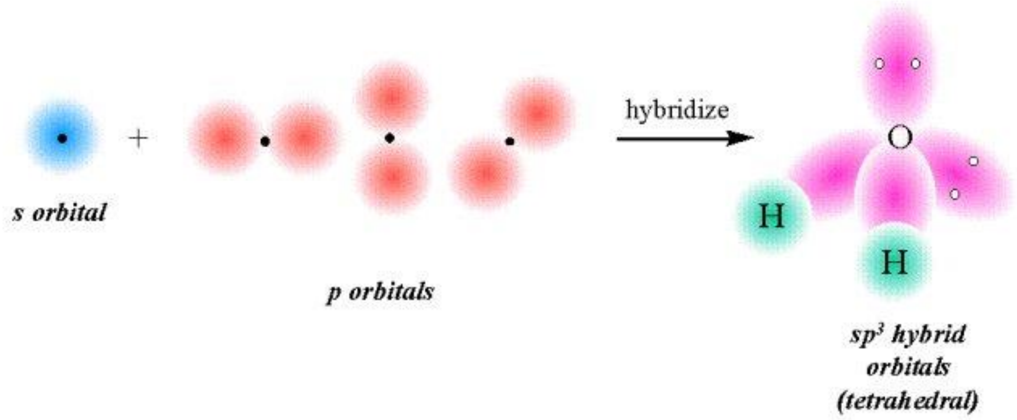
Note:

promote a valence electron from the ground state configuration to a higher energy orbital, and then hybridize the appropriate valence electron orbitals to achieve the desired valence electron geometry (i.e. the correct number of hybrid orbitals for the appropriate valence electron geometry)

H_2O

Oxygen

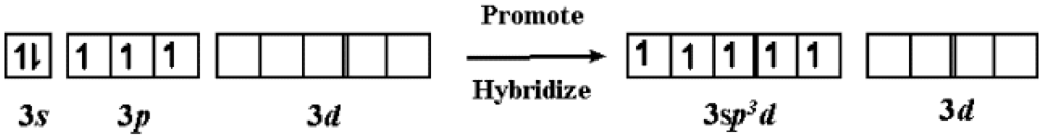


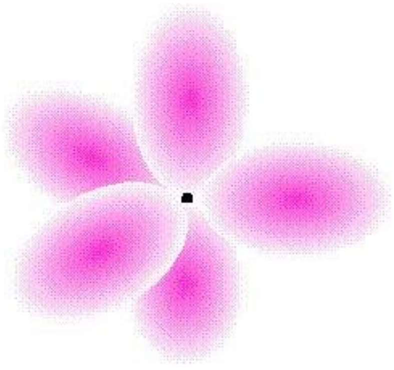


Hybridization Involving *d* Orbitals

Atoms in the third period and higher can utilize *d* orbitals to form hybrid orbitals

PF_5





Trigonal Bipyramidal

Similarly hybridizing one s, three p and two d orbitals yields six identical hybrid **sp^3d^2** orbitals. These would be oriented in an **octahedral geometry**.

- Hybrid orbitals allows us to use **valence bond theory** to describe covalent bonds (sharing of electrons in overlapping orbitals of two atoms)
- When we know the molecular geometry, we can use the concept of hybridization to describe the electronic orbitals used by the central atom in bonding

Steps in predicting the hybrid orbitals used by an atom in bonding:

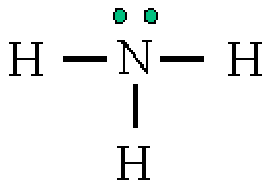
1. Draw the Lewis structure

2. Determine the electron pair geometry using the VSEPR model

3. Specify the hybrid orbitals needed to accommodate the electron pairs in the geometric arrangement

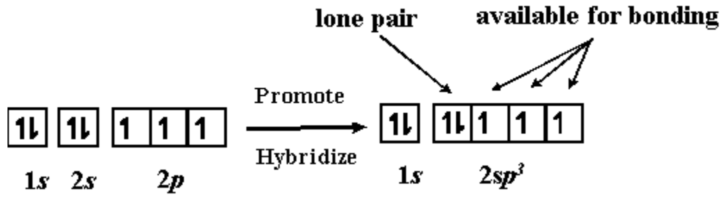
NH_3

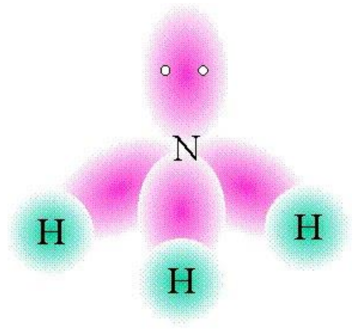
1. **Lewis structure**



2. **VSEPR** indicates ***tetrahedral geometry*** with one non-bonding pair of electrons (structure itself will be ***trigonal pyramidal***)

3. Tetrahedral arrangement indicates four equivalent electron orbitals





sp^3 hybrid orbitals (tetrahedral)

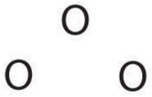
Valence Electron Pair Geometry	**Number of Orbitals**	**Hybrid Orbitals**
Linear	2	*sp*
Trigonal Planar	3	sp^2
Tetrahedral	4	sp^3
Trigonal Bipyramidal	5	sp^3d
Octahedral	6	sp^3d^2

Resonance:

Resonance is a mental exercise within the Valence Bond Theory of bonding that describes the delocalization of electrons within molecules. It involves constructing multiple Lewis structures that, when combined, represent the full electronic structure of the molecule. **Resonance structures** are used when a single Lewis structure cannot fully describe the bonding; the combination of possible resonance structures is defined as a **resonance hybrid**, which represents the overall delocalization of electrons within the molecule. In general, molecules with multiple resonance structures will be more stable than one with fewer and some resonance structures contribute more to the stability of the molecule than others - formal charges aid in determining this.

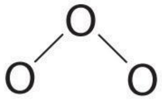
Resonance is a way of describing delocalized electrons within certain molecules or polyatomic ions where the bonding cannot be expressed by a single Lewis formula. A molecule or ion with such delocalized electrons is represented by several resonance structures. The nuclear skeleton of the Lewis Structure of these resonance structures remains the same, only the electron locations differ. Such is the case for ozone (O3O3), an allotrope of oxygen with a V-shaped structure and an O–O–O angle of 117.5°. Let's motivate the discussion by building the Lewis structure for ozone.

1. We know that ozone has a V-shaped structure, so one O atom is central:



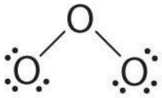
2. Each O atom has 6 valence electrons, for a total of 18 valence electrons.

3. Assigning one bonding pair of electrons to each oxygen–oxygen bond gives



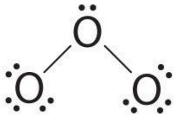
with 14 electrons left over.

4. If we place three lone pairs of electrons on each terminal oxygen, we obtain



and have 2 electrons left over.

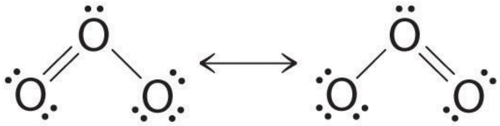
5. At this point, both terminal oxygen atoms have octets of electrons. We therefore place the last 2 electrons on the central atom:



6. The central oxygen has only 6 electrons. We must convert one lone pair on a terminal oxygen atom to a bonding pair of electrons—but which one? Depending on which one we choose, we obtain either

Which is correct? In fact, neither is correct. Both predict one O–O single bond and one O=O double bond. As you will learn, if the bonds were of different types (one single and one double, for example), they would have different lengths. It turns out, however, that both O–O bond distances are identical, 127.2 pm, which is shorter than a typical O–O single bond (148 pm) and longer than the O=O double bond in O_2 (120.7 pm).

Equivalent Lewis dot structures, such as those of ozone, are called **resonance structures**. The position of the *atoms* is the same in the various resonance structures of a compound, but the position of the *electrons* is different. Double-headed arrows link the different resonance structures of a compound:



The double-headed arrow indicates that the actual electronic structure is an *average* of those shown, not that the molecule oscillates between the two structures.

When it is possible to write more than one equivalent resonance structure for a molecule or ion, the actual structure is the average of the resonance structures.

The electrons appear to "shift" between different resonance structures and while not strictly correct as each resonance structure is just a limitation of using the Lewis structure perspective to describe these molecules. A more accurate description of the electron structure of the molecule requires considering multiple resonance structures simultaneously.

DELOCALIZATION AND RESONANCE STRUCTURES RULES

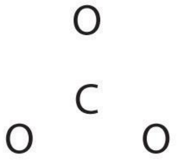
1. Resonance structures should have the same number of electrons, do not add or subtract any electrons. (check the number of electrons by simply counting them).
2. Each resonance structures follows the rules of writing Lewis Structures.
3. The hybridization of the structure must stay the same.
4. The skeleton of the structure can not be changed (only the electrons move).
5. Resonance structures must also have the same number of lone pairs.

Example:

Identify the resonance structures for the carbonate ion: CO_3^{2-} .

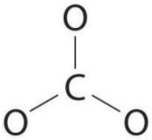
Solution

1. Because carbon is the least electronegative element, we place it in the central position:

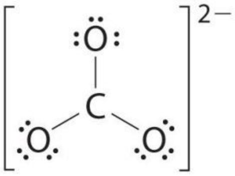


2. Carbon has 4 valence electrons, each oxygen has 6 valence electrons, and there are 2 more for the −2 charge. This gives 4 + (3 × 6) + 2 = 24 valence electrons.

3. Six electrons are used to form three bonding pairs between the oxygen atoms and the carbon:

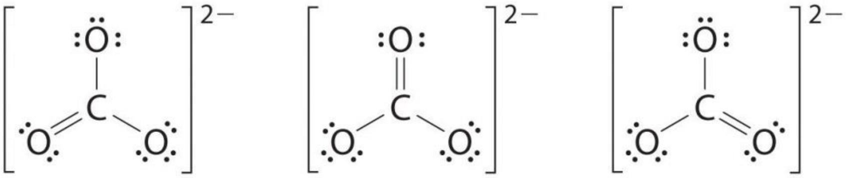


4. We divide the remaining 18 electrons equally among the three oxygen atoms by placing three lone pairs on each and indicating the −2 charge:

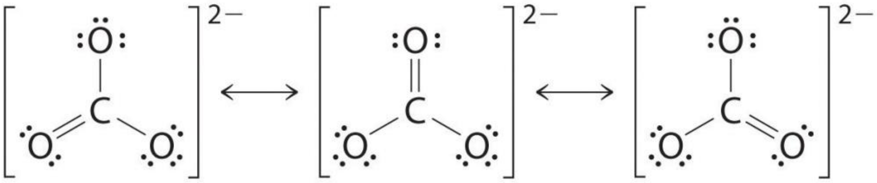


5. No electrons are left for the central atom.

6. At this point, the carbon atom has only 6 valence electrons, so we must take one lone pair from an oxygen and use it to form a carbon–oxygen double bond. In this case, however, there are *three* possible choices:



As with ozone, none of these structures describes the bonding exactly. Each predicts one carbon–oxygen double bond and two carbon–oxygen single bonds, but experimentally all C–O bond lengths are identical. We can write resonance structures (in this case, three of them) for the carbonate ion:



The actual structure is an average of these three resonance structures.

Like ozone, the electronic structure of the carbonate ion cannot be described by a single Lewis electron structure. Unlike O_3, though, the actual structure of CO_3^{2-} is an average of *three* resonance structures.

Using Formal Charges to Identify viable Resonance Structures

While each resonance structure contributes to the total electronic structure of the molecule, they may not contribute equally. Assigning Formal charges to atoms in the molecules is one mechanism to identify the viability of a resonance structure and determine its relative magnitude among other structures. The formal charge on an atom in a covalent species is the net charge the atom would bear if the electrons in all the bonds to the atom were equally shared. Alternatively the formal charge on an atom in a covalent species is the net charge the atom would bear if all bonds to the atom were nonpolar covalent bonds. To determine the formal charge on a given atom in a covalent species, use the following formula:

Formal Charge=(number of valence electrons in free orbital)−(number of lone-pair electrons)−1/2(number bond pair electrons)

RULES FOR ESTIMATING STABILITY OF RESONANCE STRUCTURES

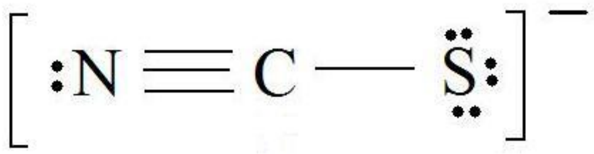
1. The **greater the number of covalent bonds**, the greater the stability since more atoms will have complete octets
2. The structure with the **least number of formal charges** is more stable
3. The structure with the **least separation of formal charge** is more stable
4. A structure with a **negative charge on the more electronegative atom** will be more stable
5. **Positive charges on the least electronegative atom** (most electropositive) is more stable
6. Resonance forms that are equivalent have no difference in stability and contribute equally (eg. benzene)

EXAMPLE : THIOCYANATE ION

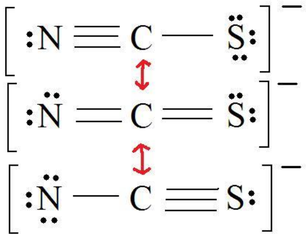
Consider the thiocyanate (CNS−CNS−) ion.

Solution

1. Find the Lewis Structure of the molecule. (Remember the Lewis Structure rules.)



2. Resonance: All elements want an octet, and we can do that in multiple ways by moving the terminal atom's electrons around (bonds too).

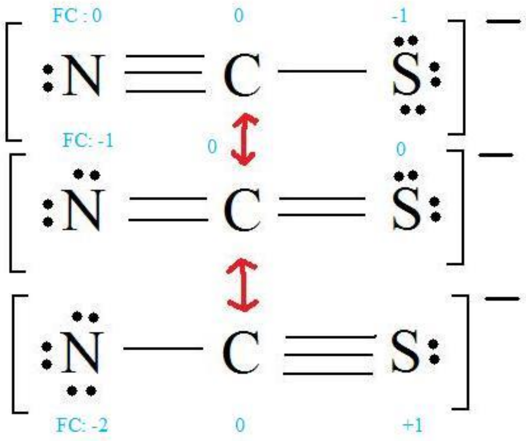


3. Assign Formal Charges via Equation .

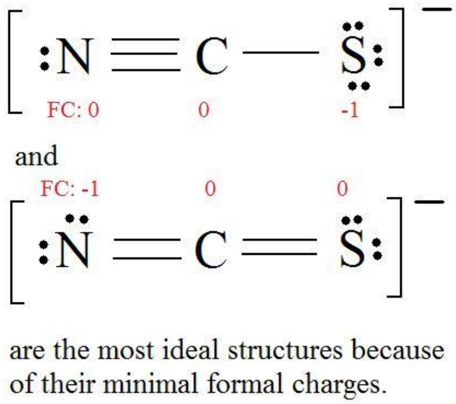
Formal Charge = (number of valence electrons in free orbital) - (number of lone-pair electrons) - (1/2 number bond pair electrons)

Remember to determine the number of valence electron each atom has before assigning Formal Charges

C = 4 valence e^-, N = 5 valence e^-, S = 6 valence e^-, also add an extra electron for the (-1) charge. The total of valence electrons is 16.

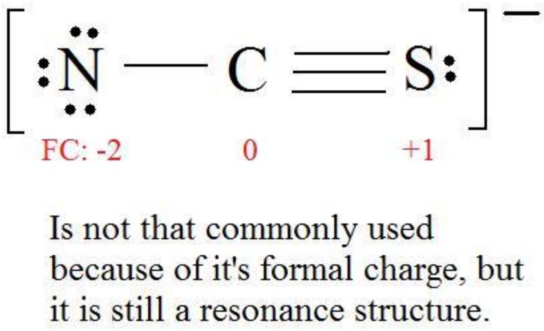


4. Find the most ideal resonance structure. (Note: It is the one with the least formal charges that adds up to zero or to the molecule's overall charge.)



and

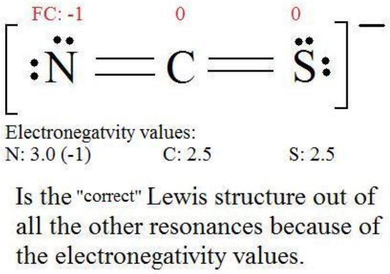
are the most ideal structures because of their minimal formal charges.



Is not that commonly used because of it's formal charge, but it is still a resonance structure.

5. Now we have to look at electronegativity for the "Correct" Lewis structure.

The most electronegative atom usually has the negative formal charge, while the least electronegative atom usually has the positive formal charges.



Electronegatvity values:
N: 3.0 (-1) C: 2.5 S: 2.5

Is the "correct" Lewis structure out of all the other resonances because of the electronegativity values.

It is useful to combine the resonance structures into a single structure called the **Resonance Hybrid** that describes the bonding of the molecule. The general approach is described below:

1. Draw the Lewis Structure & Resonance for the molecule (using solid lines for bonds).
2. Where there **can** be a double or triple bond, draw a dotted line (-----) for the bond.
3. Draw only the lone pairs found in all resonance structures, do not include the lone pairs that are not on all of the resonance structures.

Example: Benzene is a common organic solvent that was previously used in gasoline; it is no longer used for this purpose, however, because it is now known to be a carcinogen. The benzene molecule (C6H6C6H6) consists of a regular hexagon of carbon atoms, each of which is also bonded to a hydrogen atom. Use resonance structures to describe the bonding in benzene.

Given: molecular formula and molecular geometry

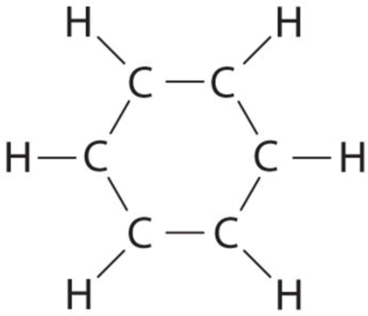
Asked for: resonance structures

Strategy:

A. Draw a structure for benzene illustrating the bonded atoms. Then calculate the number of valence electrons used in this drawing.
B. Subtract this number from the total number of valence electrons in benzene and then locate the remaining electrons such that each atom in the structure reaches an octet.
C. Draw the resonance structures for benzene.

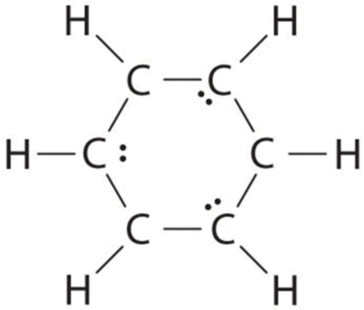
Solution:

A Each hydrogen atom contributes 1 valence electron, and each carbon atom contributes 4 valence electrons, for a total of (6 × 1) + (6 × 4) = 30 valence electrons. If we place a single bonding electron pair between each pair of carbon atoms and between each carbon and a hydrogen atom, we obtain the following:



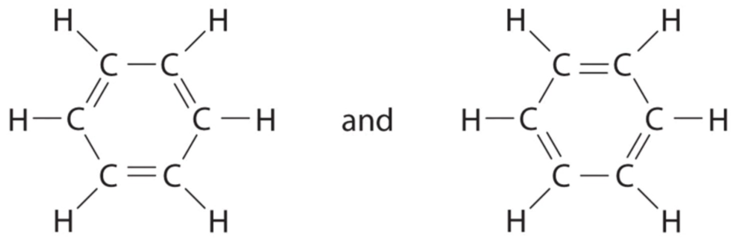
Each carbon atom in this structure has only 6 electrons and has a formal charge of +1, but we have used only 24 of the 30 valence electrons.

B If the 6 remaining electrons are uniformly distributed pairwise on alternate carbon atoms, we obtain the following:

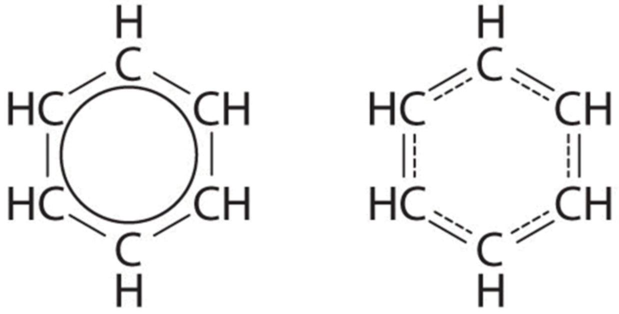


Three carbon atoms now have an octet configuration and a formal charge of −1, while three carbon atoms have only 6 electrons and a formal charge of +1. We can convert each lone pair to a bonding electron pair, which gives each atom an octet of electrons and a formal charge of 0, by making three C=C double bonds.

C There are, however, two ways to do this:



Each structure has alternating double and single bonds, but experimentation shows that each carbon–carbon bond in benzene is identical, with bond lengths (139.9 pm) intermediate between those typically found for a C–C single bond (154 pm) and a C=C double bond (134 pm). We can describe the bonding in benzene using the two resonance structures, but the actual electronic structure is an average of the two. The existence of multiple resonance structures for aromatic hydrocarbons like benzene is often indicated by drawing either a circle or dashed lines inside the hexagon:



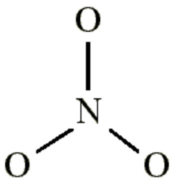
Benzene

Example: Draw the possible resonance structures for the Nitrate ion NO_3^-

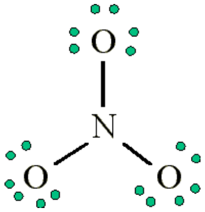
Solution

1. Count up the valence electrons: (1*5) + (3*6) + 1(ion) = **24** electrons

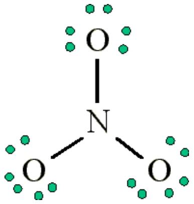
2. Draw the bond connectivities:



3. Add octet electrons to the atoms bonded to the center atom:

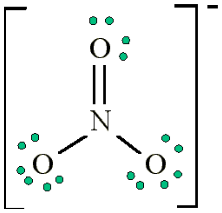


4. Place any leftover electrons (24-24 = **0**) on the center atom:



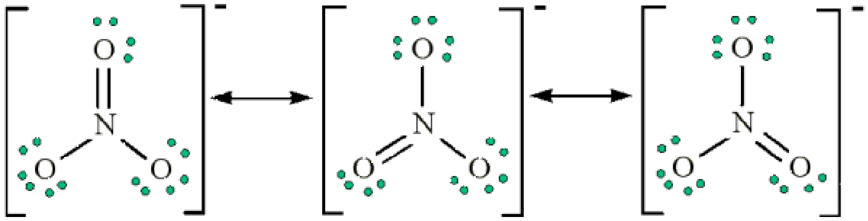
5. Does the central atom have an octet?

- **NO**, it has 6 electrons
- Add a multiple bond (first try a double bond) to see if the central atom can achieve an octet:



6. Does the central atom have an octet?

- YES
- Are there possible resonance structures? YES



Note: We would expect that the bond lengths in the NO_3^- ion to be somewhat shorter than a single bond.