

To help understand molecules (or radicals or ions), VSEPR shapes, and properties (such as polarity and bond length), we will draw the Lewis (or electron dot) structure. You will also practice this in lab.

The Lewis structure is a model that gives a description of where the atoms, charges, bonds, and lone pairs of electrons, may be found.

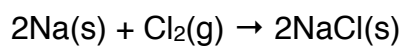
Ionic bonds involve the transfer of electrons.

Covalent bonds share electrons between atom centers.

Most real bonds are somewhere between ionic and covalent.

Ionic compounds, formed from a metal and a nonmetal, have ionic bonds.

A metal with a low ionization energy, such as sodium, combines with a nonmetal with high electron affinity to form a salt (an ionic compound): NaCl.



To a large extent, Na in NaCl is Na^+ , and Cl in NaCl is Cl^- . This is an ionic bond.

Covalent compounds, formed among nonmetals, form when 2 nuclei attract the same electrons.

A bond, ionic or covalent, is a balance of attractive and repulsive forces. The nucleus of one atom attracts the electrons from the other atom. The electrons repel, and the nuclei repel each other. A bond forms when the attractive forces are larger than the repulsive forces.

To begin drawing a Lewis structure, count the valence electrons. The molecule, HCl, has eight valence electrons, one from hydrogen and 7 from chlorine. Chlorine has more electrons, but only 7 of them are valence. The number valence electrons is the same as the group number for elements in Group A (Hydrogen is in group IA and chlorine is in group VIIA). From quantum theory, valence electrons are the outermost (highest n) s and p electrons. Recall that the d and f electrons go into inside shells, so they are not valence electrons initially. Neither chlorine nor hydrogen has electrons in d or f subshell. Because they are both in Group A, we can use the group number to get the valence

electrons. The Lewis structure for HCl looks like this: $\text{H}-\ddot{\text{Cl}}:$

There is a bond (–) between H and Cl. A bond is made of 2 electrons. Each pair of atoms must be held together by at least one bond. After placing the bond, there are still 6 of the 8 electrons left. Hydrogen, a first-row element, takes only 2 electrons to fill its valence shell, so the remaining 6 electrons are given in pairs to Cl. By sharing, hydrogen has the 2 electrons to fill its valence shell, and chlorine has the eight electrons to fill its valence shell.

The octet rule gives guidance to start building molecules and other chemical species. The octet rule is that atoms try to get 8 valence electrons by forming bonds. Elements in the second row of the periodic table never get more than 8 electrons. There are many exceptions to the octet rule, H gets 2 electrons, B often gets 6 electrons, while elements in the third row and higher often get more than 8 electrons.

For elements in the third row and higher, we also will build Lewis structures that have minimum formal charges (elements in the second row never get more than 8 electrons). The formal charge $FC = \text{Group Number} - \text{Nonbonding electrons} - 1/2 \text{ bonding electrons}$ or $FC = G\# - NBE - 1/2 BE$. When formal charges are necessary, we build structures with negative formal charges on electronegative atoms and positive formal charges on less electronegative atoms. (Electronegativity follows the same trend as ionization energy, except that the noble gases have no electronegativity.) Overall, we try not to have any formal charges (or a minimum number of them) for the preferred structure.

Calculate the formal charge on H and Cl in $\text{H}-\ddot{\text{Cl}}:$. Answer: $FC(\text{H}) = 1 - 0 - 1/2(2) = 0$. The formal charge on hydrogen is zero. Because the HCl molecule has no charge, we already know that the formal charge on Cl will be zero. $FC(\text{Cl}) = 7 - 6 - 1/2(2) = 0$. By following the outline above, we arrived at the structure with zero formal charge.

When a molecule or species involves more than 2 atoms, we follow this set of rules to build a Lewis structure.

- 1) The central atom is the one with the lowest electronegativity (never hydrogen).
- 2) Count the total number of valence electrons
- 3) Form single (or sigma, σ) bonds between the central atom and the surrounding atoms, deducting 2 electrons from the total for each bond placed.
- 4) Place any remaining electrons symmetrically as lone pairs to complete the octets on the most electronegative atoms first, and after that, to the central atom.
- 5) If needed, form double and triple bonds (symmetrically, if possible) to satisfy the octet rule. Some atoms, like B, will have 6 electrons instead of 8.
- 6) Calculate the formal charge for all atoms, and attempt to minimize the magnitude of the charges by forming double and triple bonds when third row and higher elements are the central atom.
- 7) When multiple bonds are present, consider equivalent resonance structures that contribute to the overall structure. Note that resonance can also be considered in Step 5 for the structure that satisfies the octet rule.

The Lewis structure is a model that gives insight about how a molecule is put together. The relatively straightforward rules give reasonable predictions. Real molecules sometimes behave differently from the predictions made with the Lewis model or formal charge model.

Draw the Lewis structure for H_2O . Answer: 1) The central atom is O because H cannot be. 2) There are 8 valence electrons. 3) $\text{H}-\text{O}-\text{H}$ uses 4 electrons from the total, and 4 remain. 4) H has a full shell with 2 electrons, so O gets the 4 electrons to fill its octet.

This gives $\text{H}-\ddot{\text{O}}-\text{H}$ 5) Form no double or triple bonds because the octet rule was satisfied. 6) $\text{FC}(\text{H})=1-0-1/2(2)=0$ (for both), and $\text{FC}(\text{-O})=6-4-1/2(4)=0$. 7) No equivalent resonance is possible because all are single bonds.

Draw the Lewis structure for CO_3^{2-} . Answer: 1) The central atom is C because C is less electronegative than O. 2) There 24 valence electrons C(4), O(3x6), and 2 for the -2

charge. 3) Form 3 single bonds (6 electrons) to get $\text{O}-\overset{\text{O}}{\underset{|}{\text{C}}}-\text{O}$, with 18 electrons

remaining. 4) Place the 18 electrons, 6 to each O to fill the octet, giving $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}-\text{C}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. 5) The 3 bound oxygens have complete octets (8 electrons), but C does not (6 electrons). Form a double (or pi, π) bond to carbon using a lone pair on one of the

bound O atoms, giving $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}-\text{C}=\ddot{\text{O}} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. All atoms now have an octet. 6) $\text{FC}(\text{O})=6-6-1/2(2)=-1$ (for both), $\text{FC}(\text{O}=\text{O})=6-4-1/2(4)=0$, and $\text{FC}(\text{C})=4-0-1/2(8)=0$. The sum of the formal charges adds to -2, which is equal to the charge. This is a check that the structure is correct. We can now draw the structure with the formal charges placed on

the atoms where they belong: $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ | \\ \ominus\text{:}\ddot{\text{O}}-\text{C}=\ddot{\text{O}} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$ 7) There were two other oxygen atoms where we could have drawn a double bond in step 5, the top and the left oxygen, which

leads to these structures: $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ || \\ \ominus\text{:}\ddot{\text{O}}-\text{C}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$ and $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}=\text{C}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. There are three equivalent resonance structures for the carbonate ion. These equivalent resonance structures differ only in the placement of electrons. No atoms moved.

Draw the Lewis structure for SO_2 . Answer: 1) S is the central atom. 2) There are 18 valence electrons. 3) Form single bonds. $\text{O}-\overset{\text{O}}{\underset{|}{\text{S}}}-\text{O}$ uses 4 electrons, leaving 14 to

place. 4) Place the 14 electrons: $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}-\text{S}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$ 5) Form 1 double bond to satisfy the

octet rule for S: $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ || \\ \text{:}\ddot{\text{O}}-\text{S}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. This is the structure that satisfies the octet rule (and it would have an equivalent resonance structure with the double bond on the other side. 6) $\text{FC}(\text{O})=6-6-1/2(2)=-1$, $\text{FC}(\text{S})=6-2-1/2(3)=+1$, $\text{FC}(\text{O}=\text{O})=6-4-1/2(4)=0$. The

structure with the formal charges drawn would be: $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ || \\ \ominus\text{:}\ddot{\text{O}}-\text{S}^{\oplus}-\ddot{\text{O}}\text{:} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. Because there is a +1 and a -1 formal charge, and the positive charge is on the central atom, form a

second double bond from the second oxygen, giving $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ || \\ \text{:}\ddot{\text{O}}=\text{S}^{\oplus}=\ddot{\text{O}} \\ | \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$. The formal charges

are all zero: $FC(O)=6-4-1/2(2)=0$ (for both), and $FC(S)=6-2-1/2(8)=0$. This structure has minimum formal charge. Note that S has 10 electrons. This is acceptable because S is in the third row of the periodic table. Remember that second-row elements get a maximum of 8 electrons. 7) Because both oxygens formed double bonds, there would be no equivalent resonance structures for the Lewis structure with minimum formal charge.

Which structure is correct for the real molecule, the one that satisfied the octet rule or the one that had minimum formal charge? On an exam, the right answer is the one asked for in the question. If the question asks questions about the structure that satisfies the octet rule, then that is the structure to draw. If the question does not specify or asks for the minimum formal charge, draw that structure. When done correctly, the formal charge method shows the predicted location of charges on an ion. A better (but not very helpful) explanation for the real molecule would be that the real molecule is some combination of these structures. For example, there would be some partial negative charge on the oxygen and a partial positive charge on the sulfur (but not $O=-1$ and $S=+1$ and not $2O=-1/2$ and $S=+1$). The purpose of these models is to give you a way to predict the 3D structure and the properties of the structures you draw. Better predictions will require better models and more understanding.

Structures with boron as the central atom often violate the octet rule because boron gets 6 electrons.

Draw the Lewis structure for BH_3 . 1) B is the central atom. 2) There are 6 electrons to

place. 3) Form single bonds: $H-\overset{\overset{H}{|}}{B}-H$. All electrons have been placed, and H will not form double bonds. This is the structure for BH_3 . 6) The formal charges for all atoms are zero. $FC(H)$ was done before. $FC(B) = 3-0-1/2(6)=0$.

Atoms in the third row and below often have more than 8 electrons. We saw this for SO_2 when we drew the structure with minimum formal charge. In some cases we see exceeding the octet rule for the central atom at step 4.

Draw the Lewis structure for SCl_4 . 1) S is the central atom. 2) There are 34 electrons to

place. 3) Form single bonds $Cl-\overset{\overset{Cl}{|}}{S}-Cl$, using 8 electrons. There are 26 electrons left to place. 4) Giving 6 electrons to each Cl to satisfy the octet rule uses 24 electrons, so 2

are left over for the central atom: $Cl-\overset{\overset{\cdot\cdot}{\cdot\cdot}Cl}{\underset{\cdot\cdot}{\cdot\cdot}S}-Cl$. 5) The octet rule is already satisfied or

exceeded, so do not form double or triple bonds. 6) The formal charge on each atom is 0. $FC(Cl^-) = 7 - 6 - 1/2(2) = 0$ (for all four). $FC(S) = 6 - 2 - 1/2(8) = 0$. There is no possibility for equivalent resonance structures because all atoms have single bonds.

Once you can draw Lewis structures, you can apply the VSEPR model to determine the 3D shape of the structure that you drew. Molecules, ions, and species adopt 3D shapes to minimize electron repulsions (for both electrons in bonds and in lone pairs). To determine the 3D shape, count the number of regions of electron density around the central atom (note that double and triple bonds count as 1 region of electron density for VSEPR). We can determine the 3D shape that includes all regions of electron density around the central atom (including lone pairs), or we can determine the 3D shape of just the atomic centers (ignoring lone pairs around the central atom). The first method gives the electron pair geometry (or shape) that you can look up in Table 1, while the second method gives the molecular geometry (or shape) that you can look up in Table 2. Using Table 2 additionally requires separately counting the number of bonding regions and the number of lone pairs around the central atom. Recall that double and triple bonds count as one region for the VSEPR model.

Table 1: Electron-pair geometry and molecular geometry if central atom has all atoms attached.

Bonding Regions	Electron-Pair Geometry	Faces	Bond Angle(s)
2	linear	0	180°
3	trigonal planar	2	120°
4	tetrahedral	4	109.5°
5	trigonal bipyramidal	6	90°, 120°
6	octahedral	8	90°

Table 2: Molecular geometry depends on the total number of bonding regions and lone pairs around the central atom, as well as the number of lone pairs and bonding regions. The table is organized by the sum of lone pairs and bonding regions. Recall that double and triple bonds count as one region for the VSEPR model.

Sum of Lone Pairs and Bonding Regions				Molecular Geometry	Bond Angle
Bonding Regions	= Bonding Regions + Lone Pairs				
2	2	0		linear	180°
3	3	0		trigonal planar	120°
	2	1		bent	
4	4	0		tetrahedral	109.5°
	3	1		pyramidal	
	2	2		bent	
5	5	0		trigonal bipyramidal	120°, 90°

	4	1	see saw	
	3	2	t-shaped	
	2	3	linear	
6	6	0	octahedral	90°
	5	1	square pyrimidal	
	4	2	square planar	

Question. What is the electron-pair geometry and the molecular geometry of H₂O?

Answer. The first step is to draw the Lewis structure, which we did above. The Lewis structure has 4 regions of electron density, 2 bonds and 2 lone pairs. Four regions of electron density gives a tetrahedral or 3D shape from Table 1 for the electron-pair geometry. From Table 2, the molecular geometry is bent (4 bonding regions, 2 bonds and 2 lone pairs).

Question. What is the electron-pair geometry and the molecular geometry of CO₃²⁻?

Answer. From the Lewis structure drawn above, the central atom (C) has 3 bonding regions and 0 lone pairs (remember that double and triple bonds count as 1 region). Tables 1 and 2 give trigonal planar for the electron-pair geometry and for the molecular geometry.

Question. What is the electron-pair geometry and the molecular geometry of BH₃?

Answer. From the Lewis structure drawn above, the central atom (B) has 3 bonding regions and 0 lone pairs. Tables 1 and 2 give trigonal planar for the electron-pair geometry and for the molecular geometry.

Question. What is the electron-pair geometry and the molecular geometry of SCl₄?

Answer. From the Lewis structure drawn above, the central atom (S) has 4 bonding regions and 1 lone pair, giving 5 regions of electron density. Tables 1 gives trigonal bipyramidal for the electron-pair geometry. Table 2 gives see saw as the molecular geometry.

Question. What is the electron-pair geometry and the molecular geometry of SF₆? The

Answer. Lewis structure (try drawing it) has 6 bonds and 0 lone pairs around the central S atom. Both the electron-pair geometry and the molecular geometry are octahedral.

Question. What is the electron-pair geometry and the molecular geometry of BeF₂, XeF₂, BeF₃, NH₃, CH₄, XeF₄, PF₅, ClF₃, IF₅,

Answer. You must draw the Lewis structure and use Tables 1 and 2. Do you have pencil and paper? Are you drawing the [Lewis Structure](#)? Are you applying [VSEPR theory](#) to the Lewis structure? (linear, linear), (trigonal bipyramidal, linear) (trigonal planar, trigonal planar), (tetrahedral, pyrimidal), (tetrahedral, tetrahedral), (octahedral, square planar), (trigonal bipyramidal, trigonal bipyramidal), (trigonal bipyramidal, t-shaped), (octahedral, square pyramid).

Linus Pauling empirically (meaning to explain data) discovered the concept of electronegativity based on the observed reactivity of chemicals when the form bonds. It

is one of the few models that does not yet have a theoretical explanation for why it works. Nevertheless, electronegativity is useful for chemistry. Electronegativity means the tendency of an atom to attract electrons to itself. Electronegativity follows the trend of ionization energy, except that noble gases have electronegativity values of (approximately) zero. The most electronegative elements would be fluorine, and the least electronegative element would be francium. Electronegativity must be looked up in a table, such as the one below. Rarely are such tables given on exams, so you will need to be able to work with the electronegativity trends (as well as metal ion and nonmetal-containing ion) to estimate polarity.

Electronegativity																		
H 2.1																	He --	
Li 1.0	Be 1.6											B 2.0	C 2.6	N 3.0	O 3.4	F 4.0	Ne --	
Na 0.9	Mg 1.3											Al 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2	Ar --	
K 0.8	Ca 1.0	Sc 1.4	Ti 1.5	V 1.6	Cr 1.7	Mn 1.6	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.7	Ga 1.8	Ge 2.0	As 2.2	Se 2.6	Br 3.0	Kr --	
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.3	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.3	Pd 2.2	Ag 1.9	Cd 1.7	In 1.8	Sn 2.0	Sb 2.1	Te 2.1	I 2.7	Xe --	
Cs 0.79	Ba 0.89			Hf 1.3	Ta 1.5	W 2.4	Re 1.9	Os 2.2	Ir 2.2	Pt 2.3	Au 2.5	Hg 2.0	Tl 2.0	Pb 2.3	Bi 2.0	Po 2.0	At 2.2	Rn --
Fr 0.7	Ra 0.89			Rf --	Db --	Sg --	Bh --	Hs --	Mt --	Uun --								
La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.2	Gd 1.20	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.1	Lu 1.27				
Ac 1.1	Th 1.3	Pa 1.5	U 1.38	Np 1.38	Pu 1.36	Am 1.3	Cm 1.3	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr 1.3				

Electronegativity is one of two concepts that are important to understand molecular polarity (the other is symmetry). Electronegativity differences between two atoms lead to bond polarity. When two atoms have an electronegativity difference more than about 0.4, the bond formed between those atoms is said to be polar. When the difference is above 1.5, the bond has substantial ionic character. Bond polarity causes bonds to be stronger than if electrons were shared, and the difference between the theoretical bond strength and the bond strength in the actual molecule is related to the electronegativity.

You now have two definitions for an ionic bond, one based on having metal cation and a nonmetal-containing anion, and the other based on electronegativity difference. These models can make different predictions. Real bonds have ionic character, which leads to the appearance of a salt. No bonds discovered yet are perfectly ionic.

Unlike ionic bonds, the bonds formed between diatomic molecules are nearly perfectly covalent (not polar) because there is no electronegativity difference. Other bonds will

have some degree of polarity, which means having an electrically positive and negative end, something like the poles of a magnet.

Bond polarity alone is not enough to tell if a molecule is polar because bond polarity may cancel because of symmetry. You could picture symmetry like a tractor pull. Hook a tractor up to each atom around the central atom. The horsepower of the tractor would be equal to the electronegativity of that atom. If the central atom has a net motion in one direction because of the tractor pull, the molecule is said to be polar. If not, it's nonpolar.

The diatomic molecules, H_2 , O_2 , F_2 , etc., offer an easy case to understand symmetry. They are all symmetrical. F is the most electronegative atom on the periodic table. When the bound F atoms in F_2 pull equally in opposite directions with 4.0 (the electronegativity from the table) horsepower engines, there is no net motion. The F_2 molecule is nonpolar, and the bond is also nonpolar because there is no electronegativity difference. This is one of the reasons that F_2 is a gas at room temperature, rather than a liquid or a solid.

The HCl molecule, see Lewis structure above, is polar. The magnitude of the electronegativity difference between H(2.1) and Cl(3.2) is greater than 0.4, so the bond is polar. Hooking tractors up to each end, the 3.2HP tractor for Cl would win, and the molecule would move toward Cl, so the molecule is polar.

Does the BCl_3 molecule have polar bonds? Is BCl_3 a polar molecule? The electronegativity difference between Cl (3.2) and B (2.0) is 1.2, so the B-Cl bonds are polar. To determine if the molecule is polar, we need to see if it is symmetrical by applying VSEPR theory. If the molecule has one of the 3D shapes with perfect symmetry, then the molecule is not polar; otherwise it is. The 3D shapes with perfect symmetry are given in Table 1. The linear geometry for 5 and 6 electron pairs and the square planar geometry for 6 electron pairs are also perfectly symmetrical.

Molecular polarity affects many physical properties such as melting point and boiling point, as well as chemical solvency and reactivity. Polarity tends to increase the melting and boiling points, and often indicates the point of attack for chemical reactions. You can predict many of these properties by determining that a molecule is polar using the above rules. You will also practice this skill in lab, and you will need it for CHEM II and Organic Chemistry.