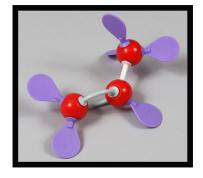
Super Models



VSEPR-ID (Octet Rule) MOLECULAR MODEL KIT

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Caution: Atom centers and connectors are choking hazards. Do not eat or chew model parts.

Kit Contents:

- 5 white 1-hole hydrogen atom centers
- 3 blue 4-hole nitrogen atom centers
- 4 red 4-hole oxygen atom centers
- 3 green 4-hole halogen atom centers
- 2 black 4-hole carbon atom centers
- 2 yellow 4-hole sulfur or phosphorous atom centers
- 1 yellow 6-hole sulfur atom center
- 8 tan, 27 mm connectors for single bonds
- 8 grey, 43 mm connectors for double or triple bonds
- 10 purple-lone-pair orbitals (paddles)
- Lab procedures and answer sheets

Related Kits Available: Coordination Chemistry Molecular Model Kit General Chemistry Molecular Model Kit VSEPR II (Expanded Octet) Molecular Model Kit

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Using the VSEPR Model Kit

I. THE PURPOSE OF VSEPR THEORY.

Pairs of valence electrons on an atom interact with each other increasing the potential energy of the atom. According to Valence-Shell-Electron-Pair-Repulsion (VSEPR) theory, there will be a reduction in the energy of a molecule by increasing the distance (angle) between electron pairs on each atom in that molecule. Electron pair interaction increases energy according to the following series: LP-LP > LP-BP > BP-BP, where LP = lone pair, and BP = bonded pair. LP-LP, a lone pair interacting with another lone pair, therefore, produces the highest amount of energy.

By using the Localized Electron (LE) theory of bonding, Lewis structures, formal charges, resonance, and VSEPR theory, we can determine the most probable placement of atoms and lone pairs of electrons in a molecule. These concepts work best when applied to atoms in groups 1, 2, and 13 through 18 (groups IA through VIIIA in the older periodic table system).

These principles do not apply to salt, metal, or van der Waals bonding.

II. VALENCE ELECTRONS, THE OCTET RULE, AND EXCEPTIONS.

Electrons which are used for bonding are called valence electrons, and the shell (highest energy level) that contains them is called the valence shell.

Atoms of the main group elements will become most stable (resist change) when they have a total of eight electrons in their outer shell s and p subshells. This is known as the octet rule.

Note that there are three categories of exceptions to the octet rule:

1) Electron deficiency. For example, hydrogen and helium are most stable with two electrons in their valence shell (the duet rule). Some elements of groups 2 and 3 are able to form stable compounds with six valence electrons (e.g. $BeCl_2$, BCl_3 , and $AlCl_3$).

2) Odd numbers of electrons. For example, nitrogen atoms in some molecules have seven valence electrons (e.g. NO_2 , NO).

3) The elements beyond period two may participate in bonding using more than eight electrons (forming an expanded octet). Some examples are sulfur in H_2SO_4 and phosphorus in H_4PO_4 and the transition metals in groups 3 through 12 (IB through VIIIB). These exceptions are due to d orbitals becoming available for bonding.

III. MOLECULAR ORBITAL (MO) AND VALENCE BOND (VB) THEORIES.

MO theory is an advanced-mathematical description of bonding in which electrons are shared by all of the atoms in a molecule, and its principles will not be covered in this manual.

VB theory, which is easier to learn, proposes that valence electrons are localized on individual atoms as Lone Pairs (LP), or nonbonding (NB) electrons, or they are shared as Bonding Pairs (BP) between atoms. This description of the placement of electrons on and between atoms is called the Localized Electron (LE) theory.

IV. HOW TO DRAW LEWIS STRUCTURES

Step 1.

From the molecular formula of the molecule, write the symbols of the atoms with dashed lines between them. The least electronegative should be used as the central atom. Hydrogen atoms will always be terminal (on an end), since the atoms can usually only have one bond. The same is true for the halogens, except in some molecules which are composed of halogens exclusively. Fluorine, the most electronegative element will always be terminal. When the chemical formula of a compound is written, very often the order in the formula is the same as the order of atoms in the Lewis structure (e.g. HSCN).

Step 2.

Using a periodic table, find the number of valence electrons of all the participating atoms. The group number in the older "A" system will be the number of valence electrons. If you use the new numbering system, subtract ten from group numbers 13 through 18 to get the valence number. Subtract two for each dash put between the atoms (each dash represents a pair of shared electrons). Subtract one for each positive charge if you are dealing with a positively charged ion. Add one for each negative charge if you are drawing the Lewis structure of a negatively charged ion.

Step 3.

Next, place the valence electrons in pairs, around the atoms starting with the most electronegative elements first until each atom has an octet (exceptions will be the elements listed in II. 1) and 2) above. If there are left over electrons, put them on the central atom.

Step 4.

If some atoms have less than an octet, move lone pairs in to form an octet.

Step 5.

Check the structure for formal charges. If the structure is a neutral molecule, the formal charge on each atom will be zero, but if some atoms have charges, they should be as low as possible, and the charge should fit with the electronegativity of the atom. For example, in a molecule with O and N atoms, the O would be the atom assigned the negative formal charge should one exist.

Step 6.

Make resonance hybrids, if needed.

Example:

1. Draw the Lewis structure for HCN (hydrocyanic acid).

Step 1.	H-C-N	
Step 2.	$1 C x 4 e^{-} = 4 e^{-}$ $1 N x 5e^{-} = 5 e^{-}$ $1 H x 1e^{-} = 1 e^{-}$	10 e ⁻ (total valence electrons) <u>- 4 e⁻ (2 bonds x 2 e⁻ used/bond)</u> 6 e ⁻ to distribute
Total valen	$rece = 10 e^{-1}$	

Step 3.

Step 4. Hydrogen with two electrons has its required duet. Nitrogen has an octet. Carbon lacks an octet, so we move lone pairs from nitrogen into the bond with nitrogen. Nitrogen doesn't lose electrons, but carbon will gain them.

$$H - C - \underbrace{N}_{\uparrow} = H - C \equiv N$$

Both carbon and nitrogen now have an octet.

Step 5. Determine the formal charge on each atom. See the following discussion.

V. OXIDATION STATE vs FORMAL CHARGE.

The **oxidation state** of an atom is an indication of how many electrons it "owns" within a molecule. When two atoms bond, the one with the highest electronegativity is assumed to possess its own nonbonding electrons and the bonding electrons as well. This approach tends to view the atoms as ions even in covalent compounds.

For HCN atoms the electronegativity trend is: H < C < N.

Oxidation State = Valence Electrons – Bonding Electrons – Lone Pair Electrons. Boxes or circles drawn around the elements and the electrons they "own" help to visualize assignment and counting of electrons.

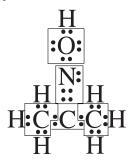
H, 1-0 = +1; C, 4-2 = +2; N, 5-6-2 = -3. The net charge is 0 as it should be, since HCN is not an ion.

In the following example, to find the oxidation state of each atom in C_3H_7NO (acetone oxime) we draw boxes around each atom and the electrons it is considered to own.

For C_3H_7NO atoms the electronegativity trend is: H < C < N < O.

7H, 1 - 0 = +7; 2C, (terminal) 8 - 14 = -6; 1C, (central) 4 - 2 = +2; 1N, 5 - 4 - 2 = -1; 1O, 6 - 4 - 4 = -2. The net charge is 0 as it should be, since C₃H₇NO is not an ion.

Note that the central C shares bonding electrons with the two terminal C atoms, since all C atoms have the same electronegativity.



3

Formal charges on atoms are used as an aid for drawing correct Lewis structures. Oxidation states are not used.

Formal charges of atoms in a compound presume electrons between atoms are being equally shared. An atom, will therefore, "own" its nonbonding electrons and one half of all its bonding electrons. Use the following formula to find formal charges.

Formal charge = Valence Electrons – Nonbonding Electrons – ½ Bonding Electrons.

Let's look again at HCN. This time boxes will outline nonbonding electrons and $\frac{1}{2}$ of the bonding electrons of each atom.

HEC

For H, 1 - 1 = 0; for C, 4 - 4 = 0; for N, 5 - 5 = 0. There are no atoms with a formal charge which means we have drawn the correct Lewis structure.

When calculating formal charges, these situations will indicate that the structure you have drawn may be incorrect.

- 1) Large charges; charges greater than +2 or -2.
- 2) Positive charges on highly electronegative elements, or negative charges on elements which are not very electronegative.

Here is an example of finding the correct Lewis structure of a positively charged ion: NH_4^{1+} (the ammonium ion).

 $1 \text{ N x } 5e^- = 5 e^- - 1 e^- \text{ (subtract 1e for + charge on ion)}$ $\frac{4 \text{ H x } 1e^- = 4 e^-}{4 \text{ Pe}^-} = \frac{-8 e^- (4 \text{ bonds x } 2 e^- \text{ used/bond})}{9 e^- \text{ used}}$ Total valence electrons $9 e^- = 9 e^- \text{ used}$ $9 e^- \text{ used}$

4, H 1 – 1 = 0; 1 N, 5 – 4 = +1. The formal charge on the N matches the charge on the ion, so the structure is correct.

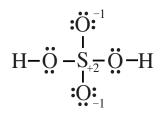
The next example illustrates bonding with elements in the 3rd period and beyond (i.e. periods $4, 5, \ldots$ Recall that these atoms have empty d subshells that can accept bonding electrons.

* H_2SO_4 , sulfuric acid, is one of the most important chemicals produced worldwide. Students can make the Lewis structure of the compound and then try to make it with a tetrahedral S atom. They will find that there aren't enough holes in the S atom to make the molecule. We have included an octahedral atom center (with 6 holes) so that the structure can be made. This illustrates the necessity of using d orbitals in 3rd row element (and beyond) compounds.

$$1 \text{ S x } 6 \text{ e}^- = 6 \text{ e}^ 32 \text{ e}^-$$
 (total valence electrons) $4 \text{ O x } 6 \text{ e}^- = 24 \text{ e}^ -12 \text{ e}^-$ (6 bonds x 2 e^- used/bond) $2 \text{ H x } 1 \text{ e}^- = 2 \text{ e}^ 20 \text{ e}^-$ to distribute

Total valence electrons $32 e^{-1}$

The two H have two electrons each for a duet. Each O has an octet, as does S. It appears that we are finished, but we didn't calculate the formal charges yet. We can do that now, and this is what we find.



We have formal charges which sum to zero, and that is good. However, we would like to see no charges if possible, and it is possible because the central atom is S, and it is found in period 3. We move lone pairs of electrons from the oxygen atoms into their bond with sulfur. Each O loses a negative charge, and the S has its +2 charge cancelled.

$$H - \ddot{\mathbf{O}} - \overset{\mathbf{O}}{\overset{\mathbf{I}}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}}{\overset{\mathbf{I}}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}{\overset{\mathbf{I}}}{\overset{\mathbf{I}}$$

The S atom now has 12 electrons surround it, but that is acceptable because S has empty d orbitals.

Below are five different Lewis structures for CO_2 (carbon dioxide). Which one is the best, i.e. most likely to exist?

The following is another problem in picking the best Lewis structure for a molecule. In this case, we look at N_2O , nitrous oxide, or laughing gas used in dentistry.

a)
$$\ddot{O} = N = \ddot{N}$$
 d) $:O \equiv N - \ddot{N}$:
b) $\ddot{N} = O = \ddot{N}$ e) $: \ddot{N} - O \equiv N$:
c) $: \ddot{O} - N \equiv N$:

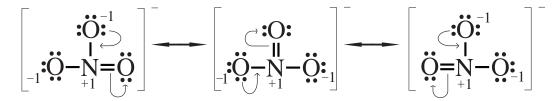
There is one more molecular strategy that can overcome the problem of formal charges. It is the chemical equivalent of a mule, and it is called resonance.

VI. RESONANCE.

 NO_3^{-} , the nitrate ion, will be used to illustrate resonance.

$$\mathbf{\ddot{O}}^{-1} = \mathbf{\ddot{O}}^{-1}$$

Each atom has an octet, and one of the negative charges matches the ionic charge, while the other negative charge cancels the positive charge on the N atom. There is not a way to get rid of the positive charge and one of the negative charges. If the negative charge can be shared among the three oxygen atoms, the energy expense of holding the charge can be lowered. The sharing is called resonance, and the Lewis structures below give an imaginary picture of how it takes place. (Chemists use the double pointed arrows for resonance only. These are not ordinary chemical reactions)



These are not actual changes. The three forms of the nitrate ion do not switch back and forth with each other, but it is difficult to make drawings that reflect the true situation. In reality, the three forms blend together to form one structure, a hybrid, at the same time.

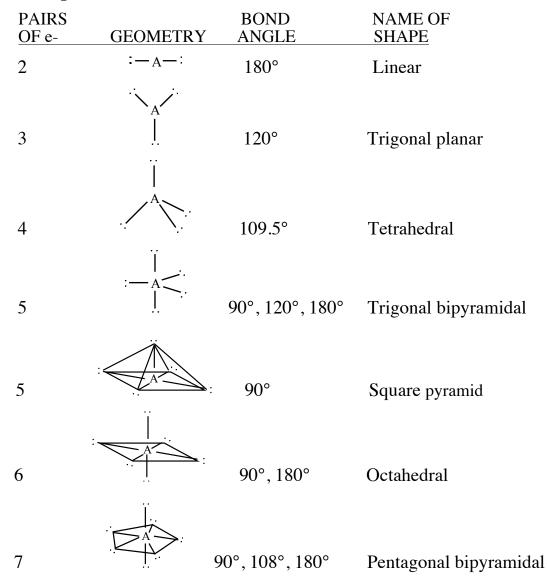
Consider a similar blending of characteristics in the biological world. The mating of a horse with a donkey produces a hybrid we call a mule. A mule is not a horse at one moment in time and a donkey at another. A mule has characteristics of both parents at all times.

Resonance hybrids present a similar situation chemically. How do chemists know that resonance hybrids exist as one blended structure? Measurements of the lengths of the bonds between the O atoms and the central N atom indicate that each bond is shorter than a single bond but longer than a double bond, and each bond is exactly like the other two. Below is the best Lewis structure that can be made for a hybrid molecule or ion. The dotted lines are partial bonds, and the three negative charges of -2/3 + -2/3 + -2/3 add up to -2. The +1 charge on N cancels -1, leaving a charge of -1 on the ion.

$$\begin{bmatrix} :O: \\ :O$$

VII. APPLICATION OF VSEPR THEORY.

I. Geometries of **pairs of electrons** around a central atom (A).



- II. When placing **additional atoms** (B) on all of the electron pairs of the central atom (A).
 - A. Treat double bonds as though they were single bonds.
 - B. Naming molecules with no lone pairs.

PAIRS OF e- 2	CLASS AB ₂	ANGLE 180°	NAME OF MOLECULE Linear
3	AB ₃	120°	Trigonal planar
4	AB_4	109.5°	Tetrahedral
5	AB ₅	90°, 120°, 180°	Trigonal bipyramidal
6	AB_6	90°, 180°	Octahedral

- III. When placing atoms (B) and one or more lone pairs of electrons (E) on a central atom (A).
 - A. The name of the molecule is based on the atoms only, not the atoms and the lone pairs.
 - B. Treat double bonds as though they were single.
 - C. To determine the best shape of the molecule, if more than one possibility exists, use these simple rules:
 - 1. in a trigonal bipyramid, put lone pairs in an equatorial position;
 - 2. in a pentagonal bipyramid, put lone pairs in an axial placement;
 - 3. for an octahedron, lone pairs should be opposite (trans to) each other;
 - 4. put the least electronegative additional atoms (B) in equatorial positions.
 - D. Example. What is the correct shape of ICl₃?





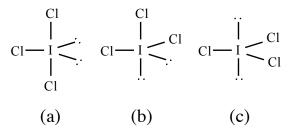
2. Pick the correct shape.

There are five pairs of electrons around the iodine, so the geometry of the shape of the central atom and its electrons is trigonal bipyramidal.

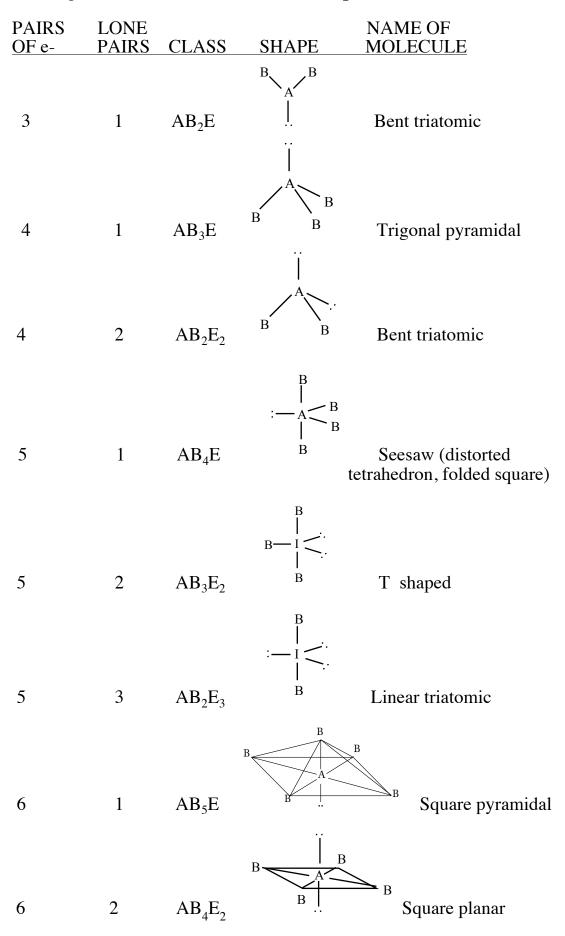


3. Draw the electrons and atoms residing on the central atom.

The possible placements of the two lone pairs and the three chlorine atoms are:



5. Pick the shape with the lowest energy. Because it has the lowest energy, (a) is the most likely form of the compound.



D. Naming molecules with one or more lone pairs.

- IV. Practice.
 - A. We apply the same principles to drawing and naming molecules and polyatomic ions.
 - B. Use the four steps from III. D., above.
 - C. Draw the following, and then name their geometries. Place a purple paddle into each hole without another atom center attached. The paddle represents a **lone pair of electrons**.

EASY (Models can be built with VSEPR I and VSEPR II Kits)

1. F ₂	5. HCN	8. CO_3^{2}
2. N_2O	6. HSCN	9. OCl ₂
3. $H_2^{-}S$	7. PH_4^{1+}	10. CH ₂ O
4. PF ₃		

To introduce students to the increased bonding possibilities of third row elements and beyond, you might have them draw the Lewis structure for SO_3 , and then attempt to use a tetrahedral sulfur atom to build a model of the molecule. It will not be possible to make the molecule since the central sulfur atom has an expanded octet of 12 valence bonding electrons surrounding it.

HARD (Models can be built only with VSEPR II Kit)

11. SF ₆	15. ICl_4^{1-}	18. BrF ₅
12. $IO_2F_2^{1-*}$	16. ClF_3	19. ICl_2^{1-}
13. XeF_4	$17. PCl_{5}$	20. I_3^{1-} †
14 $S_{\alpha}C_{1}$	2	C C

14. $SeCl_4$

* The least electronegative element should be in an equatorial position. Use an octahedral atom center for the central iodine atom.

[†] Use a trigonal bipyramidal atom center for the central iodine atom.

VSEPR I Lab Instructions

1. Obtain one VSEPR I Kit for your group. The atoms are color coded as follows. White = hydrogen Blue = nitrogen Red = oxygen Green = any halogen Black = carbon Yellow = sulfur

The purple paddle shaped item = a **nonbonding pair of electrons**. If your model has an atom with unfilled holes, place the purple paddles into the holes.

The short connectors are for single bonds, while the longer connectors are for double and triple bonds.

- 2. Make one copy of the lab the Master copy and have the teacher stamp only that one sheet. Each student should fill out a sheet, but only the Master copy will be used for the final grade.
- 3. Use a pencil to fill in all blank boxes except the "Model (checked by instructor)" column. This is where your instructor stamps or initials that the models are correct. Fill in the entire first horizontal row and bring the model to the instructor for verification.
- 4. In the columns labeled Shape, and Angle, write the shape name such as linear, bent, etc., and the angle. The shape is determined by the position of the atoms, not the electrons.
- 5. In the column labeled "Bonds, Polar/Non," write either Polar or Non-polar in the blank to describe individual bonds in the molecule.
- 6. In the column labeled "Molecule, Polar/Non," write either Polar or Non-polar in the blank to describe the whole molecule.
- 7. In the column labeled "# of bonds," a single bond counts as one bond, a double counts as two bonds, and a triple bond counts as three bonds.
- 8. In the column labeled "Resonance," write either Yes or No in the blank to describe whether the molecule could exhibit resonance.

LAB ASSESMENTS FOLLOW

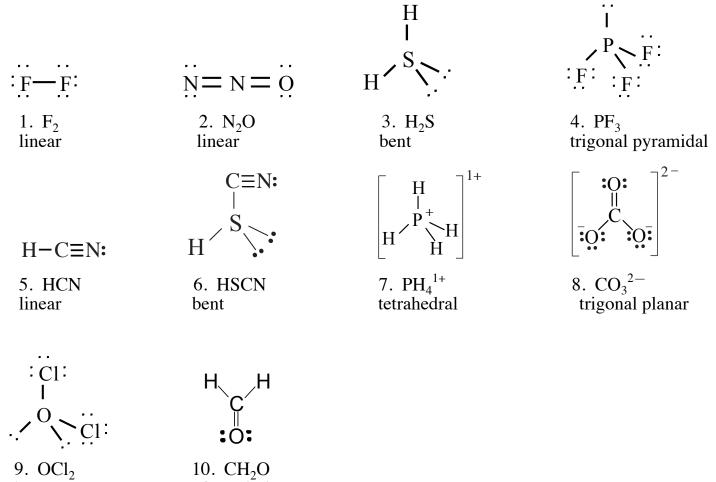
OCTET RULE LAB

Names	OCTET RULE LAB Date F							Period	
1	2	3	4	5	6	7	8	9	10
Molecular	Lewis		Bond	#Lone	#	Resonance	Bonds	Molecule	Model
Formula	Structure	Shape	Angle	Pairs	Bonds	y/n	Polar?	Polar?	Checked
H ₂									
Cl ₂									
H ₂ O									
HC1									
O ₂									
O ₂ CO ₂									
NH ₃									
NH ₄ ¹⁺									
O ₃									
CH ₄									
CH_4 NO_2^{1-} NO_3^{1-}									
NO_3^{1-}									
N ₂									
$\frac{H_2C_2}{CS_2}$									
CS ₂							-14 2015 1		

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NAME:	DATE	CLASS
1. What factor determines the shape of a	a molecule?	
2. What are three properties a molecule	must have in order	
 3. What is the cause of polar bonds? 4. Can a molecule be polar without polar 		
5. Can a molecule with polar bonds be	100001019 10000000000000000000000000000	your answer.
 6. What is the formal charge of each at a, b, c, d, e, f 7. Determine the formal charges of each at a set of each at at a set of each at a set of each at a set of each	t	$O_{, Middle O_{, Right O_{.}}$
8. What is the net formal charge on C_3	H ₇ OH?	

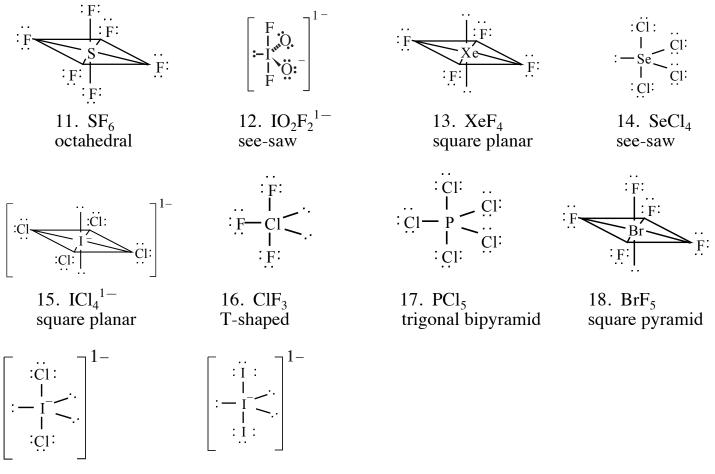
ANSWERS TO EASY STRUCTURES.



bent

10. CH₂O trigonal planar

ANSWERS TO HARD STRUCTURES.



20. I_3^{1-} linear

ANSWERS TO LAB ASSESSMENTS

1. What factor determines the shape of a molecule? ANS. PLACEMENT OF PAIRS OF NONBONDING ELECTRONS AND ATOMS AROUND A CENTRAL ATOM.

2. What are the three things a molecule must have in order to have resonance? ANS. A DOUBLE BOND, FORMAL CHARGES, AND A LONE PAIR OF ELECTRONS.

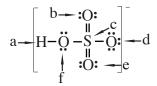
3. What is the cause of polar bonds? ANS. UNEQUAL SHARING OF BONDING ELECTRONS, OR SEPARATION OF FORMAL CHARGES, AS IN O₃.

4. Can a molecule be polar without polar bonds within the molecule? ANS. NO; THERE MUST BE A SEPARATION OF CHARGE DUE TO DIFFERENCES IN ELECTRO-NEGATIVITIES. BUT: YES; A SEPARATION OF CHARGE MAY OCCUR DUE TO TWO BONDED ATOMS WITH DIFFERENCES IN FORMAL CHARGE, AS IN O₃.

5. Can a molecule with polar bonds be nonpolar? ANS. YES, WHEN THE MOLECULE IS SYMMETRICAL.

6. What is the formal charge of each atom in

a____, b____, c____, d____, e____, f____



ANS. A 0, b 0, c 0, d -1, e 0, f 0

7. Determine the formal charges of each atom in O₃. Left O____, Middle O____, Right O____.

ANS. Left O 0, Middle O +1, Right O -1, or Left O -1, Middle O +1, Right O 0

8. What is the net formal charge on C_3H_7OH ? _____ ANS.0

RYLER'S REMEDIES:

For figuring time allotted for lab—about 2 hours.

For lost parts -1. charge 25¢ per lost part; 2. have students count parts when kits are handed out; 3. teacher counts parts when kits are turned in; 4. write numbers on baggies with a Sharpie Marker®, and assign pairs of students to a certain kit number.

For students forging teacher check marks—get some sort of a rubber stamp, e.g. happy face, or teacher signature.

OCTET RULE LAB

Names									
1	2	3	4	5	6	7	8	9	10
Molecular	Lewis		Bond	#Lone	#	Resonance	Bonds	Molecule	Model
Formula	Structure	Shape	Angle	Pairs	Bonds	y/n	Polar?	Polar?	Checked
H ₂	Н∶Н	Linear	180°	0	1	Ν	Ν	N	
Cl ₂	Cl Cl	Linear	180°	6	1	Ν	Ν	N	
H ₂ O	О. Н Н	Bent	105°	2	2	Ν	Y	Y	
HCl	H:Cl:	Linear	180°	3	1	Ν	Y	Y	
O ₂	0:0	Linear	180°	4	2	?	Ν	N	
CO ₂	:0::C::0:	Linear	180°	4	4	Ν	Y	N	
NH ₃	H N H H H	Trigonal Pyramidal	107°	1	3	N	Y	Y	
NH ₄ ¹⁺	$\begin{bmatrix} H \\ H:N:H \\ H \end{bmatrix}^{1+}$	Tetrahedral	109°	0	4	N	Y	N	
03	.0:0. .0.	Bent	117°	6	3	Y	Ν	Y	
CH ₄	Н Н:С:Н Н	Tetrahedral	109°	0	4	N	Y	N	
NO_2^{1-}		Bent	117°	6	3	Y	Y	Y	
NO_3^{1-}		Trigonal Planar	120°	8	4	Y	Y	N	
N ₂	:N:::N:	Linear	180°	2	3	Ν	N	N	
H_2C_2	H:C:::C:H	Linear	180°	0	5	N	Y	N	
CS ₂	Š∷C∷S	Linear	180°	4	4	Ν	Y	N	
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