

Super Models



VSEPR II (Expanded Octet) DALTON ATOM MOLECULAR MODEL KIT

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Recommended for ages 10-adult



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



Kit Contents:

- 6 green 4-hole halogen atom centers
- 3 red 4-hole oxygen atom centers
- 1 blue 4-hole nitrogen atom center
- 1 purple 5-hole atom centers for trigonal bipyramidal structures
- 1 silver 6-hole atom centers for octahedral structures
- 2 black 4-hole atom centers
- 1 yellow 4-hole atom centers
- 3 white 1-hole hydrogen atom centers
- 1 black 3-hole boron atom center
- 6 short rigid connectors for single bonds
- 6 long flexible connectors for double or triple bonds
- 18 lone pair purple paddles
- Lab procedures and answer sheets

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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_3PO_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. EXCEPTIONS TO THE OCTET RULE: THE EXPANDED OCTET.

Elements in groups 13 through 18, beyond neon (at. no. 10), may share eight electrons with other atoms, or, if necessary, they can share more than eight electrons with other atoms.

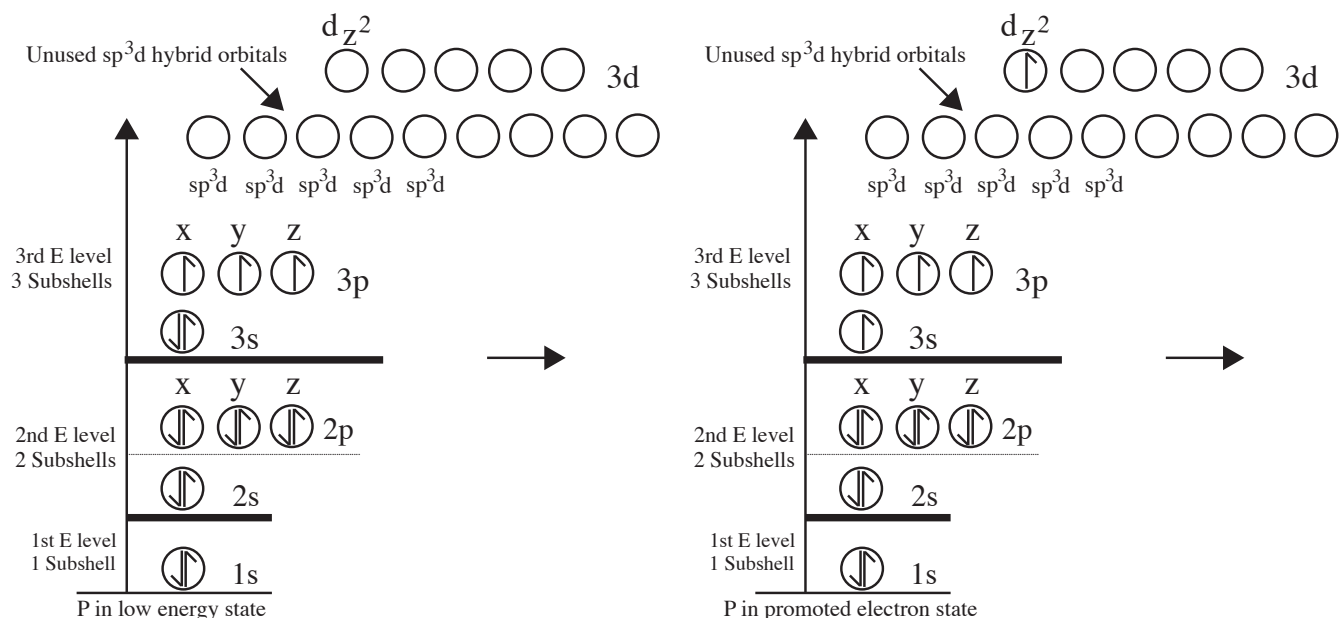
Sharing more than eight electrons depends on the availability of d orbitals in the same principal energy level (n) or in the previous principal energy level ($n-1$). The s, p, and d orbitals hybridize as illustrated in the following table.

Orbitals Hybridized	Hybrids	Steric Number (SN)
ns, np, nd	sp^3d	5
	sp^3d^2	6
	sp^3d^3	7
$(n-1)s, (n-1)p, (n-1)d$	dsp^3	5
	d^2sp^3	6
	d^3sp^3	7

The steric number refers to the total number of lone pairs of electrons plus the number of atoms or groups of atoms bonded to the central atom.

Before examining the formation of SN-5 bonding, let's look at the sp^3d hybridization of phosphorus orbitals.

Phosphorus atoms, which are not bonded or excited, have five valence electrons, two in a 3s orbital, and one in each p orbital (see "P in low energy state" below). After one of the s orbital electrons is promoted (see "P in promoted electron state" below) to the $3d_{z^2}$ orbital, the excited atom will form five equivalent sp^3d hybrid orbitals which are ready for bonding (see "P in sp^3d hybridized state" on the next page).



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.

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 formal charges 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.

Step 6.

Make resonance hybrids, if needed.

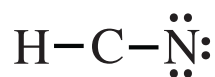
Example:

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

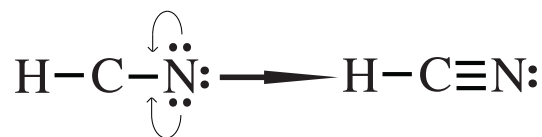


Step 2.	$1 \text{ C} \times 4 \text{ e}^- = 4 \text{ e}^-$	10 e^- (total valence electrons)
	$1 \text{ N} \times 5 \text{ e}^- = 5 \text{ e}^-$	$- 4 \text{ e}^-$ (2 bonds \times 2 e used/bond)
	$1 \text{ H} \times 1 \text{ e}^- = 1 \text{ e}^-$	6 e^- to distribute
Total valence electrons	10 e^-	

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.



Both carbon and nitrogen now have an octet.

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

VI. 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: $\text{H} < \text{C} < \text{N}$.

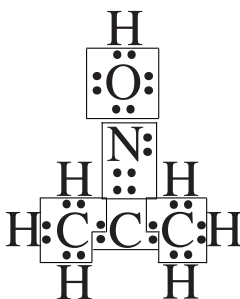
Oxidation State = Valence Electrons – Bonding Electrons – Lone Pair Electrons. Boxes or circles drawn around the elements and the electrons they “own” help to visualize assignment and counting of electrons.



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 $\text{C}_3\text{H}_7\text{NO}$ (acetone oxime) we draw boxes around each atom and the electrons it is considered to own.

For $\text{C}_3\text{H}_7\text{NO}$ atoms the electronegativity trend is: $\text{H} < \text{C} < \text{N} < \text{O}$.



7H, $1 - 0 = +1$; 2C, (terminal) $4 - 7 = -3$; 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 $\text{C}_3\text{H}_7\text{NO}$ 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.

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 – $\frac{1}{2}$ 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.

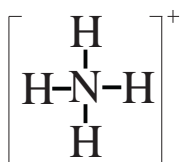


For H, $1 - 1 = 0$; for C, $4 - 4 = 0$; for N, $5 - 5 = 0$. There are no atoms with a formal charge which means we have drawn the correct Lewis structure.

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).



$$1 \text{ N} \times 5e^- = 5e^- \quad - 1e^- \text{ (subtract } 1e^- \text{ for } + \text{ charge on ion)}$$

$$4 \text{ H} \times 1e^- = 4e^- \quad - 8e^- \text{ (4 bonds} \times 2e^- \text{ used/bond)}$$

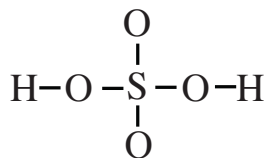
$$\text{Total valence electrons} \quad 9e^- \quad 9e^- \text{ used}$$

$9e^-$ available, $9e^-$ used. Now determine formal charges.

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, 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.

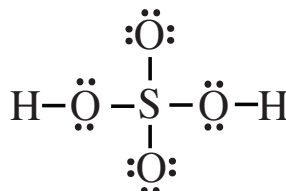


$$1 \text{ S} \times 6e^- = 6e^- \quad 32e^- \text{ (total valence electrons)}$$

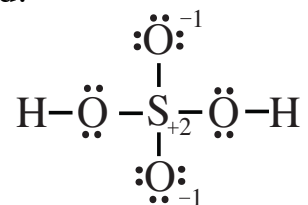
$$4 \text{ O} \times 6e^- = 24e^- \quad -12e^- \text{ (6 bonds} \times 2e^- \text{ used/bond)}$$

$$2 \text{ H} \times 1e^- = 2e^- \quad 20e^- \text{ to distribute}$$

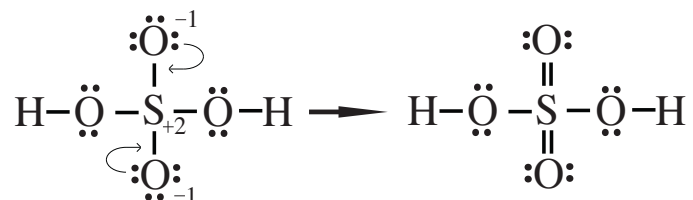
$$\text{Total valence electrons} \quad 32e^-$$



The two Hs 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.

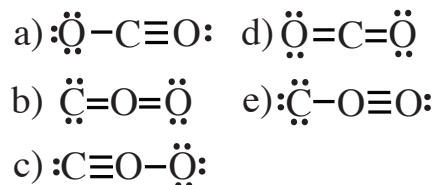


We have formal charges which sum to zero, and that is good. However, we would like to see no charges if possible, and it is possible because the central atom is S, and it is found in period 3. We move lone pairs of electrons from the oxygen atoms into their bond with sulfur. Each O loses a negative charge,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

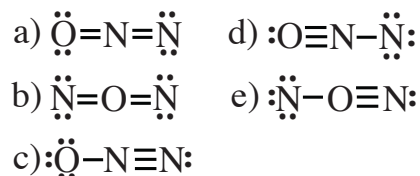


The S atom now has 12 electrons surround it, but that is acceptable because S has empty nd ($n=3$) orbitals in which electrons can reside.

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



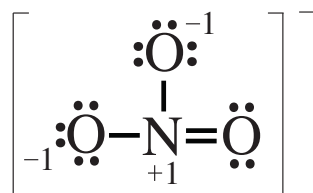
The following is another problem in picking the best Lewis structure for a molecule. In this case, we look at N_2O , nitrous oxide, or laughing gas used in dentistry.



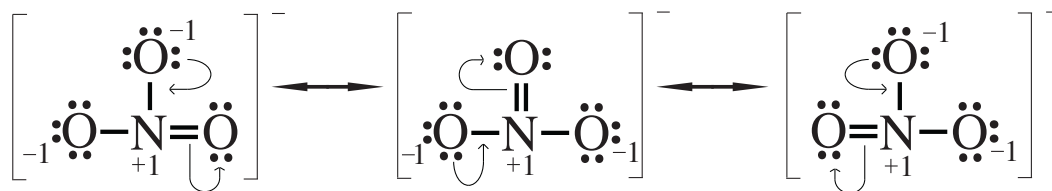
There is one more molecular strategy that can overcome the problem of formal charges. It is the chemical equivalent of a mule, and it is called resonance.

VII. RESONANCE.

NO_3^{1-} , the nitrate ion, will be used to illustrate resonance.



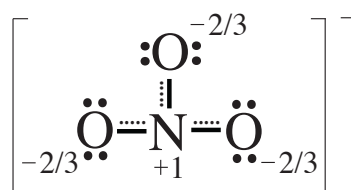
Each atom has an octet, and one of the negative charges matches the ionic charge, while the other negative charge cancels the positive charge on the N atom. There is not a way to get rid of the positive charge and one of the negative charges. If the negative charge can be shared among the three oxygen 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.

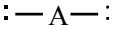
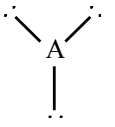
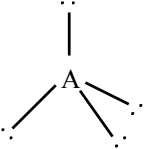
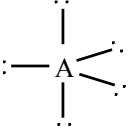
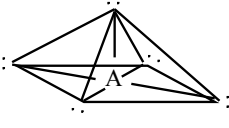
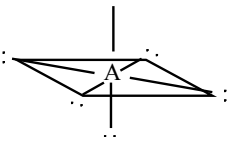
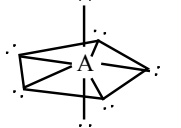
Consider a similar blending of characteristics in the biological world. The mating of a horse with a donkey produces a hybrid we call a mule. A mule is not a horse at one moment in time and a donkey at another. A mule has characteristics of both parents at all times.

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.



VIII. APPLICATION OF VSEPR THEORY.

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

PAIRS OF e ⁻	GEOMETRY	BOND ANGLE	NAME OF SHAPE
2		180°	Linear
3		120°	Trigonal planar
4		109.5°	Tetrahedral
5		90°, 120°, 180°	Trigonal bipyramidal
5		90°	Square pyramid
6		90°, 180°	Octahedral
7		90°, 108°, 180°	Pentagonal bipyramidal

II. When placing additional atoms (B) on all of the electron pairs of the central atom (A).

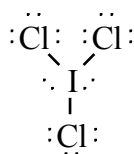
A. Treat double bonds as though they were single bonds.

B. Naming molecules with no lone pairs.

PAIRS OF e ⁻	CLASS	ANGLE	NAME OF MOLECULE
2	AB ₂	180°	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

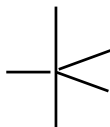
- III. When placing atoms (B) and one or more lone pairs of electrons (E) on a central atom (A).
- The name of the molecule is based on the atoms only, not the atoms and the lone pairs.
 - Treat double bonds as though they were single.
 - To determine the best shape of the molecule, if more than one possibility exists, use these simple rules:
 - in a trigonal bipyramid, put lone pairs in an equatorial position;
 - in a pentagonal bipyramid, put lone pairs in an axial placement;
 - for an octahedron, lone pairs should be opposite (trans to) each other;
 - put the least electronegative additional atoms (B) in equatorial positions.
 - Example. What is the correct shape of ICl_3 ?

1. **Draw the Lewis structure.**



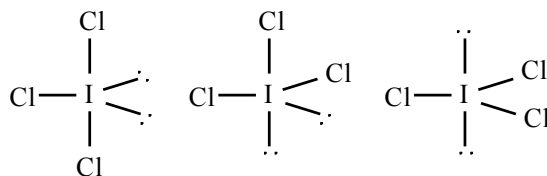
2. **Pick the correct shape.**

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:



(a)

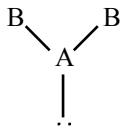
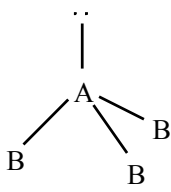
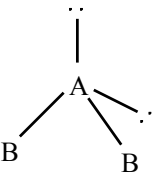
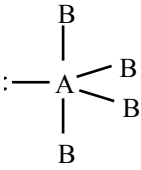
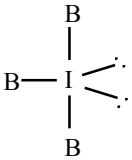
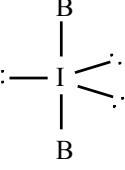
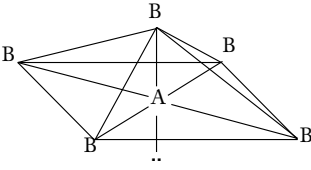
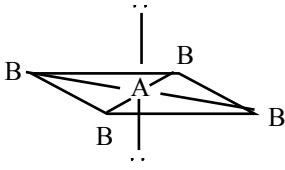
(b)

(c)

5. **Pick the shape with the lowest energy.**

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

E. Naming molecules with one or more lone pairs.

PAIRS OF e ⁻	LONE PAIRS	CLASS	SHAPE	NAME OF MOLECULE
3	1	AB ₂ E		Bent triatomic
4	1	AB ₃ E		Trigonal pyramidal
4	2	AB ₂ E ₂		Bent triatomic
5	1	AB ₄ E		Seesaw (distorted tetrahedron, folded square)
5	2	AB ₃ E ₂		T shaped
5	3	AB ₂ E ₃		Linear triatomic
6	1	AB ₅ E		Square pyramidal
6	2	AB ₄ E ₂		Square planar

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, build their models, and then name their geometries. Note that a peg without another atom center attached to it represents a lone pair of electrons.

EASY (Models can be built with VSEPR I Kit)

- | | | |
|-----------|----------------|----------------|
| 1. F_2 | 5. HCN | 8. CO_3^{2-} |
| 2. N_2O | 6. HSCN | 9. OCl_2 |
| 3. H_2S | 7. PH_4^{1+} | 10. CH_2O |
| 4. PF_3 | | |

HARD (Models can be built 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. $SeCl_4$ | | |

* 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 II Lab Instructions

1. Obtain one VSEPR II Kit for your group.
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. Draw the electron dot structure first and use it to determine the molecular structure.
5. In the column labeled “Structural Formula,” draw the three dimensional shape of the molecule or ion.
6. In the column labeled “Shape/Angle,” the shape name should go on top (such as linear, bent, etc.), and the angle in degrees goes on the bottom. The shape is determined by the position of the atoms, not the bonds.
7. In the column labeled “Formal Charge A,” write the formal charge of the central atom in the structure.
8. In the column labeled “Formal Charge B,” write the formal charge of the atoms bonded to the central atom.
9. 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.
10. Place a purple paddle, representing a lone pair of electrons, into any unfilled hole of any atom. In the column labeled “# of lone pairs,” write the number of pairs of nonbonding electrons in the entire structure.
11. In the column labeled “Hybrid Orbitals,” describe the type of hybridization of the central atom, e.g. sp^3 .

LAB ASSESMENTS FOLLOW

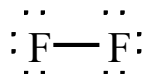
Names_____ VSEPR II Lab Date_____ Period_____

Chemical Formula	Electron Dot Structure	Structural Formula	Model Checked	Shape Angles °	Formal Charge A	Formal Charge B	# of bonds	# of lone pairs	Hybrid Orbitals
PF_5									
TeF_4									
XeF_4									
PF_3^{2-}									
XeF_2									
SF_4									
SF_5^{1-}									
SF_6									
SO_4^{2-}									

1. Valence electrons are found
 - a. only in elements beyond the second row
 - b. only in metal atoms
 - c. only in nonmetal atoms
 - d. only in the inner core of electron shells
 - e. none of the above
2. The octet rule
 - a. is followed by all atoms
 - b. is followed by some atoms, but not all
 - c. is followed by all atoms in the second row except for carbon
 - d. is always followed by third row elements
 - e. none of the above
3. An expanded octet refers to
 - a. eight electrons around a central atom in a molecule
 - b. eight electrons around a peripheral atom in a molecule
 - c. eight electrons around an atom that has a large diameter
 - d. an atom with more than eight electrons in its p orbitals
 - e. none of the above
4. In order for an atom to obtain an expanded octet, the atom must
 - a. have an expanded s orbital
 - b. have an extra p orbital
 - c. have an available d orbital
 - d. have access to expanded electrons
 - e. have only a tetrahedral shape
5. The elements that obey the octet rule
 - a. have d orbitals
 - b. have s orbitals
 - c. have p orbitals
 - d. all of the above
 - e. none of the above
6. Which of the following is the orbital hybridization for steric number 6?
 - a. sp^3d
 - b. sp^3
 - c. sp
 - d. d^3sp^3
 - e. d^2sp^3
7. What is the formal charge of S in SF_5^{1-} ?
 - a. 0
 - b. 1-
 - c. 2-
 - d. 3-
 - e. 4-

8. What is the shape of a molecule in class AB_3E ?
- bent triatomic
 - trigonal pyramidal
 - bent triatomic
 - see-saw
 - cannot be determined
9. How many lone pairs of electrons can be drawn on the electron dot structure of XeF_2 ?
- 9
 - 8
 - 7
 - 6
 - 0
10. How many total bonds (single plus double) are in a molecule of H_3PO_4 ?
- 9
 - 8
 - 7
 - 6
 - 0

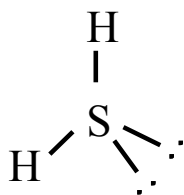
ANSWERS TO EASY STRUCTURES.



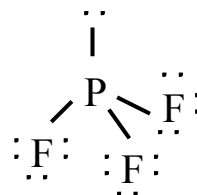
1. F_2
linear



2. N_2O
linear



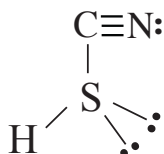
3. H_2S
bent



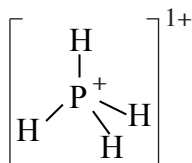
4. PF_3
trigonal pyramidal



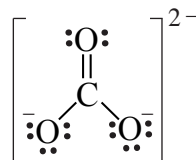
5. HCN
linear



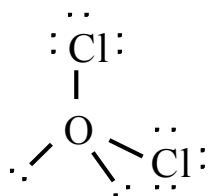
6. HSCN
bent



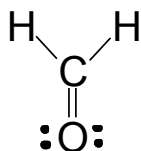
7. PH_4^{1+}
tetrahedral



8. CO_3^{2-}
trigonal planar

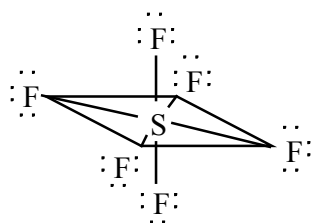


9. OCl_2
bent

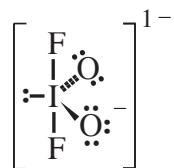


10. CH_2O
trigonal planar

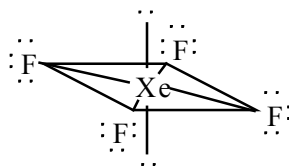
ANSWERS TO HARD STRUCTURES.



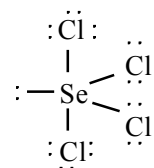
11. SF_6
octahedral



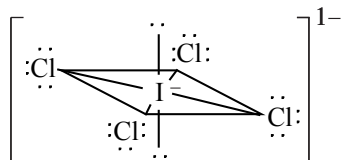
12. $\text{IO}_2\text{F}_2^{1-}$
see-saw



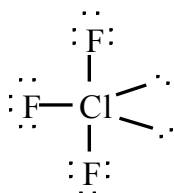
13. XeF_4
square planar



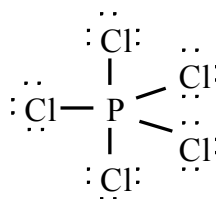
14. SeCl_4
see-saw



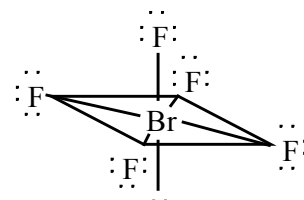
15. ICl_4^{1-}
square planar



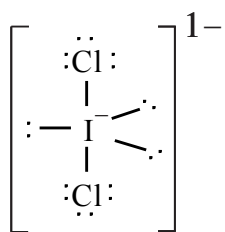
16. ClF_3
T-shaped



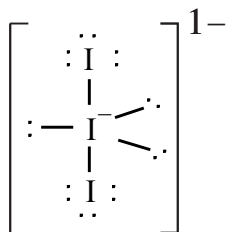
17. PCl_5
trigonal bipyramid



18. BrF_5
square pyramid



19. ICl_2^{1-}
linear



20. I_3^{1-}
linear

ANSWERS TO LAB ASSESSMENTS

Names _____

VSEPR II Lab

Date _____ Period _____

Chemical Formula	Electron Dot Structure	Structural Formula	Model Checked	Shape Angles °	Formal Charge A	Formal Charge B	# of bonds	# of lone pairs	Hybrid Orbitals
PF ₅				trigonal bipyramidal 120/90	0	0	5	15	sp ³ d
TeF ₄				See Saw 90/170	0	0	4	13	sp ³ d
XeF ₄				Square Planar 90	0	0	4	14	sp ³ d ²
PF ₃ ²⁻				T Shaped 90	-2	0	3	11	sp ³ d
XeF ₂				Linear 180	0	0	2	9	sp ³ d
SF ₄				See Saw 90/170	0	0	4	13	sp ³ d
SF ₅ ¹⁻				Square Pyramidal 90	-1	0	5	16	sp ³ d ²
SF ₆				Octahedral 90	0	0	6	18	sp ³ d ²
SO ₄ ²⁻				Tetrahedral 109.5	0	2(-1) 2(0)	6	10	sp ³

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ANSWERS TO QUIZ

1. e
2. b
3. e
4. c
5. d
6. e
7. b
8. b
9. a
10. b

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.