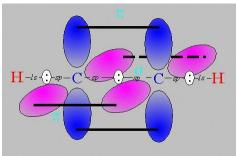
#### Homework #7

## **Chapter 14**

### **Covalent Bonding Orbitals**

- 7. Both MO theory and LE model use quantum mechanics to describe bonding. In the LE model, wavefunctions on one atom are mixed to form hybridized orbitals. In MO theory wavefunctions on all of the atoms in the structure are mixed to form new molecular orbits. When mixing orbitals in either MO or LE the same number of orbitals that you put in is the number that you get out. LE model breaks down for some structures, for instants it is not able to predict the magnetic properties of O<sub>2</sub> or the existence of B<sub>2</sub>H<sub>6</sub>. In addition, resonance structures are not explained by LE model. MO theory is able to fix all of these problems.
- 12. Single bonds have their electron density concentrated between the two atoms (on the internuclear axis). Therefore, an atom can rotate freely on the internuclear axis. Double and triple bonds have their electron density located above and to the side of the internuclear axis (see below). Therefore, in order for an atom to rotate on the internuclear axis (while the other atom is stationary) the double and/or triple bonds would need to be broken.



16. LE (Local Electron) Model Hybridizations

•	,		,				
	2(H)	С	0	Total			
Valence e⁻	2(1)	4	6	12			
Wanted e	2(2)	8	8	20			
 $bonds = \frac{wc}{e}$ $e^{-} = valence$	nted – 2 ce – 2(	2		$=\frac{20-3}{2}$ $=12-2$	= 4		
*O*    H-C-H							

 $H_2CO$  is a trigonal planer molecule. The central carbon atom is  $sp^2$  hybridized and the oxygen atom is  $sp^2$  hybridized. Two of the  $sp^2$  hydride orbitals, on the carbon, are used in C-H single bonds ( $\sigma$  bond). The C-H single bonds are formed from the overlap of the  $sp^2$  hybridized orbital on the carbon. There is a double bond between the C-O (1  $\sigma$  bond and 1  $\pi$  bond). The  $\sigma$  bond is formed from the overlap of the  $sp^2$  hybridized orbital,

on the carbon, and the sp<sup>2</sup> hybridized orbital on the oxygen. The  $\pi$  bond is formed from the overlap of the 2 unhybridized p orbitals on the carbon and the oxygen atoms. The loan pair electrons on the oxygen atom are located in sp<sup>2</sup> hybridized orbitals.

	2(H)	2(C)	Total
Valence e	2(1)	2(4)	10
Wanted e	2(2)	2(8)	20

# bonds = 
$$\frac{wanted - valence}{2} = \frac{20 - 10}{2} = 5$$
  
#  $e^- = valence - 2(\#bonds) = 10 - 2(5) = 0$   
# bonds =  $\frac{Wanted - Valence}{2} = \frac{20 - 10}{2} = 5$   
#  $e^- = Valence - 2(\#bonds) = 10 - 2(5) = 0$ 

# $H-C \equiv C-H$

H<sub>2</sub>C<sub>2</sub> is a linear molecule. The central carbon atoms are sp hybridized. On each carbon atom, one of the sp hybridized orbitals overlaps with a s orbital on the hydrogen atom to form a H-C single bonds ( $\sigma$  bonds). There is a triple bond between the carbons (1  $\sigma$  bond and 2 $\pi$  bonds). The  $\sigma$  bond is formed from the overlap of the sp hybridized orbitals on each carbon atom. The two  $\pi$  bonds are formed from the overlap of the 4 unhybridized p orbitals (2 on each carbon) on the carbons.

		С	4(F)	Total
Va	lence e⁻	4	4(7)	32
Wa	anted e⁻	8	4(8)	40

# bonds = 
$$\frac{wanted - valence}{2} = \frac{40 - 32}{2} = 4$$
  
#  $e^- = valence - 2(\#bonds) = 32 - 2(4) = 24$ 

Molecular Structure =Tetrahedral

C Hybridization=sp<sup>3</sup>

Bond Angles = 109.5°

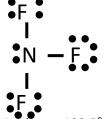
Polar/Non Polar = Non Polar

$$\# \ bonds = \frac{wanted - valence}{2} = \frac{32 - 26}{2} = 3$$

$$\# e^- = valence - 2(\#bonds) = 26 - 2(3) = 20$$

Molecular Structure = Trigonal Pyramidal

N Hybridization=sp<sup>3</sup>



Bond Angles = <109.5°

Polar/Non Polar = Polar

c)		0	2(F)	Total
٠,	Valence e	6	2(7)	20
	Wanted e	8	2(8)	24

# bonds = 
$$\frac{wanted - valence}{2}$$
 =  $\frac{24 - 20}{2}$  = 2  
#  $e^-$  =  $valence - 2$ (#bonds) =  $20 - 2$ (2) = 16

Molecular Structure = Bent

Bond Angles = <109.5°

Polar/Non\_Polar = Polar

d)		В	3(F)	Total
	Valence e	3	3(7)	24

Boron is known to not obey the octet rule.

Molecular Structure = Trigonal Planer

It is known to form only 3 bonds allowing the formal charge on B to be 0.

Bond Angles = 120°

B Hybridization=sp<sup>2</sup>

Polar/Non Polar = Non Polar

Η

Be

Н

e) BeH<sub>2</sub> is a covalent compound because the difference

in electronegativity between the Be and H is only 0.6.  $\,$ 

	Be	2(H)	Total
Valence e⁻	2	2(1)	4

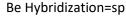
Beryllium is known to not obey the octet rule.

It is known to form only 2 bonds allowing the formal charge on Be to be 0.

Bond Angles = 180°

Molecular Structure = Linear

Polar/Non Polar = Non Polar

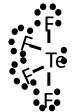


f)		Te	4(F)	Total
	Valence e	6	4(7)	34

Te must expand its octet to accommodate all of the electrons/atoms

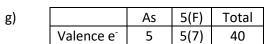
Molecular Structure = See-Saw

Te Hybridization=sp<sup>3</sup>d



Bond Angles = <120° and <90°

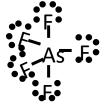
Polar/Non Polar = Polar



As must expand its octet to accommodate all of the F atoms

Molecular Structure = Trigonal Bipyramidal

As Hybridization=sp<sup>3</sup>d



Bond Angles =  $120^{\circ}$  and  $90^{\circ}$ 

Polar/Non Polar = Non Polar

h)

	Kr	2(F)	Total
Valence e	8	2(7)	22

Kr must expand its octet to accommodate all of the electrons

Molecular Structure = Linear

Kr Hybridization=sp3d

	Kr	4(F)	Total	i)
Valence e⁻	8	4(7)	36	

Kr must expand its octet to accommodate all of the electrons

Molecular Structure = Square Planer

Kr Hybridization=sp<sup>3</sup>d<sup>2</sup>



	Se	6(F)	Total
Valence e	6	6(7)	48

Se must expand its octet to accommodate all of the atoms

Molecular Structure = Octahedral

Se Hybridization=sp<sup>3</sup>d<sup>2</sup>

k)

		5(F)	Total
Valence e⁻	7	5(7)	42

I must expand its octet to accommodate all of the electrons/atoms

Molecular Structure = Square Pyramidal

I Hybridization=sp<sup>3</sup>d<sup>2</sup>

i)

	1	3(F)	Total
Valence e⁻	7	3(7)	28

I must expand its octet to accommodate all of the electrons/atoms

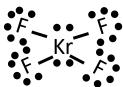
Molecular Structure = T-Shaped

I Hybridization=sp<sup>3</sup>d



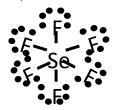
Bond Angles = 180°

Polar/Non Polar = Non Polar



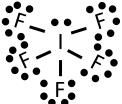
Bond Angles = 90°

Polar/Non Polar = Non Polar



Bond Angles = 90°

Polar/Non Polar = Non Polar



Bond Angles = <90° and <90°

Polar/Non Polar = Polar



Bond Angles = <90°

Polar/Non Polar = Polar

24. a)

	S	2(0)	Total
Valence e	6	2(6)	18
Wanted e⁻	8	2(8)	24

$$0-S=0 \iff 0=S-0$$

$$\# \ bonds = \frac{wanted-valence}{2} = \frac{24-18}{2} = 3$$

$$\# e^- = valence - 2(\#bonds) = 18 - 2(3) = 12$$

Molecular Structure = Bent Bond Angles = <120° S Hybridization = sp<sup>2</sup>

b)

	S	3(0)	Total
Valence e	6	3(6)	24
Wanted e	8	3(8)	32

# bonds = 
$$\frac{wanted - valence}{2} = \frac{32 - 24}{2} = 4$$
  
#  $e^- = valence - 2(\#bonds) = 24 - 2(4) = 16$ 

$$0 = S - O \iff 0 - S = O \iff 0 - S - O$$

Molecular Structure = Trigonal Planer Bond Angles = 120° S Hybridization = sp<sup>2</sup>

Wanted e | 2(8) | 3(8) | 40 |   
# bonds = 
$$\frac{wanted - valence}{2} = \frac{40 - 32}{2} = 4$$

$$\# e^- = valence - 2(\#bonds) = 32 - 2(4) = 24$$

Molecular Structure = Tetrahedral

 $\frac{32}{2(4)} = 4$ Bond Angles = 109.5° S Hybridization = sp<sup>3</sup>

d)		2(S)	8(O)	e⁻	Total
	Valence e	2(6)	8(6)	+2	62
	Wanted e⁻	2(8)	8(8)		80

$$\# bonds = \frac{wanted - valence}{2} = \frac{80 - 62}{2} = 9$$

$$\# e^- = valence - 2(\#bonds) = 62 - 2(9) = 44$$

Molecular Structure = Tetrahedral (around S) Bent (around central O)

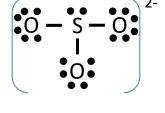
Bond Angles = 109.5° (around S) and <109.5° (around central O) S Hybridization = sp<sup>3</sup>

٥١		S	3(0)	e <sup>-</sup>	Total
e)	Valence e	6	3(6)	+2	26
	Wanted e	8	3(8)		32

# bonds = 
$$\frac{wanted - valence}{2} = \frac{32 - 26}{2} = 3$$
  
#  $e^- = valence - 2(\#bonds) = 26 - 2(3) = 20$ 

Molecular Structure = Trigonal Pyramidal

S Hybridization =  $sp^3$ 



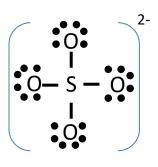
Bond Angles = <109.5°

t/					
')		S	4(O)	e <sup>-</sup>	Total
	Valence e	6	4(6)	+2	32
	Wanted e⁻	8	4(8)		40

# bonds = 
$$\frac{wanted - valence}{2} = \frac{20 - 12}{2} = 4$$
  
# bonds =  $\frac{wanted - valence}{2} = \frac{40 - 32}{2} = 4$   
#  $e^- = valence - 2(\#bonds) = 32 - 2(4) = 24$ 

Molecular Structure = Tetrahedral

S Hybridization = sp<sup>3</sup>



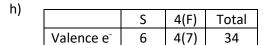
Bond Angles = 109.5°

$$\#\ bonds = \frac{wanted-valence}{2} = \frac{20-12}{2} = 4$$

# bonds = 
$$\frac{wanted - valence}{2} = \frac{24 - 20}{2} = 2$$
  
#  $e^- = valence - 2(\#bonds) = 24 - 2(2) = 20$ 

Molecular Structure = Bent

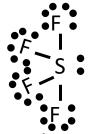
Bond Angles =  $<109.5^{\circ}$  S Hybridization =  $sp^{3}$ 



Sulfur must expand its octet to accommodate all of the electrons/atoms

Molecular Structure = See-Saw

Bond Angles =  $<90^{\circ}$  and  $<120^{\circ}$ 



S Hybridization =  $sp^3d$ 

i)		S	6(F)	Total
	Valence e	6	6(7)	48

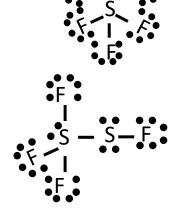
Sulfur must expand its octet to accommodate all of the electrons/atoms Molecular Structure = Octahedral

Bond Angles = 
$$90^{\circ}$$
 S Hybridization =  $sp^3d^2$ 

j)		2(S)	4(F)	Total
	Valence e	2(6)	4(7)	40

Sulfur must expand its octet to accommodate all of the electrons/atoms Molecular Structure = See-Saw and Bent

Bond Angles =  $<90^{\circ}$ ,  $<120^{\circ}$ , and  $<109.5^{\circ}$ 



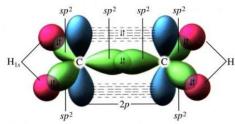
S Hybridization = sp<sup>3</sup>d and sp<sup>3</sup>

25.		4(H)	2(C)	Total
	Valence e	4(1)	2(4)	12
	Wanted e	4(2)	2(8)	24

# bonds = 
$$\frac{wanted - valence}{2} = \frac{24 - 12}{2} = 6$$
  
#  $e^- = valence - 2(\#bonds) = 12 - 2(6) = 0$ 

$$C = CH$$

The hybridization around both carbons is  $sp^2$  hybridized, making the shape trigonal planer around each carbon. The  $\sigma$  bond of the double bond is formed form the overlap of a  $sp^2$  hybridized (green) orbital on each C. The  $\pi$  bond of the double bond is formed from the overlap of the p orbitals (blue) that are in the plane of the page. Therefore, the remaining  $sp^2$  hybrid orbitals are all in plane with each other. Making the H's in the same plane so that they can form  $\sigma$  bonds with the carbons from the overlap of the s orbitals on the hydrogens and the  $sp^2$  hybridized orbitals on the carbons.



26. In order for the central carbon atom to form two double bonds, one of the double bonds must be formed with p orbitals into/out of the page and the other double bond must be formed with p orbitals in the plane of the page. Therefore, the hydrogens on either end will be oriented 90° from each other.



27.

	6(H)	2(0)	4(C)	Total
Valence e⁻	6(1)	2(6)	4(4)	34
Wanted e⁻	6(2)	2(8)	4(8)	60

$$\#\ bonds = \frac{wanted-valence}{2} = \frac{60-34}{2} = 13$$

$$\# e^{-} = valence - 2(\#bonds) = 34 - 2(13) = 8$$

CCO bond angles all = 120°

carbon hybridization (list in order of appearance in structure) =  $sp^3$ ,  $sp^2$ ,  $sp^2$ ,  $sp^3$ 

$$\sigma$$
 bonds = 11  $\pi$  bonds = 2

In this structure only the carbons that are circled have to be in the same plane and the carbons that are squared have to be in the same plan. If the  $\sigma$  bond between the two carbons that have double bonded oxygen's is aligned carefully then all of the carbons can be in the same plane.

	8(H)	2(0)	4(C)	Total
Valence e	8(1)	2(6)	4(4)	36
Wanted e	8(2)	2(8)	4(8)	64

$$\# \ bonds = \frac{wanted - valence}{2} = \frac{64 - 36}{2} = 14$$

$$\#e^{-} = valence - 2(\#bonds) = 36 - 2(14) = 8$$

CCO bond angles =  $109.5^{\circ}$  and  $120^{\circ}$ 

C hybridization (list in order of appearance in structure) =  $sp^3$ ,  $sp^3$ ,  $sp^2$ ,  $sp^3$ 

$$\sigma$$
 bonds = 13  $\pi$  bonds = 1

п п •	$\mathcal{J}_{ullet}$ $\square$
120.°	120.°
H-C-C-	C - C - H
H - C - C - C - C - C - C - C - C - C -	
103.5	
•••	11
H :0:	Н
.*.	
H	
an3 an2 an3	

Ц

28.

	3(H)	Ν	3(C)	Total
Valence e	3(1)	5	3(4)	20
Wanted e	3(2)	8	3(8)	38

$$\# bonds = \frac{wanted - valence}{2} = \frac{38 - 20}{2} = 9$$

$$\# e^- = valence - 2(\#bonds) = 20 - 2(9) = 2$$

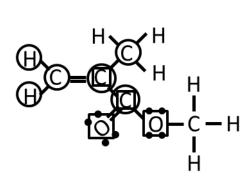
carbon hybridization (listed in the order that they appear in the structure) =  $sp^2$ ,  $sp^2$ , sp

$$\sigma$$
 bonds = 6  $\pi$  bonds = 3

All atoms are in the same plane.

	8(H)	0	5(C)	Total
Valence e⁻	8(1)	2(6)	5(4)	40
Wanted e	8(2)	2(8)	5(8)	72

# bonds = 
$$\frac{wanted - valence}{2} = \frac{72 - 40}{2} = 16$$
  
#  $e^- = valence - 2(\#bonds) = 40 - 2(16) = 8$ 



carbon hybridization (listed in the order that they appear in the structure) =  $sp^2$ ,  $sp^2$ ,  $sp^3$ ,  $sp^2$ ,  $sp^3$  Bond angles:  $d = 120.^\circ$ ,  $e = 120.^\circ$ ,  $f = <109.5^\circ$ 

 $\sigma$  bonds = 14  $\pi$  bonds = 2

Atoms with circles around them have to be in the same plane. Atoms with squares around them have to be in the same plane. Depending on the rotation, the atoms with the circles and the atoms with the squares can be in the same plane.

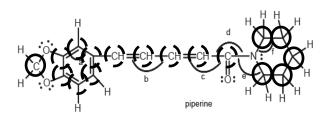
29.

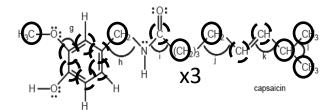
- a) 6 carbon atoms are sp<sup>3</sup> hybridized (carbons cycles in solid circle)
- b) 4 carbon atoms are sp<sup>2</sup> hybridized (carbons cycles in dashed line)
- c) The boxed nitrogen atom is sp hybridized
- d) 33  $\sigma$  bonds
- e)  $5 \pi$  bonds

f) 180°

- g) <109.5°
- h) sp<sup>3</sup>

30. a)





b) piperine

6 carbon atoms sp<sup>3</sup> hybridized (circled with solid line)

11 carbons atoms sp<sup>2</sup> hybridized (circles with dashed line)

0 carbon atoms sp hybridized

### capsaicin

9 carbon atoms sp<sup>3</sup> hybridized (circled with solid line)

9 carbons atoms sp<sup>2</sup> hybridized (circles with dashed line)

0 carbon atoms sp hybridized

c) piperine

The nitrogen is sp<sup>3</sup> hybridized.

### capsaicin

The nitrogen is sp<sup>3</sup> hybridized.

d)	a.	120°	b.	120°	c.	120°
	d.	120°	e.	<109.5°	f.	109.5°
	g.	120°	h.	109.5°	i.	120°
	j.	109.5°	k.	120°	l.	109.5°

34. a)



The bonding orbital is seen above. This is the bonding orbital because there is electron density between the nucleuses of the atoms (black dots).





The antibonding orbital is seen above. This is the antibonding orbital because there is no electron density between the nucleuses of the atoms (black dots).

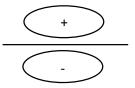
b) The bonding molecular orbital is at a lower energy than the antibonding orbital because the electrons in the area between the nuclei are attracted to two nuclei instead of one.

35. a)



This is a  $\sigma_p$  molecular orbital. The phases of the wavefunctions were the same causing an increase in electron density between the nuclei. It is a sigma molecular orbital because there is cylindrical symmetry. It is a bonding molecular orbital because there is electron density between the nuclei.

b)

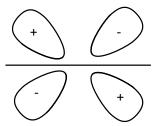


This is a  $\pi_p$  molecular orbital. It is a pie molecular orbital because there is not cylindrical symmetry. It is a bonding molecular orbital because there is electron density above and below the nuclei.



This is a  $\sigma_p^*$  molecular orbital. It is a sigma molecular orbital because there is cylindrical symmetry. It is antibonding because there is no electron density between the nuclei.

d)



This is a  $\pi_p^*$  molecular orbital. It is a pie molecular orbital because there is no cylindrical symmetry. It is antibonding because there is no electron density above and below the nuclei.

42. bond order = 
$$\frac{\text{\# bonding } e^- + \text{\# antibonding } e^-}{2}$$

If the bonding order is greater than zero then the species is predicted to be stable.

a) 
$$H_2^+ = (\sigma_{1s})^1$$

bond order = 
$$\frac{1-0}{2} = \frac{1}{2}$$
 stable

$$H_2 = (\sigma_{1s})^2$$

bond order = 
$$\frac{2-0}{2}$$
 = 1 stable

$$H_2^- = (\sigma_{1s})^2 (\sigma_{1s}^*)^1$$

bond order = 
$$\frac{2-1}{2} = \frac{1}{2}$$
 stable

$$H_2^{2-} = (\sigma_{1s})^2 (\sigma_{1s}^*)^2$$

bond order = 
$$\frac{2-2}{2}$$
 = 0 not stable

b) 
$$N_2^{2^-} = (\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2 (\pi_{2p})^4 (\sigma_{2p})^2 (\pi_{2p}^*)^2$$

bond order = 
$$\frac{10-6}{2}$$
 = 2 stable

$$O_2^{2^-} = (\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s}^*)^2 (\sigma_{2s}^*)^2 (\sigma_{2p})^2 (\pi_{2p})^4 (\pi_{2p}^*)^4$$

bond order = 
$$\frac{10-8}{2}$$
 = 1 stable

$$F_2^{2-} = (\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2 (\sigma_{2p}^*)^2 (\sigma_{2p}^*)^4 (\sigma_{2p}^*)^4 (\sigma_{2p}^*)^2$$

bond 
$$order = \frac{10-10}{2} = 0$$
 not stable

c) Be<sub>2</sub> = 
$$(\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2$$

Be<sub>2</sub> = 
$$(\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2$$
  
bond order =  $\frac{4-4}{2}$  = 0 not stable

$$B_2 = (\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s})^2 (\sigma_{2s}^*)^2 (\pi_{2p})^2$$

bond order = 
$$\frac{6-4}{2}$$
 = 1 stable

Ne<sub>2</sub> = 
$$(\sigma_{1s})^2(\sigma_{1s}^*)^2(\sigma_{2s}^*)^2(\sigma_{2s}^*)^2(\sigma_{2p}^*)^2(\pi_{2p}^*)^4(\pi_{2p}^*)^4(\sigma_{2p}^*)^2$$

$$bond\ order = \frac{10-10}{2} = 0$$
 not stable

43. bond order = 
$$\frac{\text{\# bonding } e^- - \text{\# antibonding } e^-}{2}$$

$$N_2=(\sigma_{1s})^2(\sigma_{1s}^*)^2(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2p})^2$$

$$bond\ order = \frac{10-4}{2} = 3$$

Therefore, one way to get a bond order of 2.5 is to add 1 more antibonding e

N<sub>2</sub>=(
$$\sigma_{1s}$$
)<sup>2</sup>( $\sigma_{1s}$ \*)<sup>2</sup>( $\sigma_{2s}$ )<sup>2</sup>( $\sigma_{2s}$ \*)<sup>2</sup>( $\pi_{2p}$ )<sup>4</sup>( $\sigma_{2p}$ )<sup>2</sup>( $\pi_{2p}$ \*)<sup>1</sup>

bond order =  $\frac{10-5}{2}$  = 2.5

Or another way to get a bond order of 2.5 is to remove 1 bonding  $e^ N_2^+=(\sigma_{1s})^2(\sigma_{1s}^*)^2(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2p})^1$ 

$$bond\ order = \frac{9-4}{2} = 2.5$$

46. 
$$F_{2}^{+} = (\sigma_{1s})^{2} (\sigma_{1s}^{*})^{2} (\sigma_{2s}^{*})^{2} (\sigma_{2s}^{*})^{2} (\sigma_{2p}^{*})^{2} (\pi_{2p}^{*})^{4} (\pi_{2p}^{*})^{3}$$

$$bond \ order = \frac{10 - 7}{2} = 1.5$$

1 unpaired e

$$F_2 = (\sigma_{1s})^2 (\sigma_{1s}^*)^2 (\sigma_{2s}^*)^2 (\sigma_{2s}^*)^2 (\sigma_{2p})^2 (\pi_{2p})^4 (\pi_{2p}^*)^4$$

$$bond\ order = \frac{10 - 8}{2} = 1$$

No unpaired e

$$F_{2}^{-} = (\sigma_{1s})^{2} (\sigma_{1s}^{*})^{2} (\sigma_{2s})^{2} (\sigma_{2s}^{*})^{2} (\sigma_{2p})^{2} (\pi_{2p})^{4} (\pi_{2p}^{*})^{4} (\sigma_{2p}^{*})^{2}$$

$$bond \ order = \frac{10 - 9}{2} = 0.5$$

1 unpaired e

Increasing F-F bond length

$$F_2^+ < F_2 < F_2^-$$

48. a) 
$$CN^{+}=(\sigma_{1s})^{2}(\sigma_{1s}^{*})^{2}(\sigma_{2s})^{2}(\sigma_{2s}^{*})^{2}(\pi_{2p})^{4}$$

$$bond\ order = \frac{8-4}{2} = 2$$
Diamagnetic

b) CN=
$$(\sigma_{1s})^2(\sigma_{1s})^2(\sigma_{2s})^2(\sigma_{2s})^2(\sigma_{2s})^4(\sigma_{2p})^4$$
  
bond order =  $\frac{9-4}{2}$  = 2.5

Paramagnetic

C) 
$$CN^{-}=(\sigma_{1s})^{2}(\sigma_{1s}^{*})^{2}(\sigma_{2s})^{2}(\sigma_{2s}^{*})^{2}(\pi_{2p})^{4}(\sigma_{2p})^{2}$$

$$bond\ order = \frac{10-4}{2} = 3$$
Diamagnetic

Increasing bond length

$$CN^- < CN < CN^+$$

**Increasing Bond Energy** 

55. Delocalized  $\pi$  bonding: Is when electrons are spread out over several atoms instead of being concentrated between/around 2 atoms. This phenomenon happens anytime that you have resonance structures. It also explains why you only see 1 bond length in structures that have two types of bonds.

$$H \quad H \quad H \quad H \quad H$$

$$C = C \quad C - H$$

$$C - C \quad C = C$$

$$C = C \quad C = C$$

$$C = C \quad C = C$$

$$C = C \quad C = C$$

In  $C_6H_6$  the delocalized bonding electrons are spread out over the entire ring causing the carbon –carbon bond length to be in-between a single and a double bond length. All carbon-carbon bond lengths are the same.

$$0-S=0 \iff 0=S-0.$$

In  $SO_2$ , the electrons are spread over both of the sulfur oxygen bonds causing the sulfur-oxygen bond length to be in-between a single and a double bond length. All sulfur-oxygen bond lengths are the same.

57.

The LE model says that the central carbon atom is  $sp^2$  hybridized and that the  $sp^2$  hybrid orbitals on the carbon atoms overlap with either the  $sp^2$  (double bonded O atom) or  $sp^3$  (single bonded O atoms) to form 3 sigma bonds. The carbon atom has one unhybridized p orbital that overlaps with a p orbital on the double bonded oxygen atom to form  $1\pi$  bond. This localized  $\pi$  bond moves from one position to another. In the molecular orbital model all of the oxygen atoms have p orbitals that form a delocalized  $\pi$  bonding network with the  $\pi$  electrons spread out over the molecule.

$$\begin{array}{c} CH_3 \\ CH_2 \\ CH$$

All of the carbon atoms are sp<sup>3</sup> hybridized except for the two with "\*" by them, they are sp<sup>2</sup> hybridized. All of the carbon atoms are not in the same plane; sp<sup>3</sup> hybridized structures have bond angles of 109.5 and only 2 atoms, of the four, can be in the same plane.