CHEM110 Tutorial 4 (Week 4) – Chapter 5 Chemical Bonding and Molecular Structure

1. For each of the following pairs, identify which elements tends to attract electron density from the other in a covalent bond: (a) C and N (b) S and H (c) Zn and I (d) S and As

The more electronegative element will attract the electron density from the other. Therefore the answers here are: (a) N (b) S (c) I (d) S

2. Show the direction of bond polarity for the following bonds using δ+/δ- notation: (a) Si–O (b) N–C (c) Cl–F (d) Br–C

Here the more electronegative atom will attract the electron density of the other atom rendering it more negative (δ-). The less electronegative atom will therefore have a partial positive charge (δ+); the answers for each are given below:

(a) dipole ←
Si—O
δ+ δ–

(b) dipole →
N—C
δ– δ+

(c) dipole ←
Cl—F
δ+ δ–

(d) dipole →
Br—C
δ– δ+

3. Determine the Lewis structures of: (a) NH_3 (b) NH_4^+ (c) H_2N^-

(a) Firstly calculate the number of valence electrons (from the periodic table)

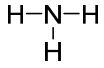
NH_3

N = 5

H = 1 × 3 = 3

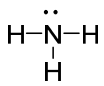
Total = 8 e^-

Next for single bond framework (H on the outside)



6 e- used in bonds therefore 2 left.

Assign remaining electrons onto N



8 e- used in bonds therefore 0 left to assign.

Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$N_{fc} = 5 - 2 - \frac{1}{2}(6)$

$N_{fc} = 0$

$H_{fc} = 1 - 0 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore the Lewis structure is that shown above

(b) Firstly calculate the number of valence electrons (from the periodic table)

NH_4^+

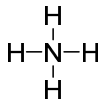
N = 5

H = 1 × 4 = 4

Postive charge = 1 less e^-

Total = 8 e^-

Next for single bond framework (H on the outside)



8 e- used in bonds therefore 0 left.

Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$N_{fc} = 5 - 0 - \frac{1}{2}(8)$

$N_{fc} = +1$

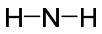
$H_{fc} = 1 - 0 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore the Lewis structure is that shown above

(c) Firstly calculate the number of valence electrons (from the periodic table)

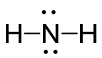
NH_2^-
N = 5
H = 1 × 2 = 2
Negative charge = 1 more e^-
Total = 8 e^-

Next for single bond framework (H on the outside)



4 e- used in bonds therefore 4 left.

Assign remaining electrons onto N



8 e- used in bonds therefore 0 left to assign.

Finally calculate formal charges and reduce if required:
FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)
$N_{fc} = 5 - 4 - \frac{1}{2}(4)$
$N_{fc} = -1$

$H_{fc} = 1 - 0 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore the Lewis structure is that shown above

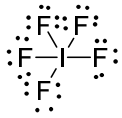
4. Determine the Lewis structure of: (a) IF_5 (b) SO_3 (c) $OPCl_3$ (d) XeF_2

(a) Firstly calculate the number of valence electrons (from the periodic table)
IF_5
I = 7
F = 7 × 5 = 35
Total = 42 e^-

Next for single bond framework (most electronegative atom on the outside; in this case F)

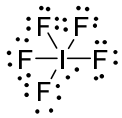
10 e- used in bonds therefore 32 left.

Place 6 valence e^- on each outer atom (except H)



40 e- used therefore 2 left to assign.

Place final e^- on the central I atom



42 e- used.

Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$I_{fc} = 7 - 2 - \frac{1}{2}(10)$

$I_{fc} = 0$

$F_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore no changes are required to the Lewis structure shown above

(b) Firstly calculate the number of valence electrons (from the periodic table)

SO_3

S = 6

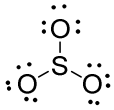
O = 6 × 3 = 18

Total = 24 e^-

Next for single bond framework (most electronegative atom on the outside; in this case F)

6 e- used in bonds therefore 18 left.

Place 6 valence e^- on each outer atom (except H)



24 e- used therefore 0 left to assign.

Finally calculate formal charges and reduce if required:

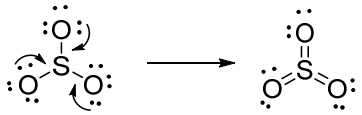
FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$S_{fc} = 6 - 0 - \frac{1}{2}(6)$

$S_{fc} = +3$

$O_{fc} = 6 - 6 - \frac{1}{2}(2) = -1$

Therefore S can share some more electrons present on each O to minimize formal charges on each atom.



Recalculate formal charges to confirm they have been minimised

$S_{fc} = 6 - 0 - \frac{1}{2}(12)$

$S_{fc} = 0$

$O_{fc} = 6 - 4 - \frac{1}{2}(4) = 0$

This is now the correct Lewis structure

(c) Firstly calculate the number of valence electrons (from the periodic table)

$OPCl_3$

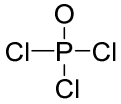
O = 6

P = 5

Cl = 7× 3 = 21

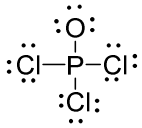
Total = 32 e^-

Next for single bond framework (most electronegative atoms on the outside; in this case Cl and O)



8 e- used in bonds therefore 24 left.

Place 6 valence e^- on each outer atom (except H)



32 e- used in bonds therefore 0 left to assign.

Finally calculate formal charges and reduce if required:

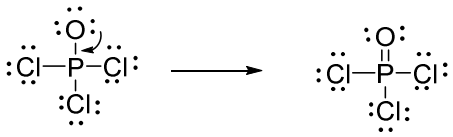
FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$P_{fc} = 5 - 0 - \frac{1}{2}(8) = +1$

$O_{fc} = 6 - 6 - \frac{1}{2}(2) = -1$

$Cl_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

Therefore O can share some more electrons with each P to minimize formal charges on each.



$P_{fc} = 5 - 0 - \frac{1}{2}(10) = 0$

$O_{fc} = 6 - 6 - \frac{1}{2}(4) = 0$

(d) Firstly calculate the number of valence electrons (from the periodic table)

XeF_2

Xe = 8

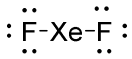
F = 7 × 2 = 14

Total = 22 e^-

Next for single bond framework (most electronegative atom on the outside; in this case F)

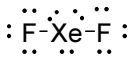
4 e- used in bonds therefore 18 left.

Place 6 valence e^- on each outer atom (except H)



16 e- used therefore 6 left to assign.

Place final 6e^- on the central Xe atom



22 e- used.

Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

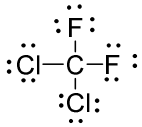
$Xe_{fc} = 8 - 6 - \frac{1}{2}(4) = 0$

$F_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore no changes are required to the Lewis structure shown above

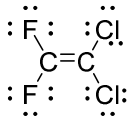
5. Sketch and name the shapes of the following molecules: (a) CF_2Cl_2 (b) SiF_4 (c) PBr_3

(a)

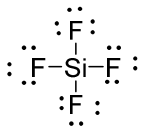


CF_2Cl_2 is tetrahedral

Note the original sheet had the typo CF_2CH_2
in this case each of the carbon atoms would have trigonal planar geometry i.e.

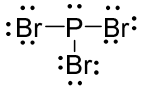


(b)



SiF_4 is tetrahedral

(c)



6. Iodine forms three compounds with chlorine: (a) ICl (b) ICl_3 (c) ICl_5. Determine the Lewis structure, describe the shape and draw a ball-and-stick model of each compound.

(a) Firstly calculate the number of valence electrons (from the periodic table)

ICl
I = 7
Cl = 7
Total = 14 e^-

Next for single bond framework

I—F

2 e- used in bonds therefore 12 left.

Place 6 valence e^- on each outer atom (except H)

42 e- used therefore 0 left to assign.

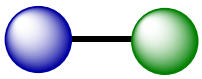
Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$I_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

$Cl_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore no changes are required to the Lewis structure shown above



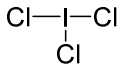
Linear

(c) Firstly calculate the number of valence electrons (from the periodic table)

ICl_3
I = 7
Cl = 7 × 3 = 21

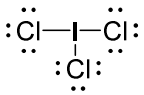
Total = 28 e^-

Next for single bond framework (most electronegative atom on the outside; in this case Cl)



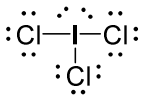
6 e- used in bonds therefore 22 left.

Place 6 valence e^- on each outer atom (except H)



24 e- used therefore 4 left to assign.

Place final e^- on the central I atom



28 e- used.

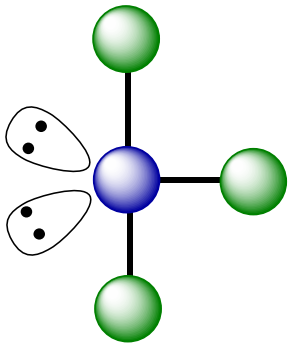
Finally calculate formal charges and reduce if required:

FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)

$I_{fc} = 7 - 4 - \frac{1}{2}(6) = 0$

$Cl_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

Formal charges are already minimized therefore no changes are required to the Lewis structure shown above

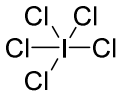


T-shaped

(c) Firstly calculate the number of valence electrons (from the periodic table)

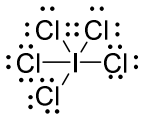
ICl_5
I = 7
Cl = 7 × 5 = 35
Total = 42 e^-

Next for single bond framework (most electronegative atom on the outside; in this case Cl)



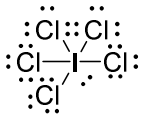
10 e- used in bonds therefore 32 left.

Place 6 valence e^- on each outer atom (except H)



40 e- used therefore 2 left to assign.

Place final e^- on the central I atom

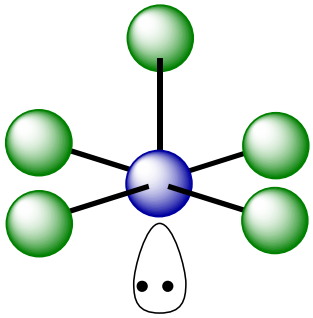


42 e- used.

Finally calculate formal charges and reduce if required:
FC = (Valence e^- for the atomic state of the atom) – (Valence e^- in Lewis structure) - $\frac{1}{2}$(shared e^-)
$I_{fc} = 7 - 2 - \frac{1}{2}(10) = 0$

$Cl_{fc} = 7 - 6 - \frac{1}{2}(2) = 0$

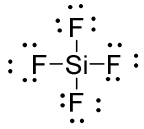
Formal charges are already minimized therefore no changes are required to the Lewis structure shown above



Square pyramidal

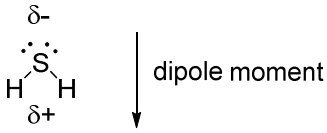
7. Determine the Lewis structures of the following compounds, and determine which have dipole moments. For each molecule that has a dipole moment, draw a ball-and-stick model and include an arrow to indicate the direction of the dipole moment. (a) SiF_4 (b) H_2S (c) XeF_2 (d) $GaCl_3$ (e) NF_3

(a) SiF_4



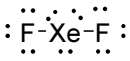
SiF_4 is tetrahedral as each F atom bonded to Si is equivalent it has no dipole moment

(b) H_2S



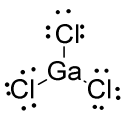
H_2S electron geometry is tetrahedral, its molecular geometry is bent. The molecule has a dipole moment pointing from the partially negatively charged S towards the side of the molecule bearing the H atoms

(c) XeF_2



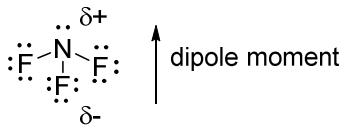
XeF_2 has five sets of electron pairs around Xe, with its 3 lone pairs in equatorial positions, so the molecule is linear without a dipole moment.

(c) $GaCl_3$



$GaCl_3$ has three sets of electron pairs around Ga, so the molecule is trigonal planar and has no dipole moment.

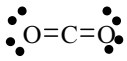
(d) NF_3

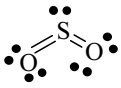


NF_3 molecular geometry is pyramidal and has a dipole moment.

8. Carbon dioxide has no dipole moment, but sulfur dioxide has $\mu = 5.44 \times 10^{-30}$ C m. Use Lewis structures to account for this difference in dipole moments.

The Lewis structure of CO_2 shows no lone pairs on the C atom, thus there are only two sets of electron pairs around C resulting in a linear shape. The two C═O bonds point opposite each other, so bond polarities cancel. The Lewis structure of SO_2 below shows a lone pair on the S atom, resulting in a bent molecule whose polar bonds do not cancel each other.





9. Determine the hybridization of an inner atom in a molecule that has each of the following characteristics: (a) 2 lone pairs and 2 ligands (b) 3 ligands and 1 lone pair (c) 3 ligands and no lone pairs

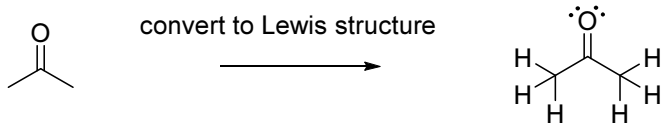
(a) 4 electron domains around a central atom – tetrahedral: there sp^3
(b) 4 electron domains around a central atom – tetrahedral: there sp^3
(c) 3 electron domains around a central atom – tetrahedral: there sp^2

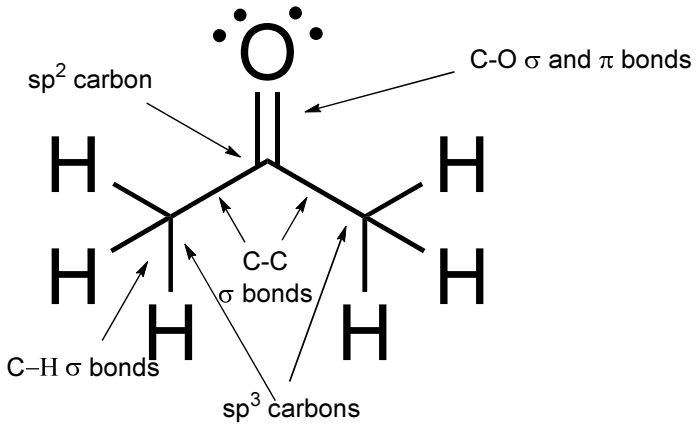
10. Name the hybrid orbitals formed by combining each of the following sets of atomic orbitals: (a) 3*s* and three 3*p* orbitals (b) 2*s* and one 2*p* orbital

(a) sp^3 – s + 3p
(b) sp - s + p

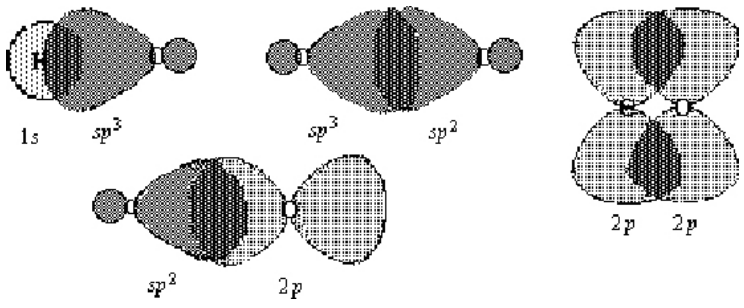
11. Describe the bonding in the common solvent acetone, $(CH_3)_2CO$, and include sketches of all the bonding orbitals.

To determine the bonding pattern from a line structure, first convert the line structure into a molecular structure by adding C and H atoms. Molecular structures contain information to deduce the steric numbers of C, N and O inner atoms without determining the complete Lewis structure. Acetone has three inner C atoms. Two have only single bonds (one C—C and three C—H) and are tetrahedral. The atom bonded to O has one π bond is trigonal planar. In the entire molecule, there are 6 sp^3 (C) – 1s (H) σ bonds, 2 sp^3 (C) – sp^2 (C) σ bonds, 1 sp^2 (C) – 2p (O) σ bond, 1 π bond between C and O, 2 lone pairs in 2s and 2p orbitals on O. The orbital overlap diagrams for acetone are:

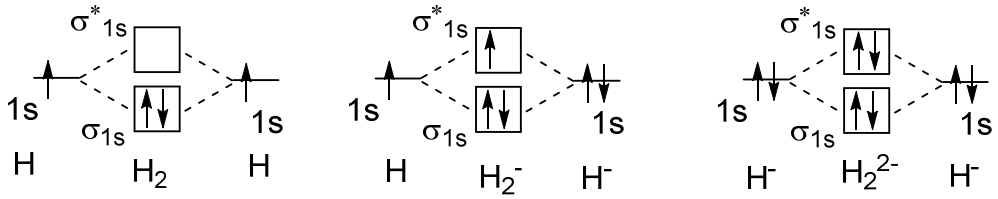




Orbital overlap diagrams shown below



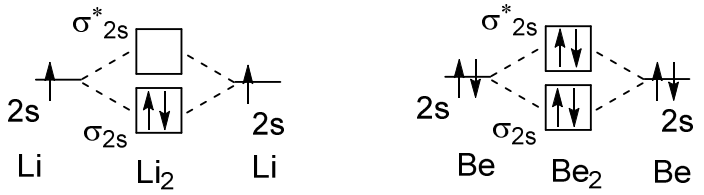
12. Use molecular orbital diagrams to rank the bond energies of the following diatomic species from weakest to strongest: H_2, H_2^-, H_2^{2-}



	H_2	H_2^-	H_2^{2-}
e^- in bonding MOs	2	2	2
e^- in antibonding MOs	0	1	2
BO calc.	BO = ½ (2 – 0)	BO = ½ (2 – 1)	BO = ½ (2 – 2)
BO	1	½	0
	Strongest	middle strength	Weakest (No bond)

13. Dilithium molecules can be generated by vaporizing lithium metal at very low pressure. DO you think it is possible to prepare diberyllium? Explain your reasoning using MO diagrams for Li_2 and Be_2.

Li: each atom has 1 valence electron in the 2s atomic orbital
Be: each atom has 2 valence electrons in the 2s atomic orbital
We combined then to form the MO diagrams of each diatomic molecule as below.

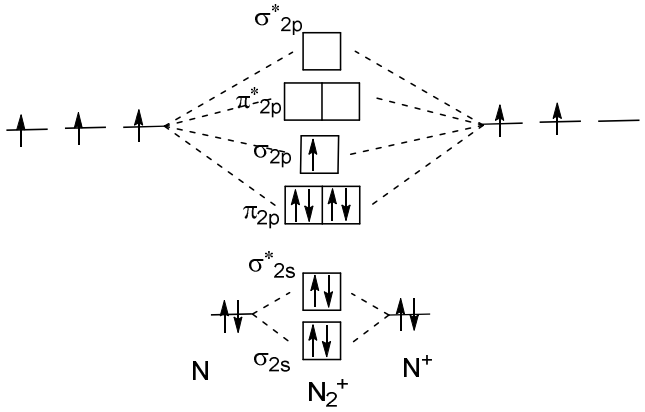


	Li_2	Be_2
e^- in bonding MOs	2	2
e^- in antibonding MOs	0	2
BO calc.	BO = ½ (2 – 0)	BO = ½ (2 – 2)
BO	1	0

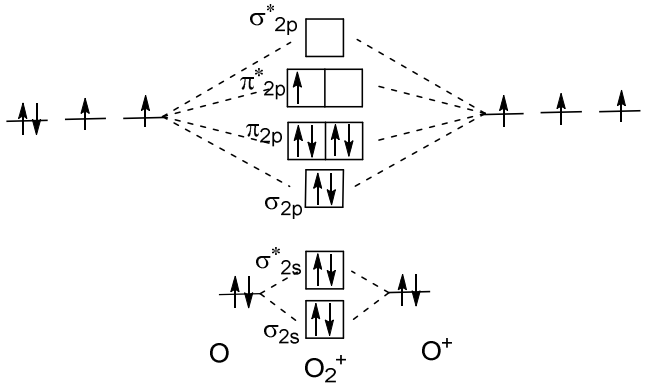
It is not possible to make Be_2

14. Use electron configurations to decide if the following species are paramagnetic or diamagnetic: (a) N_2^+ (b) O_2^+

N has 5 valence electrons; N^+ therefore has 4; The MO diagram is as follows



O has 6 valence electrons; O^+ therefore has 5; The MO diagram is as follows



As both molecules possess unpaired electrons they are both paramagnetic