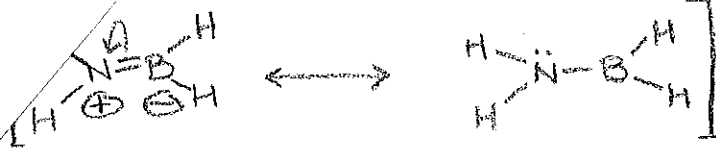
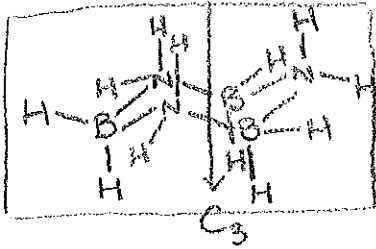


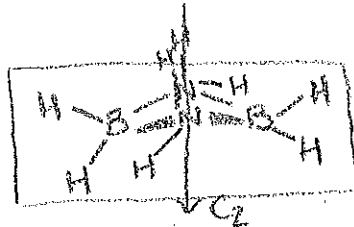
PROBLEM SET #3



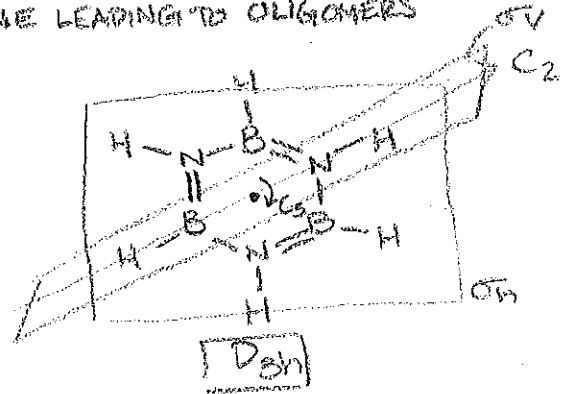
↳ LONE PAIR ON N MAY DONATE TO EMPTY P ORBITAL OF B ON ANOTHER MOLECULE OF AMINO BORANE LEADING TO OLIGOMERS



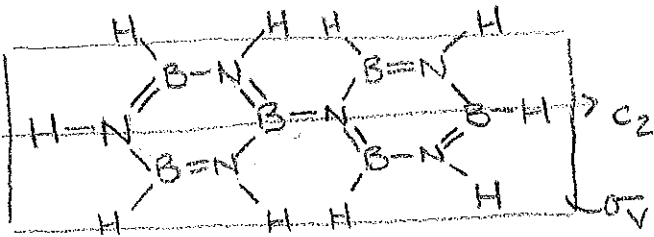
C_{3v}



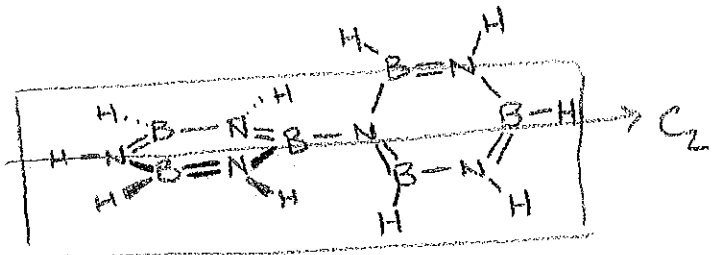
C_{2v}



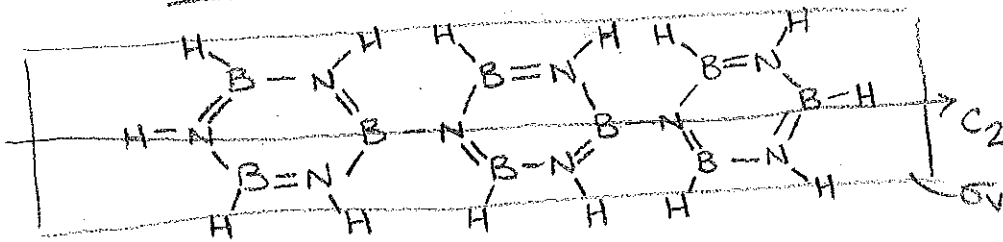
D_{3h}



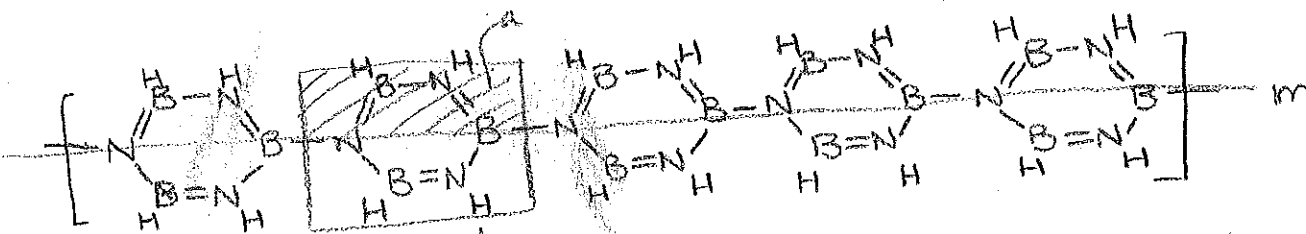
C_{2v}



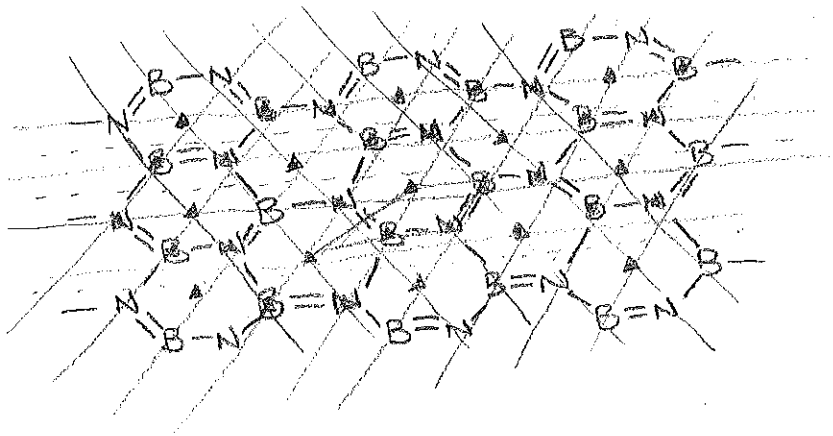
C_{2v}



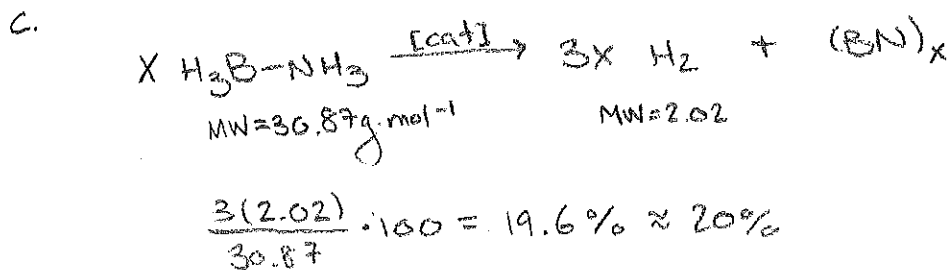
C_{2v}



CLASS 2

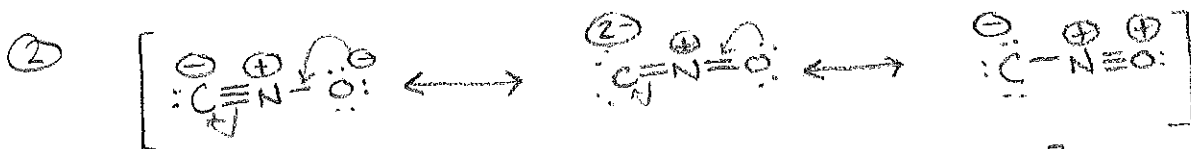


P3m1

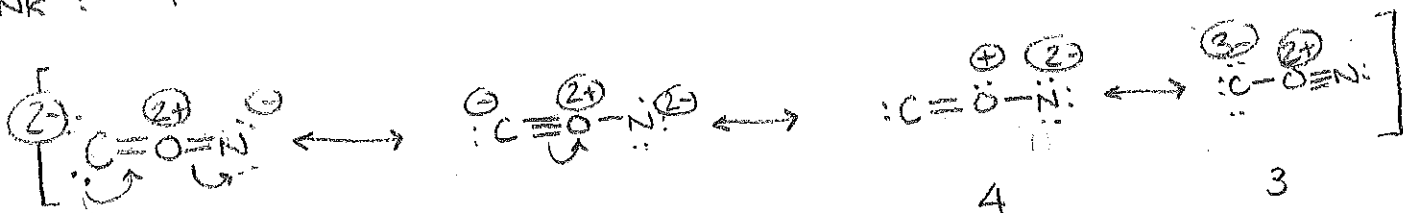


d. C_{2v} ; 2 TYPES Mn

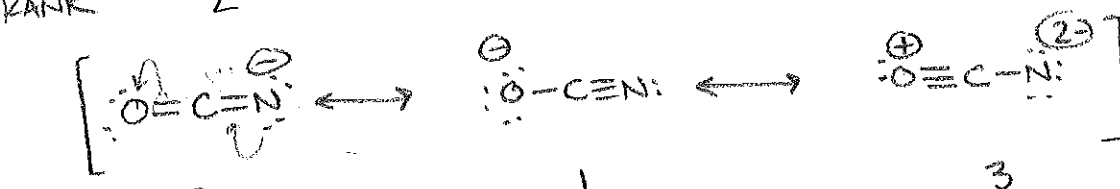
D_{4h} ; 1 TYPE Mn



RANK : 1 2 3



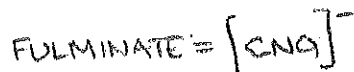
RANK 2 1 4 3



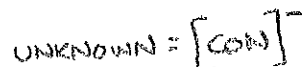
RANK 2 1 3



↳ LOW CHARGE SEPARATION

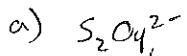


↳ MEDIUM CHARGE SEPARATION

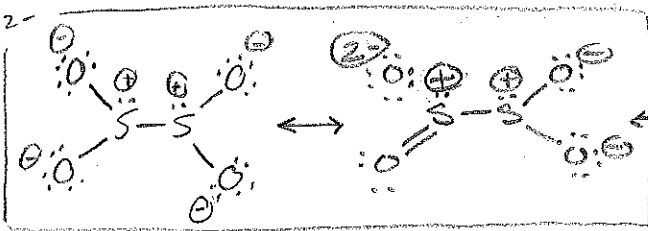


↳ HIGH AMOUNTS OF CHARGES ON ATOMS, O REQUIRES 4 BONDS TO SATISFY OCTET RULE

PART 2

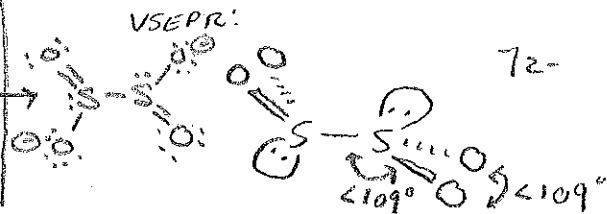


$$\begin{aligned} 2S &= 12 \\ 4O &= 24 \\ \ominus &= 2 \\ \hline &38 \end{aligned}$$



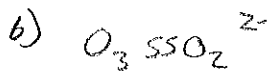
PREFERRED - OBEYS OCTET RULE

VSEPR:

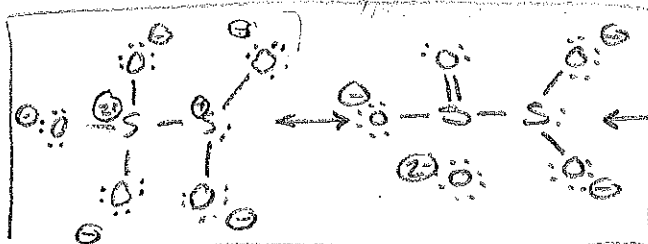


72-

C_{2h}

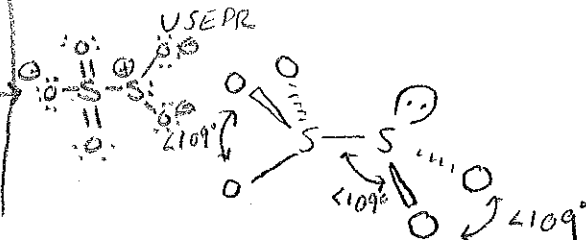


$$\begin{aligned} 2S &= 12 \\ 5O &= 30 \\ \ominus &= 2 \\ \hline &44 \end{aligned}$$

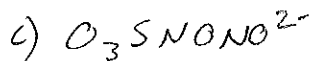


PREFERRED - OBEYS OCTET RULE

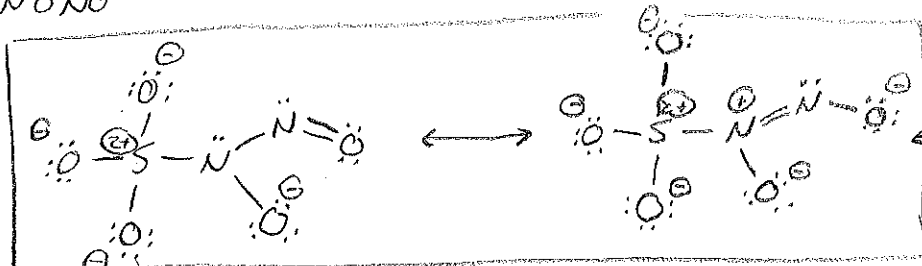
USEPR



C_s



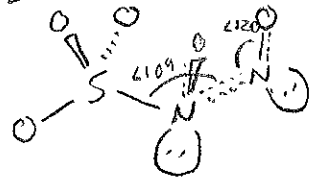
$$\begin{aligned} 1S &= 6 \\ 5O &= 30 \\ 2N &= 10 \\ \ominus &= 2 \\ \hline &48 \end{aligned}$$



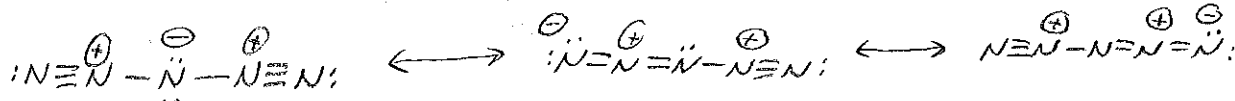
PREFERRED - OBEYS OCTET RULE

↳ BEST: MINIMIZES FORMAL CHARGES

VSEPR:

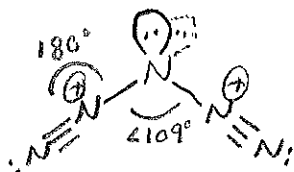


$$\begin{aligned} 5N &= 25 \\ \oplus &= -1 \\ \hline &24 \end{aligned}$$



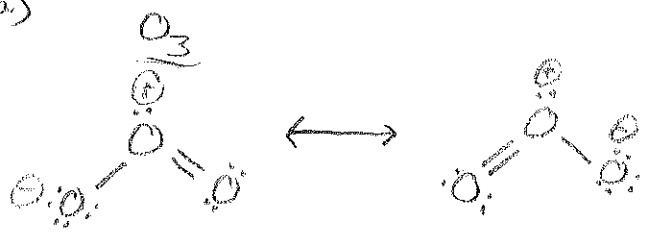
↳ BEST: FORMAL CHARGES OF OPPOSITE SIGN ADJACENT

VSEPR



3

a)



OX STATE
O: 0

O₂



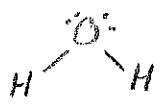
OX STATE
O: 0

O



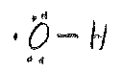
OX STATE
O: 0

H₂O



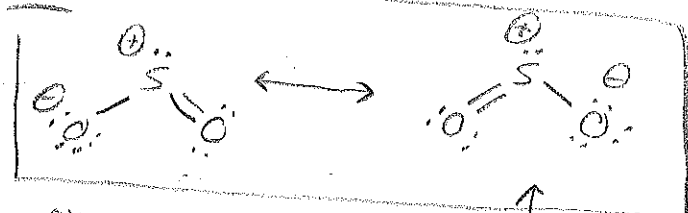
OX STATE
O: 2-
H: 1+

OH



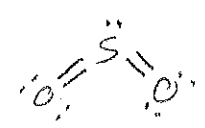
OX STATE
O: 1-
H: 1+

SO₂

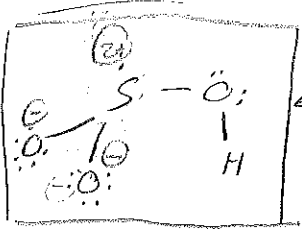


PREFERRED
OBEYS
OCTET
RULE

OX STATE:
O: 2-
S: 4+



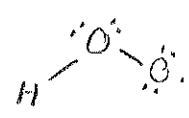
HO₂SO₂



PREFERRED
DOES NOT EXCEED OCTET
OX STATE

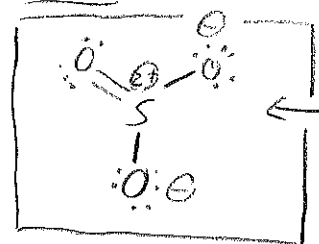
O: 2-
H: 1+
S: 5+

HO₂



OX STATE: O: 1/2-
H: 1+

SO₃

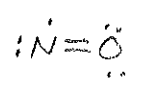


PREFERRED - OBEYS
OCTET RULE



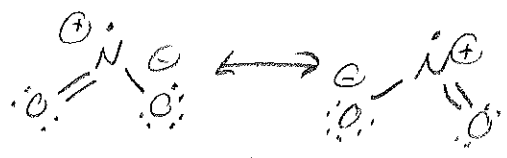
OX STATE
O: 2-
S: 6+

NO



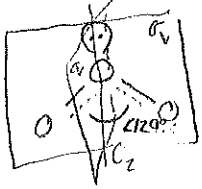
OX STATE:
N: 2+
O: 2-

NO₂



OX STATE
N: 4+
O: 2-

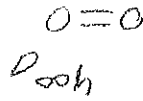
b) $\frac{O_3}{1 \text{ lp} + 2 \text{ BONDS} = \text{BENT}}$



C_{2v}

O_2

$2 \text{ lp} + 1 \text{ bond} = \text{LINEAR}$

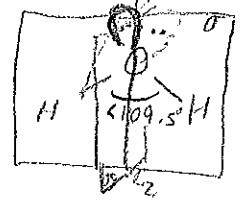


O

N/A

H_2O

$2 \text{ lp} + 2 \text{ BONDS} = \text{BENT}$



C_{2v}

OH

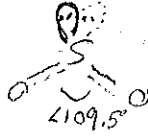
$1 \text{ bond} = \text{LINEAR}$



$C_{\infty v}$

SO_2

$2 \text{ lp} + 2 \text{ BONDS} = \text{BENT}$

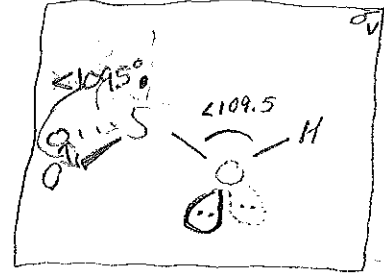


C_{2v}

$HOSO_2$

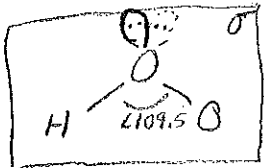
$S \text{ } 0 \text{ lp} + 3 \text{ BONDS} = \text{TRIGONAL PLANAR}$

$O \text{ } 2 \text{ lp} + 2 \text{ BONDS} = \text{BENT}$



HO_2

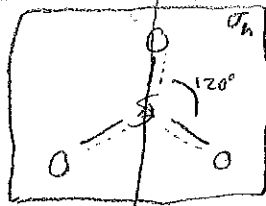
$2 \text{ lp} + 2 \text{ BONDS} = \text{BENT}$



C_s

SO_3

$0 \text{ lp} + 3 \text{ BONDS} = \text{TRIGONAL PLANAR}$



D_{3h}

NO

$1 \text{ bond} = \text{LINEAR}$



$C_{\infty v}$

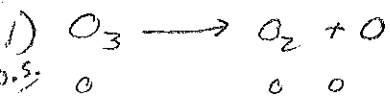
NO_2

$1 \text{ lp} + 2 \text{ BONDS} = \text{BENT}$

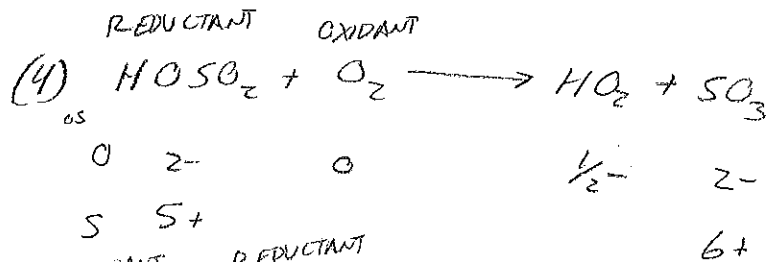


C_{2v}

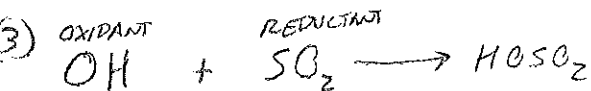
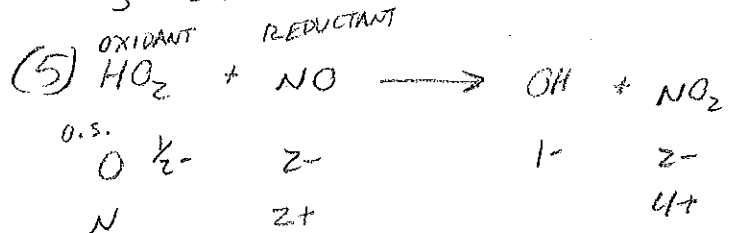
c)



REDOX NEUTRAL



OXIDANT REDUCTANT



0	-1	2-	2-
S	+	4+	5+

For Problem 4, Part A:

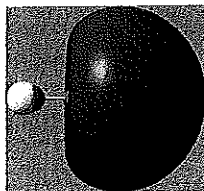
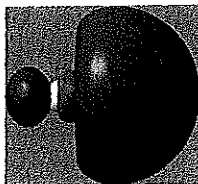
i) F-H

ii) F-Li

iii) Cl-H

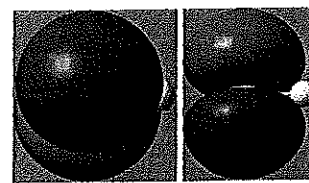
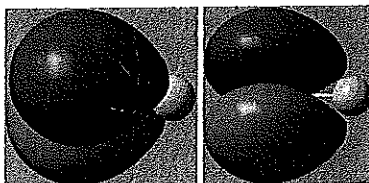
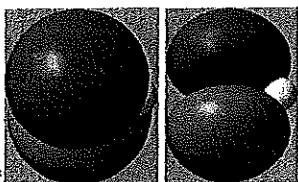
Axial
Symmetry
σ

LUMO*

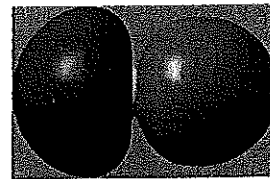
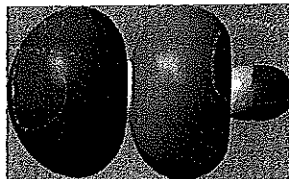
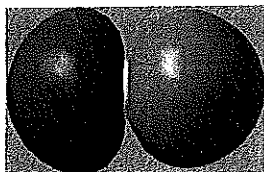


HOMO*

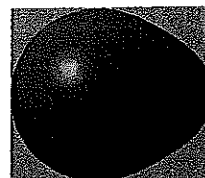
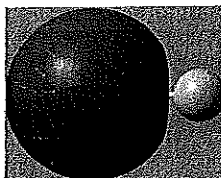
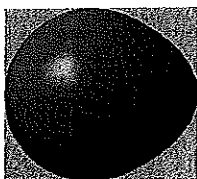
(degenerate set of two molecular orbitals)



HOMO-1



HOMO-2

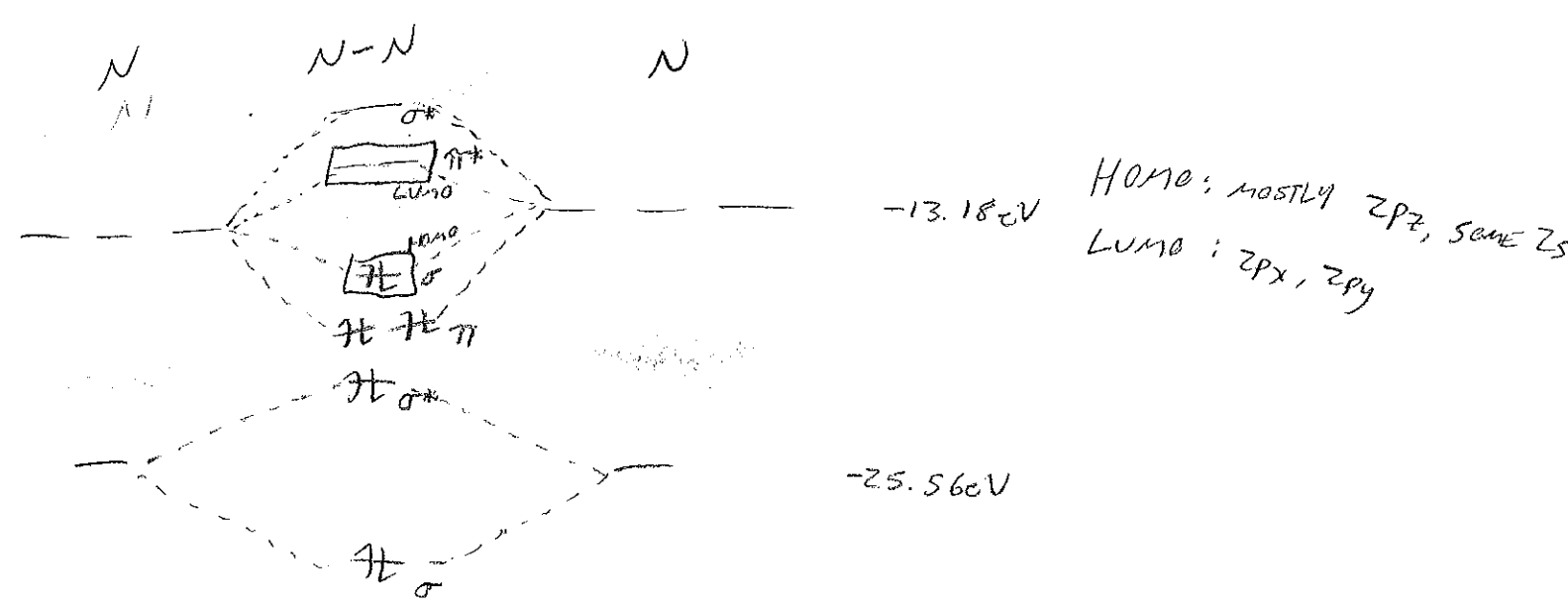
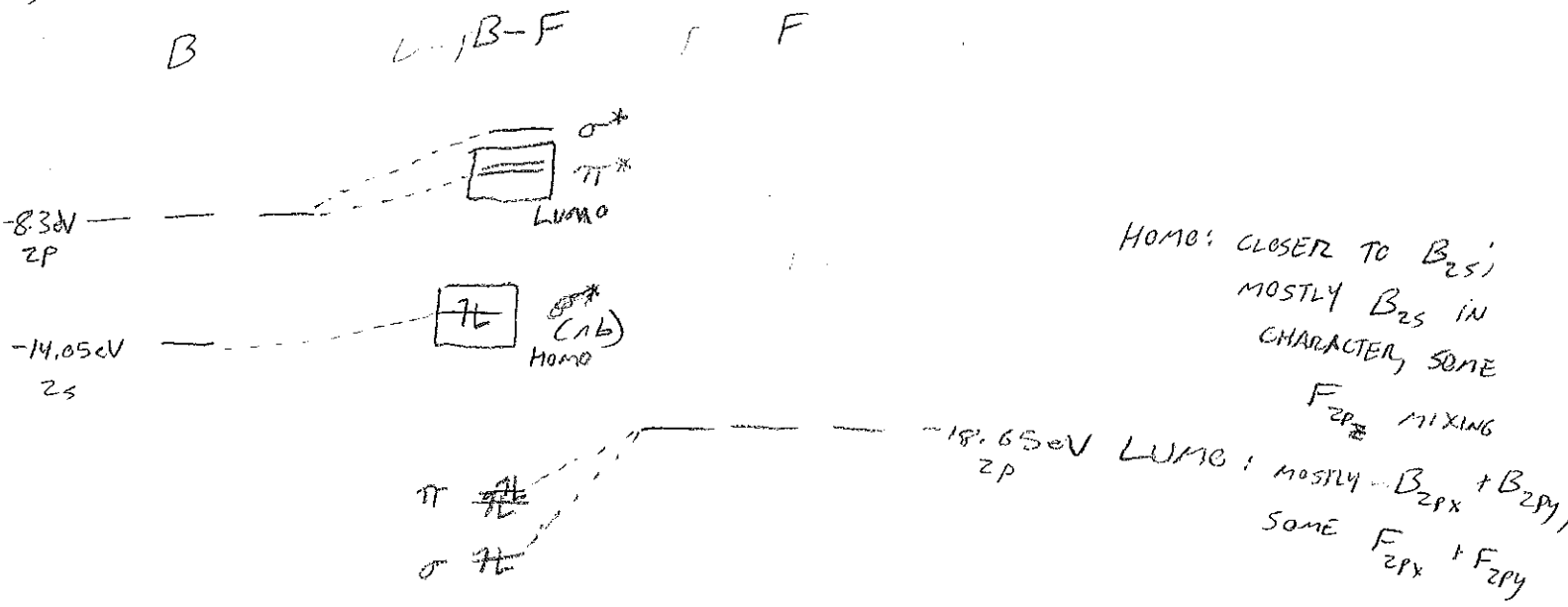


*LUMO = lowest unoccupied molecular orbital

*HOMO = highest occupied molecular orbital

The bonding in LiF is ionic in character due to the large energy difference between the Li orbitals (-5.39 eV, 2s) and the F orbitals (-40.17 eV, 2s and -18.65 eV, 2p). The lowest energy MOs contain contribution from the most electronegative atom F, while the highest energy MOs contain contribution from Li, the least electronegative atom. The bonding in HF is more covalent in character due to the closer energy differences between the H orbital (-13.61 eV, 1s) and the F orbitals, hence there is more mixing in the MOs. In HCl the bonding is more covalent than HF, as the Cl orbitals (-25.23 eV, 3s and -13.67 eV, 3p) are closer in energy to the H orbital and hence there is more mixing in the MOs. While there is more mixing, the lowest energy orbitals still contain a larger of contribution from the more electronegative atom Cl and the higher energy orbitals contain more contribution from H.

B)



c) HOMO IN N_2 IS LOWER ENERGY THAN IN BF
 ALSO, HOMO'S ARE SIMILAR TO B, N AO'S SO TREND IN DIATOMICS' IE SHOULD BE SIMILAR TO TREND IN IE FOR ELEMENTS

d) i is N_2 ii is BF_3
 FOR ii, LOWER ENERGY MO'S CONTAIN MOSTLY CONTRIBUTION FROM ELECTRONS OF F WHILE HIGHER MO'S CONTAIN CONTRIBUTION FROM LESS ELECTRONS OF B.

e) HOMO IN BF HAS A LARGE LOBE ON B, WHERE N_2 HAS HOMO THAT IS MORE DELOCALIZED \Rightarrow HOMO OF BF WILL BETTER OVERLAP WITH BH_3 .
 BF HOMO IS ALSO HIGHER ENERGY AND MORE REACTIVE.