

Molecular Modelling Investigation
Chemistry 2
NIVA International School 2010-2011

Name: _____

Date: _____

Thoroughly read the entire procedure before starting the lab.

Note: This lab will be submitted without a lab report. Instead, complete the investigation as described and submit it on Friday, November 5, 2010.

Materials: Molecular Model Kit

Chemicals: None

Procedure:

1. Build the compounds that are shown in the table in Section 1 using the molecular model kits provided.
2. Complete Section 1 by filling out the table as the headings indicate, ensuring that all fields have been completed. **(15 Marks)**
 - a. IUPAC name for each compound
 - b. A rough sketch of the completed model
 - c. Electron pair geometry (only the name is necessary)
 - d. Molecular geometry (include the name and the bond angle(s))
 - e. VSEPR Hybridization
3. Complete Section 2 by drawing the appropriate orbital diagrams on the provided axes. **(15 Marks)**
4. Complete Section 3 by drawing the molecular orbital diagrams for the indicated molecules in the spaces provided. **(10 Marks)**

Marking Scheme

Section 1 - /15

Section 2 - /15

Section 3 - /10

TOTAL /40

Section 1 - Model Kits

Name	Formula	Sketch	Electron Pair Geometry	Molecular Geometry	VSEPR Hybridization
	CS_2				
	NCl_3				
	H_2Se				

Name	Formula	Sketch	Electron Pair Geometry	Molecular Geometry	VSEPR Hybridization
	CCl_4				
	SeBr_6				
	NbBr_5				

Section 2 - Sketching Orbitals

1. Molecule: CH_4

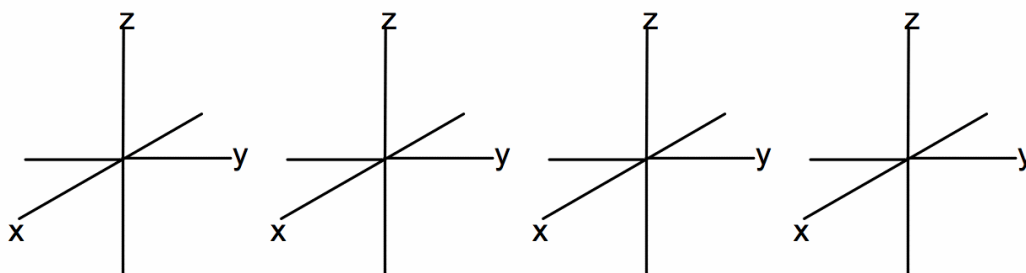
Atomic Orbitals Involved: _____

Hybridization: _____

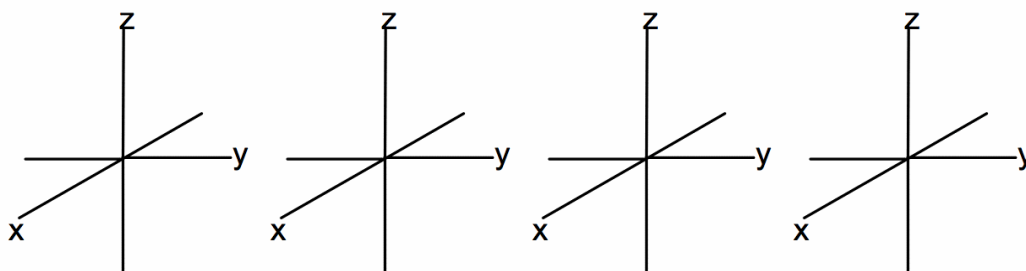
Molecular Orbitals Formed: _____

Sketch and label all atomic orbitals and molecular orbitals on the properly labeled axes shown below. Include lone pairs of electrons if needed. The molecular orbital diagram should show constructive interference of hybridized orbitals, where appropriate.

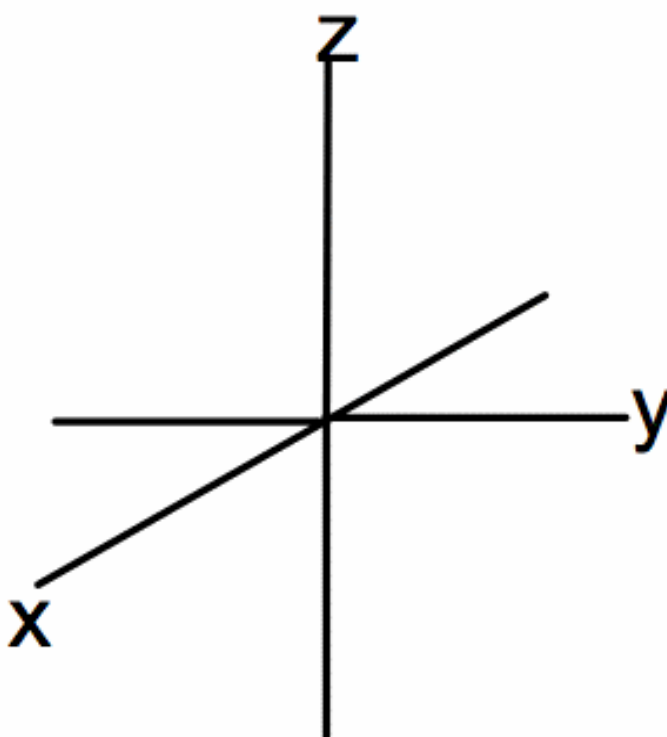
1 Carbon



4 Hydrogen



Resultant Molecular Orbital Configuration



2. Molecule: SCl_2

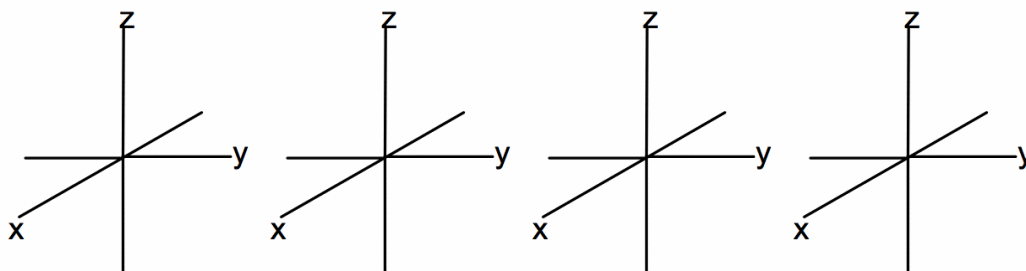
Atomic Orbitals Involved: _____

Hybridization: _____

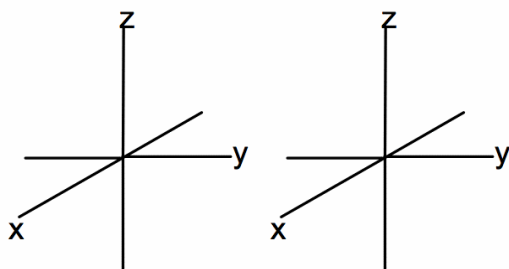
Molecular Orbitals Formed: _____

Sketch and label all atomic orbitals and molecular orbitals on the properly labeled axes shown below. Include lone pairs of electrons if needed. The molecular orbital diagram should show constructive interference of hybridized orbitals, where appropriate.

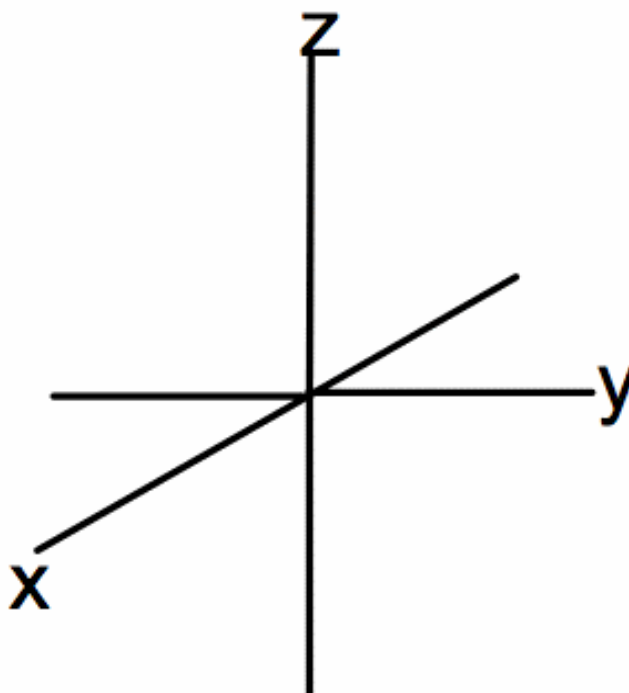
1 Sulfur



2 Chlorine



Resultant Molecular Orbital Configuration



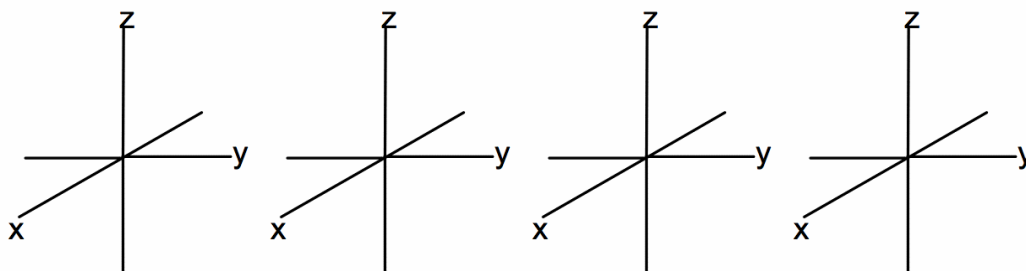
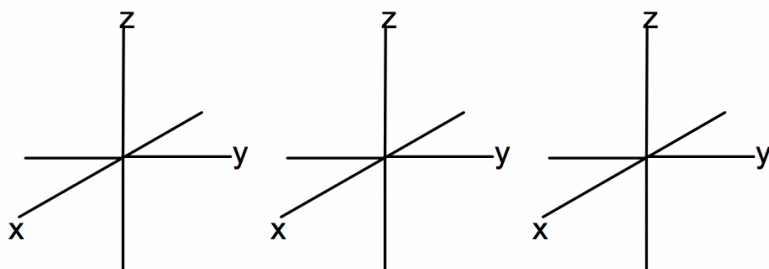
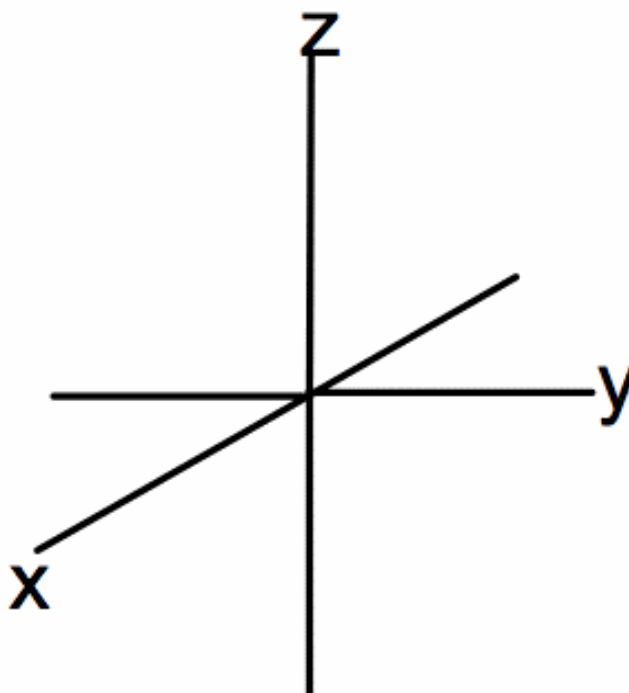
3. Molecule: NF_3

Atomic Orbitals Involved: _____

Hybridization: _____

Molecular Orbitals Formed: _____

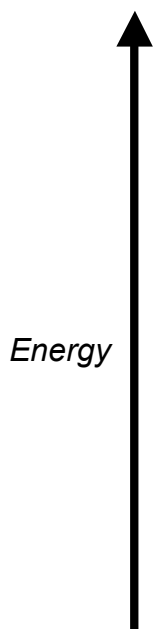
Sketch and label all atomic orbitals and molecular orbitals on the properly labeled axes shown below. Include lone pairs of electrons if needed. The molecular orbital diagram should show constructive interference of hybridized orbitals, where appropriate.

1 Nitrogen2s, 2p_x, 2p_y, 2p_z**3 Fluorine**2p_y**Resultant Molecular Orbital Configuration**

Section 3 - Molecular Orbital Diagrams

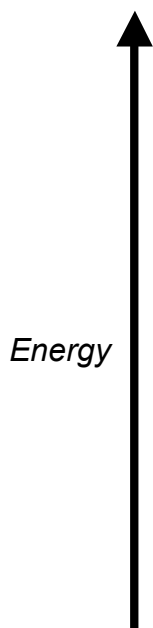
Draw accurate molecular orbital diagrams for the following molecules. Be sure to place the energy levels correctly and to identify the each orbital as either a σ orbital, π orbital, bonding orbital and/or antibonding orbital. Calculate the bond order for each species and decide whether the molecule is stable or unstable.

1. Ne_2



Bond Order = _____

2. N_2



Bond Order = _____