VALENCE BOND (VB) THEORY

AND

MOLECULAR ORBITAL (MO) THEORY

LAB

This lab contains a series of handouts that you should complete. Neatness counts!

Useful handouts from the *Chemistry 222 Companion* or the CH 222 website (http://mhchem.org/222):

- Geometry and Polarity Guide
- MO Diagram - B_2 through N_2
- MO Diagram - O_2 through Ne_2

VALENCE BOND THEORY AND MOLECULAR ORBITAL THEORY LAB - *Worksheet* **Name:**

Complete the sections below by providing the appropriate information in the spaces provided. *Neatness counts!*

Part One: Valence Bond Theory *Complete the following sections using Valence Bond Theory.*

Molecule/Ion	Lewis Structure (& Isomers, if any)		
SeI_2		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Molecule/Ion	Lewis Structure (& Isomers, if any)		
$AsCl_5$		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Molecule/Ion	Lewis Structure (& Isomers, if any)		
CO_3^{2-}		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Molecule/Ion	Lewis Structure (& Isomers, if any)		
ClO_3^{-1}		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Molecule/Ion	Lewis Structure (& Isomers, if any)		
ClO_4^{-1}		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Molecule/Ion	Lewis Structure (& Isomers, if any)		
$XeOF_4$		***Electron Pair Geometry:*** ***Molecular Geometry:*** ***Polar or Nonpolar:***	***Hybridization:*** ***Bond Order:*** ***Resonance Forms? (Y/N)***

Part Two: Molecular Orbital Theory *Complete the following sections using Molecular Orbital Theory. Draw a complete Molecular Orbital diagram to answer these questions (include all 1s and 2s interactions, no short hand notation) and provide the missing information.*

Molecule / Ion: **Li_2**

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Molecule / Ion: **Be_2**

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Molecule / Ion: **B_2**

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Molecule / Ion: $\mathbf{N_2}$

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Molecule / Ion: $\mathbf{F_2}$

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Molecule / Ion: **Ne_2**

Molecular Orbital Diagram:

Bond Order: _____ Number of sigma bonds: _____ Number of pi bonds: _____

(Circle) **Paramagnetic** *or* **Diamagnetic** Should this molecule exist? *(Circle)* **Yes** *or* **No**

Part Three: Theory Comparison *Complete the following sections using both Valence Bond (VB) Theory and Molecular Orbital (MO) Theory.* ***Use shorthand notation for MO Diagrams****. Provide all of the missing information.*

Molecule / Ion: **CN^{-1}**

Valence Bond Lewis Structure:

Molecular Orbital Diagram using shorthand notation:

Bond Order (VB): _____

Bond Order (MO): _____

Number of sigma bonds (VB): _____

Number of sigma bonds (MO): _____

Number of pi bonds (VB): _____

Number of pi bonds (MO): _____

(VB) Paramagnetic? *(circle)* **Yes No**

(MO) Paramagnetic? *(circle)* **Yes No**

Molecule / Ion: **NO^{+1}** *(Use the MO Diagram for O, F and Ne on this problem)*

Valence Bond Lewis Structure:	Bond Order (VB): _____
	Bond Order (MO): _____
	Number of sigma bonds (VB): _____
Molecular Orbital Diagram using shorthand notation:	Number of sigma bonds (MO): _____
	Number of pi bonds (VB): _____
	Number of pi bonds (MO): _____
	(VB) Paramagnetic? *(circle)* **Yes No**
	(MO) Paramagnetic? *(circle)* **Yes No**

Molecule / Ion: **NO** *(Use the MO Diagram for O, F and Ne on this problem)*

Valence Bond Lewis Structure:	Bond Order (VB): _____
	Bond Order (MO): _____
	Number of sigma bonds (VB): _____
Molecular Orbital Diagram using shorthand notation:	Number of sigma bonds (MO): _____
	Number of pi bonds (VB): _____
	Number of pi bonds (MO): _____
	(VB) Paramagnetic? *(circle)* **Yes No**
	(MO) Paramagnetic? *(circle)* **Yes No**

Molecule / Ion: **O_2**

Valence Bond Lewis Structure:	Bond Order (VB): _____
	Bond Order (MO): _____
	Number of sigma bonds (VB): _____
Molecular Orbital Diagram using shorthand notation:	Number of sigma bonds (MO): _____
	Number of pi bonds (VB): _____
	Number of pi bonds (MO): _____
	(VB) Paramagnetic? *(circle)* **Yes No**
	(MO) Paramagnetic? *(circle)* **Yes No**

Molecule / Ion: **OF^{-1}**

Valence Bond Lewis Structure:	Bond Order (VB): _____
	Bond Order (MO): _____
	Number of sigma bonds (VB): _____
Molecular Orbital Diagram using shorthand notation:	Number of sigma bonds (MO): _____
	Number of pi bonds (VB): _____
	Number of pi bonds (MO): _____
	(VB) Paramagnetic? *(circle)* **Yes No**
	(MO) Paramagnetic? *(circle)* **Yes No**

Molecule / Ion: $\mathbf{Ne_2^{+2}}$

Valence Bond Lewis Structure:	Bond Order (VB): _____
	Bond Order (MO): _____
	Number of sigma bonds (VB): _____
Molecular Orbital Diagram using shorthand notation:	Number of sigma bonds (MO): _____
	Number of pi bonds (VB): _____
	Number of pi bonds (MO): _____
	(VB) Paramagnetic? *(circle)* **Yes No**
	(MO) Paramagnetic? *(circle)* **Yes No**