

Chem 6 sample exam 3 (100 points total)

- @ This is a closed book exam to which the Honor Principle applies.
- @ The last page contains the MO energy level ordering for diatomic molecules, some electronegativity information, and the periodic table. You can detach it for easy reference.
- @ Please write clearly and **SHOW YOUR WORK**. If you need to write on the back of the exam paper, please indicate this clearly.
- @ Some questions are more challenging than others. Allot your time accordingly, and try to answer **EVERY** question.
- @ Please put your name both below and on p. 2.

NAME (please print) _____

1. (10 pts, 2 each) Indicate whether or not each of the following molecules has a dipole moment. **Briefly explain** your answers.

(a) CO

(b) BBr₃

(c) BrF₃

(d) XeF₄

(e) PF₅

2. (10 pts, 5 each) Give Lewis dot structures for the following molecules, including formal charges and resonance structures if necessary.

Also, predict their **idealized** 3-dimensional structures, and describe qualitatively any **deviations** of the structures from the idealized predictions.

(a) O_3 [atom connectivity is O-O-O]

(b) BrF_5

3. (10 pts, 5 each) (a) GaSbCl_6 could exist either as $[\text{SbCl}_2]^+[\text{GaCl}_4]^-$ (1) or $[\text{GaCl}_2]^+[\text{SbCl}_4]^-$ (2). Give the 3-dimensional structure of the **anions** in both cases.

(b) It is found experimentally that the **cation** is bent. Does this tell you if the correct structure is 1 or 2? **Explain** your answer.

4. (10 pts) Rank the nitrogen oxides NO, NO⁺, and NO⁻ by increasing bond order. **Explain** your answer using MO theory.

_____ < _____ < _____

smallest bond order-----> largest bond order

5. (10 pts) The ionization energy of a molecule can be defined in the same way as for an atom. The ionization energy of O_2 is **less** than that of O, but the ionization energy of N_2 is **greater** than that of N. **Explain** using MO theory.

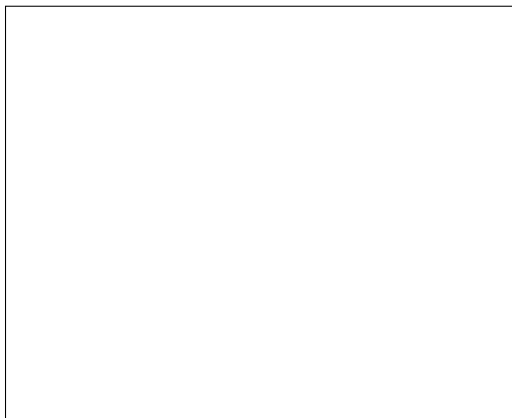
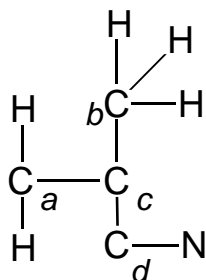
6. (10 pts, 5 each) The highest occupied molecular orbital (HOMO) for a given molecule is the highest-energy MO which contains electrons. Similarly, the lowest unoccupied molecular orbital (LUMO) is the lowest-energy MO which does not contain electrons.

(i) Identify the HOMO of C_2 , and sketch the combination of atomic orbitals used to form this MO. [If the HOMO is actually a degenerate set of MO's, just sketch one of the set.] Your sketch should show the relative contributions of the atomic orbitals to the MO.

(i) Identify the LUMO of CN, and sketch the combination of atomic orbitals used to form this MO. [If the LUMO is actually a degenerate set of MO's, just sketch one of the set.] Your sketch should show the relative contributions of the atomic orbitals to the MO.

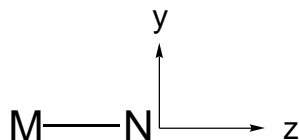
7. (10 pts) (a, 2pts) Methylacrylonitrile has the atom connectivity shown below.

Draw an acceptable Lewis structure for this molecule in the box provided.



(b, 8 pts) Give the **hybridization** and the **ideal bond angles** at each carbon atom. Identify the carbons using the labeling scheme (a-d) above.

8. (10 pts, 5 each) Consider a diatomic molecule MN, where M is a transition metal, and the z-axis is the internuclear axis. The yz plane is the plane of the paper.



(a) By sketching the appropriate combinations of atomic orbitals, show how to make a **σ -bonding MO** for MN from a M p_z orbital and a nitrogen s orbital.

(b) By sketching the appropriate combinations of atomic orbitals, show how to make a **π -antibonding MO** for MN from a M d_{yz} orbital and a nitrogen p_y orbital.

9. (10 pts) (a, 4 pts) Give the hybridization on Cl in the molecular ions ClO_4^- and ClO_3^- .

(b, 6 pts) Give the expected geometries of these ions.

10. (10 pts, 2 each) Multiple choice. **Circle** your answers.

(a) The hybridization at Xe in XeF₄ is

- (i) dsp³ (ii) sp³
(iii) d²sp³ (iv) d⁵sp²

(b) Pick the **true** statement(s) about hybridization.

- (i) H₃O⁺ and BH₄⁻ both have sp³ hybridization at the central atom.
(ii) NO₃⁻ is sp hybridized at N.
(iii) H₂O₂ [atom connectivity H-O-O-H] is sp² hybridized at both O atoms.
(iv) The carbon in CH₃⁺ is sp² hybridized, **and** the molecule is trigonal planar.

(c) Circle the molecule(s) which has (have) a dipole moment.

- (i) ClF₂⁺
(ii) XeF₂
(iii) SO₄²⁻
(iv) H-C≡C-H

(d) Pick the molecule with the largest bond order.

- (i) CN⁻ (ii) O₂
(iii) Be₂ (iv) C₂

(e) Pick the **paramagnetic** molecule(s).

- (i) O₂ (ii) N₂
(iii) CH₄ (iv) NO

ENERGY ORDERING -- DIATOMIC MO SCHEME

for Li-N: $\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2px}, \pi_{2py} < \sigma_{2pz} < \pi^*_{2px}, \pi^*_{2py} < \sigma^*_{2pz}$

for O-Ne: $\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2pz} < \pi_{2px}, \pi_{2py} < \pi^*_{2px}, \pi^*_{2py} < \sigma^*_{2pz}$

Electronegativity Info

atom	Electronegativity
B	2.04
C	2.55
N	3.04
O	3.44
F	3.98
Cl	3.16

PERIODIC TABLE

1											2																								
H 1.0079											He 4.00260																								
3		4																		5		6		7		8		9		10					
Li 6.941		Be 9.01218																		B 10.81		C 12.011		N 14.0067		O 15.9994		F 18.9984		Ne 20.179					
11		12																		13		14		15		16		17		18					
Na 22.9898		Mg 24.305																		Al 26.9815		Si 28.0855		P 30.9738		S 32.06		Cl 35.453		Ar 39.948					
19		20		21		22		23		24		25		26		27		28		29		30		31		32		33		34		35		36	
K 39.0983		Ca 40.08		Sc 44.9559		Ti 47.88		V 50.9415		Cr 51.996		Mn 54.9380		Fe 55.847		Co 58.9332		Ni 58.69		Cu 63.546		Zn 65.39		Ga 69.72		Ge 72.59		As 74.9216		Se 78.96		Br 79.904		Kr 83.80	
37		38		39		40		41		42		43		44		45		46		47		48		49		50		51		52		53		54	
Rb 85.4678		Sr 87.62		Y 88.9059		Zr 91.224		Nb 92.9064		Mo 95.94		Tc (98)		Ru 101.07		Rh 102.906		Pd 106.42		Ag 107.868		Cd 112.41		In 114.82		Sn 118.71		Sb 121.75		Te 127.60		I 126.905		Xe 131.29	
55		56		57		72		73		74		75		76		77		78		79		80		81		82		83		84		85		86	
Cs 132.905		Ba 137.33		La 138.906		Hf 178.49		Ta 180.948		W 183.85		Re 186.207		Os 190.2		Ir 192.22		Pt 195.08		Au 196.967		Hg 200.59		Tl 204.383		Pb 207.2		Bi 208.980		Po (209)		At (210)		Rn (222)	
87		88		89		104		105		106		107		108		109																			
Fr (223)		Ra 226.025		Ac 227.028		Unq (261)		Unp (262)		Unh (263)		Uns (262)		Uno (265)		Une (266)																			

58		59		60		61		62		63		64		65		66		67		68		69		70		71	
Ce 140.12		Pr 140.908		Nd 144.24		Pm (145)		Sm 150.36		Eu 151.96		Gd 157.25		Tb 158.925		Dy 162.50		Ho 164.930		Er 167.26		Tm 168.934		Yb 173.04		Lu 174.967	
90		91		92		93		94		95		96		97		98		99		100		101		102		103	
Th 232.038		Pa 231.036		U 238.029		Np (237)		Pu (244)		Am (243)		Cm (247)		Bk (247)		Cf (251)		Es (252)		Fm (257)		Md (258)		No (259)		Lr (260)	