

CHEM261 TEST
Inorganic and Structural Chemistry
Monday 7 May 2007

Time: 9:00 to 9:50 a.m.

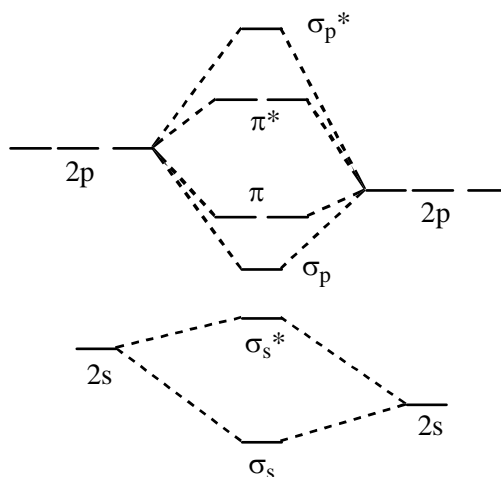
Time allowed: 50 minutes

Answer ALL five questions. There is a total of 50 marks available.

There is a periodic table at the end of the paper.

1. (15 marks)

Given below is a MO diagram for a heteronuclear diatomic molecule:



- Sketch each molecular orbital.
- Sketch the molecular orbital diagram for a homonuclear diatomic molecule, such as N_2 , when s-p mixing is taken into account.
- Give the bond orders for the following species (you can assume s-p mixing) and indicate which are paramagnetic:
 - NO^+
 - NO
 - NO^{2-}
- For F_2 , which MO is the HOMO?
- For F_2 , which MO is the LUMO?

2. (15 marks)

The valence molecular orbitals (MOs) for the π system of trigonal planar NO_3^- can be described as linear combinations of atomic orbitals as follows:

$$\Psi_1 = c_1\phi(\text{N}_{p_z}) + c_2[\phi(\text{O1}_{p_z}) + \phi(\text{O2}_{p_z}) + \phi(\text{O3}_{p_z})]$$

$$\Psi_2 = c_3[\phi(\text{O2}_{p_z}) - \phi(\text{O3}_{p_z})]$$

$$\Psi_3 = c_4\{2\phi(\text{O1}_{p_z}) - [\phi(\text{O2}_{p_z}) + \phi(\text{O3}_{p_z})]\}$$

$$\Psi_4 = c_5\phi(\text{N}_{p_z}) - c_6[\phi(\text{O1}_{p_z}) + \phi(\text{O2}_{p_z}) + \phi(\text{O3}_{p_z})]$$

- Sketch each MO and label as bonding, non-bonding or anti-bonding.
- Sketch a qualitative MO diagram for the π system only of NO_3^- and fill in the electrons. Hint, consider each atom to be sp^2 hybridised with one p orbital available for the π system.
- What is the average N–O bond order?
- What is the average C–O bond order in CO_3^{2-} ?
- Why doesn't the N p_z orbital mix with the Ψ_2 and Ψ_3 combinations?

3. (13 marks)

- Draw all valid Lewis dot structures of nitrite, NO_2^- .
- What is the geometry of NO_2^- ?
- How does valence bond theory account for the fact that the two N–O bonds in NO_2^- are the same distance?
- Assign formal charges to the atoms in one of your structures of NO_2^- .
- What is the average N–O bond order?
- Draw a valid Lewis dot structure of NO_2^+ .
- What is the geometry of NO_2^+ ?
- Are the N–O bonds in nitrite shorter or longer than the N–O bonds in NO_2^+ ? Explain your answer.

4. (4 marks)

Consider the quantum number sets for an electron in a hydrogen atom given below:

	n	l	m_l	m_s
(i)	1	0	0	$\frac{1}{2}$
(ii)	2	2	-2	$-\frac{1}{2}$
(iii)	3	2	-2	$-\frac{1}{2}$
(iv)	2	1	-1	$\frac{1}{2}$
(v)	4	3	4	$-\frac{1}{2}$
(vi)	3	2	-2	$\frac{1}{2}$
(vii)	4	3	-3	$\frac{1}{2}$

- (a) Which is/are not allowed?
- (b) Which allowed set(s) is/are associated with the electron of highest energy?
- (c) Which electron(s) is/are in a p orbital?
- (d) Which electrons could be in the same orbital?

5. (3 marks)

- (a) Sketch the radial distribution function of a 3p orbital.
- (b) How many radial and angular nodes does a 5p orbital have?

Periodic Table

1 H 1.008																2 He 4.00	
3 Li 6.94	4 Be 9.01											5 B 10.8	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.0	10 Ne 20.2
11 Na 23.0	12 Mg 24.3											13 Al 27.0	14 Si 28.1	15 P 31.0	16 S 32.1	17 Cl 35.5	18 Ar 39.9
19 K 39.1	20 Ca 40.1	21 Sc 45.0	22 Ti 47.9	23 V 50.9	24 Cr 52.0	25 Mn 54.9	26 Fe 55.9	27 Co 58.9	28 Ni 58.7	29 Cu 63.5	30 Zn 65.4	31 Ga 69.7	32 Ge 72.6	33 As 74.9	34 Se 79.0	35 Br 79.9	36 Kr 83.8
37 Rb 85.5	38 Sr 87.6	39 Y 88.9	40 Zr 91.2	41 Nb 92.9	42 Mo 95.9	43 Tc (99)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57-71 see below	72 Hf 178.5	73 Ta 181.0	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89-103 see below	104 Rf (257)	105 Db (260)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110	111	112						

57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
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89 Ac (227)	90 Th 232.0	91 Pa (231)	92 U 238.1	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (245)	98 Cf (251)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)
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