CHEM261 TEST

Inorganic and Structural Chemistry

Wednesday 27 April 2005

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

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

There is a periodic table on the last page.

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1. (4 marks)

   Sketch a p-d interaction that illustrates a **σ bonding MO** and a p-d interaction that illustrates a **π* anti-bonding MO**.

2. (10 marks)

   (a) Draw Lewis diagrams of the following species:

   (i) BrF_3

   (ii) $[XeOF_5]^-$

   (iii) N_2O

   (iv) NO_2

   (b) Calculate the formal charges on the atoms in NO_2 and suggest why this molecule forms a dimer, N_2O_4, with a weak N–N bond.

3. (6 marks)

   For each of the following wave functions, note the number of **radial** and **angular** nodes and state **which atomic orbital** it is.

   (a) $e^{-r/3}(27 - 18r + 2r^2)/81(3\pi)^{1/2}$

   (b) $(\cos\theta)re^{-r/2}/4(2\pi)^{1/2}$

4. (4 marks)

Consider the quantum number sets given:

	n	l	m_l	m_s
(i)	1	0	0	½
(ii)	2	2	–2	–½
(iii)	3	2	–2	–½
(iv)	2	1	–1	½
(v)	4	3	4	–½
(vi)	3	2	–2	½
(vii)	4	3	–3	½

(a) Which is/are not allowed?

(b) Which 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. (14 marks)

(a) Draw the MO energy level diagram for NO. You should clearly illustrate the relative energy of the starting N and O atomic orbitals and the MO labels.

(b) What is the NO bond order?

(c) Is the bond order of NO^- smaller or larger than NO?

(d) Is the bond distance in NO^+ less than or greater than in NO?

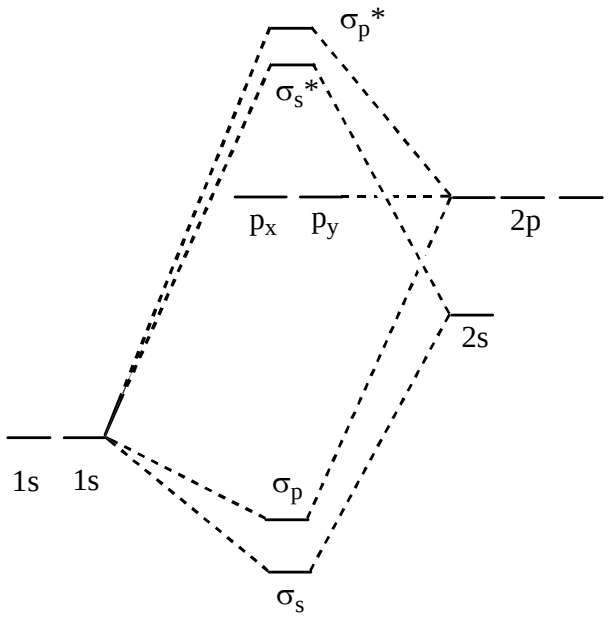
(e) Sketch the Lewis structure of NO.

(f) Justify your placement of the unpaired electron in (e).

(g) What does the MO diagram tell you about the location of the unpaired electron and the NO bond order that the Lewis diagram does not?

6. (12 Marks)

Shown below is the MO diagram for BeH_2 (without electrons shown).



(a) Sketch the Lewis diagram for BeH_2 and comment on the differences between the VB description of BeH_2 and the MO description.

(b) Sketch the MOs for σ_s and σ_p and write an equation for each as LCAOs.

(c) Which is the HOMO?

(d) Which is the SHOMO?

(e) What does the MO diagram tell you about the polarity of the Be-H bonds? (Explain how you arrive at your conclusion).

(f) Why are the p_x and p_y orbitals not involved in the bonding with the H atoms?

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

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)