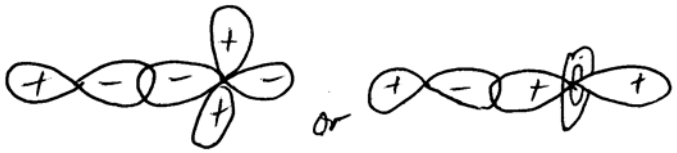
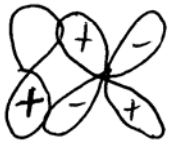
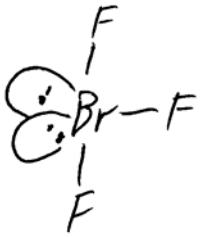
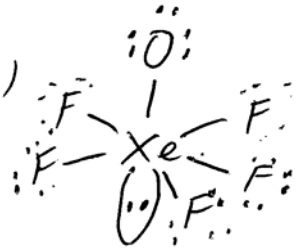
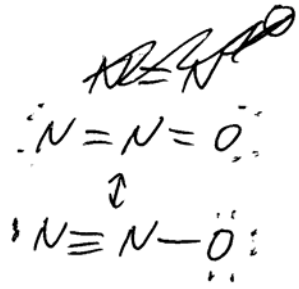
CHEM261 1st Test 2005
Model answers

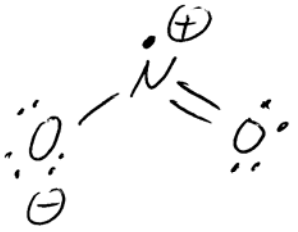
1. σ:  or

π: 

2. (a) (i) 

(ii)  (pentagonal pyramid)

(iii) 

(iv) 

(b) +ve charge on N gives an electrostatic repulsion between the N atoms.

3. (a) 2 radial and 0 angular nodes ⇒ 3s

(b) 0 radial and 1 angular node ⇒ 2p

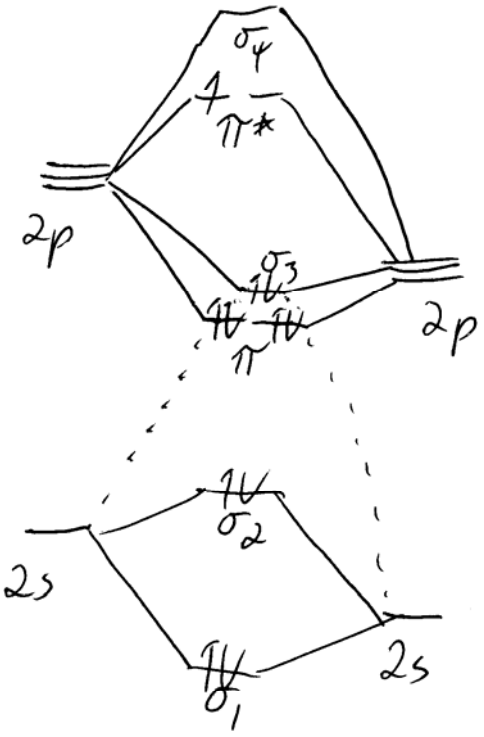
4. (a) (ii) and (v)

(b) ~~(vi)~~ (vii)

(c) (iv)

(d) (iii) and (vi)

5. (a)



N NO O

(b) 2.5

(c) smaller

(d) ~~more~~ less than

(e) :N≡O:

(f) The π* orbital with the unpaired e⁻ is closest in energy to the N(2p)

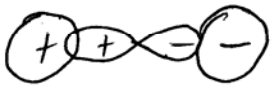
(g) The MO diagram tells you the unpaired e⁻ is on both atoms, but mostly on N. The Lewis ~~diagram~~ diagram suggests a bond order of only 2.

6. (a) H—Be—H (or H:Be:H)

VB theory says each pair of e⁻s is localised in a Be-H bond and that each Be-H bond is equivalent. MO theory says each pair of e⁻s is delocalised over all three atoms and the two pairs of e⁻s are different.

(b) σ_s : 

$$\psi_{\sigma_s} = c_1\phi_{1s_A} + c_2\phi_{2s(Be)} + c_1\phi_{1s_B}$$

σ_p : 

$$\psi_{\sigma_p} = c_3\phi_{1s_A} + c_4\phi_{2p} - c_3\phi_{1s_B}$$

(c) σ_p

(d) σ_s

(e) Polarised with the negative charge on the H atoms since the bonding MOs are closest in energy to the H 1s orbitals.

$$\overset{\delta^-}{H}-\overset{\delta^{++}}{Be}-\overset{\delta^-}{H}$$

(f) Wrong symmetry.