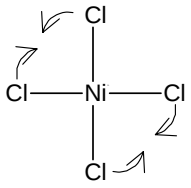
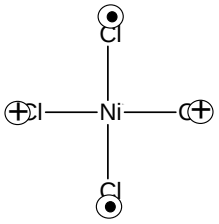
Assignment 2 Solutions - 2351 W10

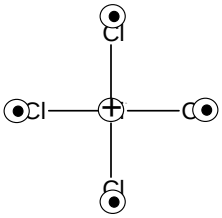
Question 1 Bearing in mind the definitions of the axes and planes (C_2 is the z-axis, C_2' is the x or y-axis, C_2'' is 45° between the x and y-axes; the σ_v is the xz or the yz-plane, the σ_d is at a 45° angle between the xz and yz plane, σ_h is the xy-plane), you should get the following for the three vibrations:



scissor bend



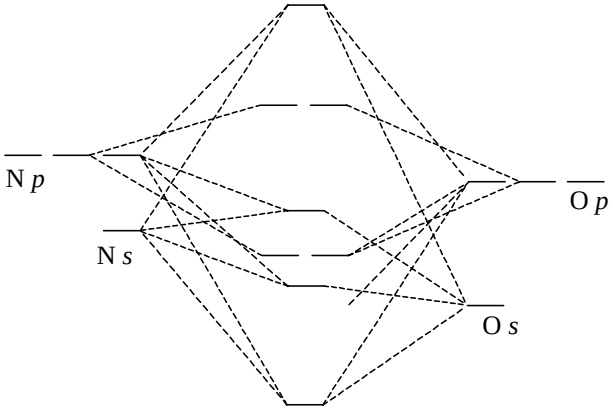
trans-pair bend



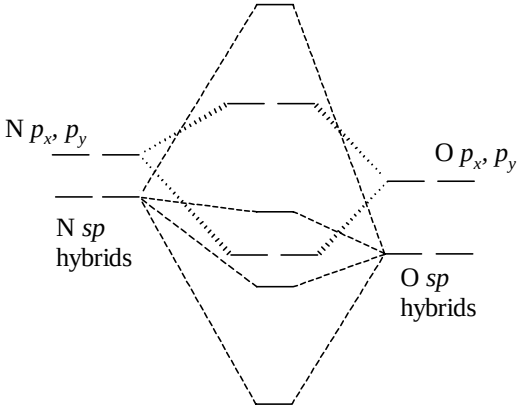
umbrella inversion

Irred. rep:	B_{2g}	B_{2u}	A_{2u}
activity:	Raman	none	IR

Question 2 Either of the following (empty) MO pictures is correct:

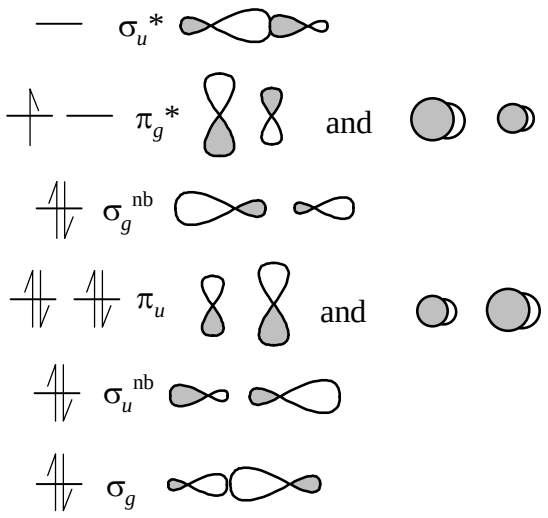


with "mixing"
(technically correct MO picture)



using *sp* hybrids

N has 5 valence electrons and O has 6, for a total of 11 electrons to be added. Filling these in, and drawing/labelling the orbitals gives the next picture, just focussing on the middle MO part of the above pictures:

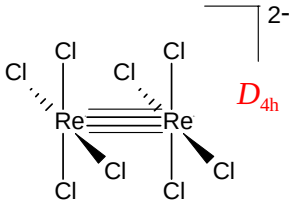


(a) There are 6 electrons in bonding orbitals, 1 in an antibonding orbital (and 4 in non-bonding), which gives a B.O. = (6 - 1)/2 = 2.5. Recall that CO has a bond order of 3, so the NO bond should be weaker.

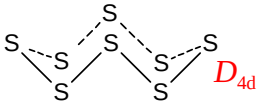
(b) NO^+ loses one antibonding electron; B.O. = (6 - 0)/2 = 3.
NO^- adds one antibonding electron; B.O. = (6 - 2)/2 = 2.
Therefore, the stronger and shorter bond is in NO^+.

(c) The NO should bond through the nitrogen because both the HOMO and LUMO have their larger electron densities on the N. Note that hard/soft arguments do not really apply here because the N and O are very close on the hard-soft scale.

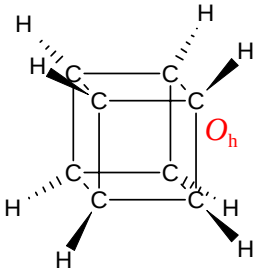
Question 3



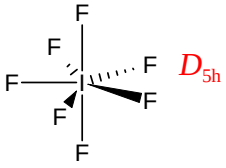
(the $RuCl_4$ units are squares)



(every S is identical - *i.e.* this is a regular up/down oscillation)



cubane - each corner is a C-H unit



pentagonal bipyramidal
equator is a regular pentagon

