

Name: _____

Answer all three questions, showing all calculations, 20 pts each.

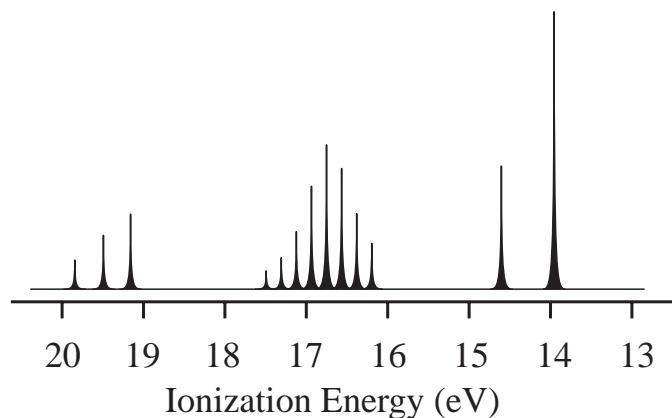
- What point group does ferrocene (bis-cyclopentadienyl iron, $(C_5H_5)_2Fe$) belong to assuming the cyclopentadienyl groups are eclipsed?
A) C_5 B) C_{5v} C) D_5 D) D_{5h} E) D_{5d}
- For an electronic transition of a diatomic molecule in which the internuclear distance changes significantly, which statements are true:
A) Franck-Condon overlap factors are greatest for highly excited vibrational final states.
B) Franck-Condon overlap factors are smallest for highly excited vibrational final states.
C) The transition is allowed only if $\Delta V = \pm 1$ D) The transition is allowed only if $\Delta V \neq 0$
E) The energy absorbed by the transition decreases as the excited vibrational state increases.
- Which of the following molecules may show IR absorption spectra (may be more than one answer)?
A) H_2 B) HCl C) CO D) CH_3Cl E) O_2

Problems - Answer any three questions, showing all calculations 30 pts each

- What are the symmetry species of the excited states which would allow an electronic transition within the point group C_{4v} (indicate what polarization produces each transition assuming the ground state wavefunction has A_2 symmetry).

C_{4v} , $4mm$	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$	$h = 8$
A_1	+1	+1	+1	+1	+1	$z, z^2, x^2 + y^2$
A_2	+1	+1	+1	-1	-1	R_z
B_1	+1	+1	-1	+1	-1	$x^2 - y^2$
B_2	+1	+1	-1	-1	+1	xy
E	+2	-2	0	0	0	$(x,y), (xz,yz), (R_x,R_y)$

- Calculate the irreducible representation of the displacement vectors for a C_{4v} molecule (square pyramidal) with the formula AB_4 . Indicate which modes are translations, rotations, IR active vibrations and Raman active vibrations.
- Consider the photoelectron spectrum for CO shown to the right. Ascribe the lines to the ionization processes involved and classify orbitals as bonding, non-bonding or anti-bonding in light of the vibrational structure seen.
- The rotational constant for CO is 1.9314 cm^{-1} and 1.6116 cm^{-1} in the ground and first excited states respectively. By how much does the internuclear distance change as a result of this transition?



Problem 3. Photoelectron spectrum of CO

- Describe the differences and similarities between fluorescence and phosphorescence.
- Construct a group multiplication table for the group C_{3h} which consists of E, C_{3L} , C_{3R} , S_{3L} , S_{3R} and σ_h .