CHEM442-001/002
College of Charleston
Spring 2001
Exam IV

Name _____

Score _____ /100

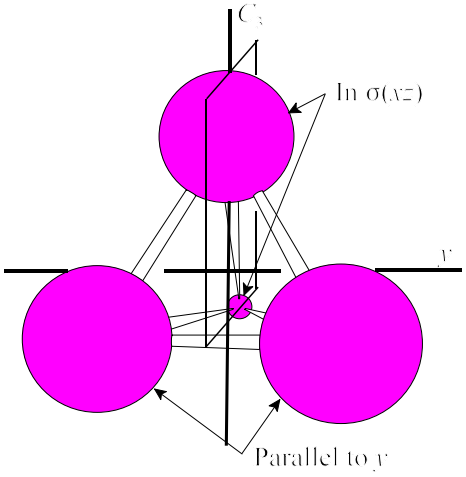
1(50). Elemental phosphorus exists as a tetrahedral molecule (point group $\mathbf{T_d}$) with the formula P_4.

$\mathbf{T}_d$ representation	$\hat{E}$	$8\hat{C}_3$	$3\hat{C}_2$	$6\hat{S}_4$	$6\hat{\sigma}_d$	
A_1	1	1	1	1	1	$x^2+y^2+z^2$
A_2	1	1	1	-1	-1	
E	2	-1	2	0	0	$(2z^2-x^2-y^2, x^2-y^2)$
T_1	3	0	-1	1	-1	(R_x,R_y,R_z)
T_2	3	0	-1	-1	1	(x,y,z), (xy,xz,yz)

Is this molecule polar? _____

Is this molecule optically active? _____

Using the direct product to prove your answer, is an electric-dipole transition from A_2 to T_2 permitted?

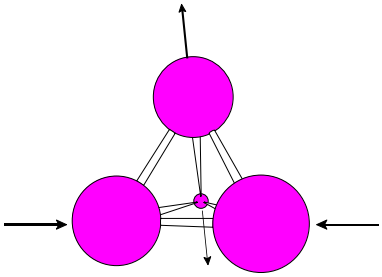


Determine the symmetry of the vibrational modes. (You may use the back of this sheet for additional workspace.)

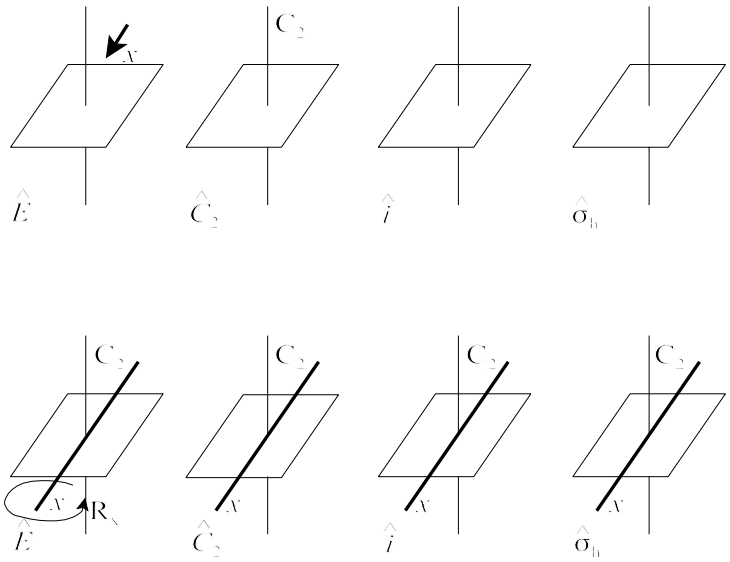
Which of the six vibrational modes are IR active? _____

Which of the six vibrational modes are Raman active? _____

The sketch shows one normal mode of vibration. Determine the symmetry of this mode. _____



2(30). Show sketches of the result of performing the $\hat{C}_2$, $\hat{i}$, $\hat{\sigma}_h$ operations on the *x* translational motion and on the R_x rotational motion. The results of the $\hat{E}$ operation are given to you.



These symmetry elements define the $\mathbf{C_{2h}}$ point group.

$\mathbf{C_{2h}}$ representation	$\hat{E}$	$\hat{C}_2$	$\hat{i}$	$\hat{\sigma}_h$	
A_g	1	1	1	1	
A_u	1	1	-1	-1	
B_g	1	-1	1	-1	
B_u	1	-1	-1	1	

Which irreducible representation should be assigned to *x*? _____

Which irreducible representation should be assigned to R_x? _____

3(10). The configuration for an excited state for a carbon atom in which one of the 2s electrons is excited to the 2p orbital is $2s^1\ 2p^3$. Assuming that all electrons in this configuration to have parallel spins, determine the atomic term symbol for the configuration. (Neglect *J*.)

4(10). The diagram shows the ground state and one excited state of a carbon atom. Draw lines connecting the states illustrating transitions which are consistent with the selection rules $\Delta S = 0$; $\Delta L = 0,\pm1$ but $L=0 \not\leftrightarrow L=0$; $\Delta J = 0,\pm1$ but $J=0 \not\leftrightarrow J=0$; $\Delta l = \pm1$.