

NAME:

Instructions:

1. Keep this exam closed until instructed to begin.
2. **Please write your name on this page but not on any other page.**
3. Please silence any noisy electronic devices you have.
4. Attached sheet(s) provide potentially useful constants and equations. You may detach these from the exam.
5. To receive full credit for your work, please
 - (a) show all your work, using only the exam papers, including the back of this sheet if necessary;
 - (b) specify the correct units, if any, for your final answers;
 - (c) use an appropriate number of significant digits for final numerical answers;
 - (d) **stop writing and close your exam immediately when time is called.**

Other notes:

- **The first page portion of the exam is worth 40 points.** Partial credit for these problems is not necessarily available.
- **Your 2 best scores of the 3 remaining problems will count towards the other 60 points.** Partial credit is available for these problems, so try each problem and do not erase any of your work.

1. **40 points.**

(a) Evaluate $b_g \otimes a_u$ in the point group C_{2h} .

(b) Is the transition from an a_{2u} MO to an a_{1u} MO in ethane (point group D_{3d}) allowed:

i. by electric dipole selection rules?

ii. by Raman selection rules?

(c) What is the symmetry representation for the C—C σ -bonding orbital in ethane?

(d) Assume that Li_2^+ follows the line for N_2 in the correlation diagram.

i. Write the MO configuration for the ground state of Li_2^+ .

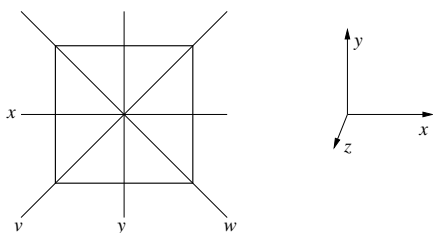
ii. Write the term symbol for the ground state of Li_2^+ .

C_{2h}	\hat{E}	\hat{C}_2	\hat{I}	$\hat{\sigma}_h$	Functions
$A_g(a_g)$	1	1	1	1	$x^2, y^2, z^2, xy; R_z$
$B_g(b_g)$	1	-1	1	-1	$xz, yz; R_x, R_y$
$A_u(a_u)$	1	1	-1	-1	z
$B_u(b_u)$	1	-1	-1	1	x, y

D_{3d}	\hat{E}	$2\hat{C}_3$	$3\hat{C}_2$	\hat{I}	$2\hat{S}_6$	$3\hat{\sigma}_d$	Functions
$A_{1g}(a_{1g})$	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A_{2g}(a_{2g})$	1	1	-1	1	1	-1	R_z
$E_g(e_g)$	2	-1	0	2	-1	0	$(x^2 - y^2, xy), (xz, yz); (R_x, R_y)$
$A_{1u}(a_{1u})$	1	1	1	-1	-1	-1	
$A_{2u}(a_{2u})$	1	1	-1	-1	-1	1	z
$E_u(e_u)$	2	-1	0	-2	1	0	(x, y)

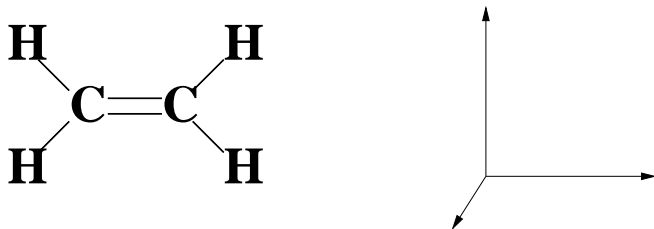
2. List all the point groups possible for the fluorobenzenes, C_6H_5F , $C_6H_4F_2$, $C_6H_3F_3$, $C_6H_2F_4$, C_6HF_5 , and C_6F_6 , with any arrangement of the F atoms.

3. One corner of a multiplication table for the group D_{4h} is left blank below. For convenience, we have labeled the four dihedral \hat{C}_2 rotation axes by v , w , x , and y , as shown. The v and w axes (like x and y) do not move when we carry out an operation. Fill in the missing entries. (You may choose any direction of rotation, and you may choose which operation is carried out first, but be consistent.)



D_{4h}	\hat{E}	$\hat{C}_4(z)$	$\hat{C}_2(w)$	\hat{I}
\hat{E}				
$\hat{C}_4(z)$				
$\hat{C}_2(w)$				
\hat{I}				

4. The *complete* MO configuration of ethene is $1a_g^2 1b_{3u}^2 2a_g^2 3a_g^2 2b_{3u}^2 1b_{1u}^2 1b_{2g}^2 1b_{2u}^2$.



- (a) Label the coordinate axes x , y , and z above, based on the representations used in this MO configuration.
- (b) Identify each of the MO's with one of the following groups of electrons:
- (A) C—H σ -bond electrons,
 - (B) C—C π -bond electrons,
 - (C) $1s$ core electrons,
 - (D) C—C σ -bond electrons.

$1a_g^2$

$1b_{3u}^2$

$2a_g^2$

$3a_g^2$

$2b_{3u}^2$

$1b_{1u}^2$

$1b_{2g}^2$

$1b_{2u}^2$

