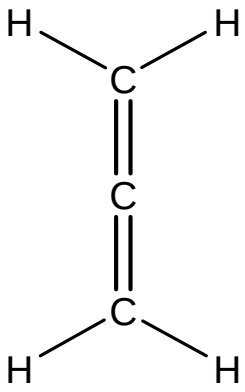
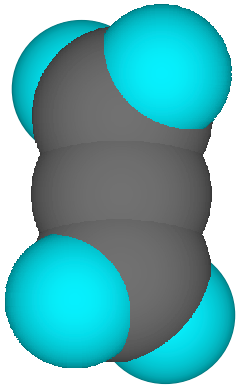
CHEM442-001
College of Charleston
Spring 1999
Exam IV

The point group for molecular allene CH_2CCH_2 is **D_{2d}**. (Note: in the molecular model shown, the two mirror planes $2\hat{\sigma}_d$ are at 45° to the plane of the paper and the two rotation axes $2\hat{C}_2'$ are in the plane of and perpendicular to the paper.



D_{2d}	$\hat{E}$	$2\hat{S}_4$	$\hat{C}_2$	$2\hat{C}_2'$	$2\hat{\sigma}_d$	
A_1	1	1	1	1	1	x^2+y^2,z^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	z,xy
E	2	0	-2	0	0	$(x,y),(R_x,R_y),(xz,yz)$



1(10). How many symmetry operations are in this group? _____

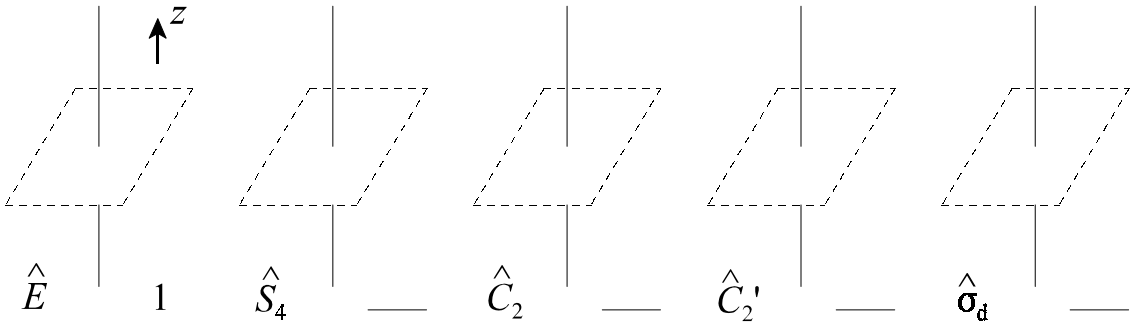
How many symmetry classes are in this group? _____

2(10). Is allene optically active? _____

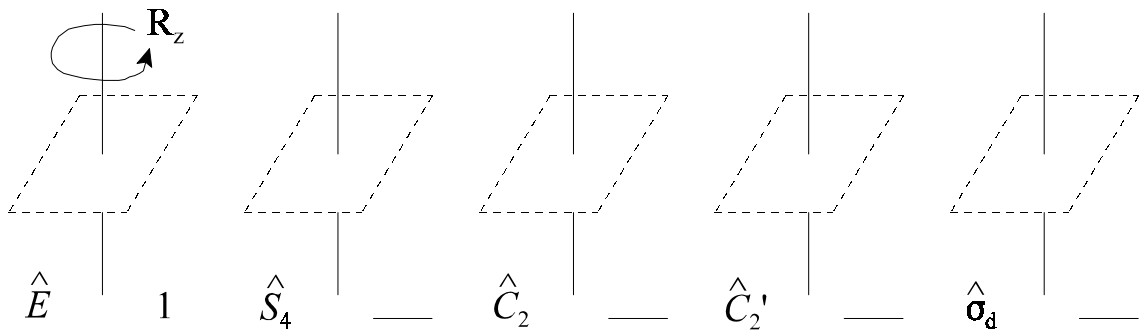
Does allene have an electric dipole moment? _____

3(10). Perform a direct product between B_1 and A_2. Will an electric dipole transition between states with these symmetries be allowed? _____

4(10). Confirm the table entries for translation along the *z* direction by completing the remaining four drawings.



5(10). Confirm the table entries for rotation about the *z* direction by completing the remaining four drawings.



6(20). Determine the irreducible representations for the vibrational motion.

7(15). Of the 15 vibrational transitions, list those that are ***ONLY*** IR active and specify the number of peaks that will be observed.

Of the 15 vibrational transitions, list those that are ***ONLY*** Raman active and specify the number of peaks that will be observed.

Of the 15 vibrational transitions, list those that are ***BOTH*** IR and Raman active and specify the number of peaks that will be observed.

8(15). Determine the irreducible representations for the π molecular orbitals. (If time permitted, the next question would be to write the wave function as $\phi = N \Sigma \pm\phi_i$.)