1. 8
2. 10
3. 8
4. 6

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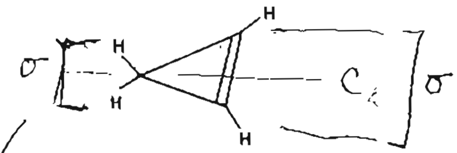
CHEM * 3870
W09
GRADING SCHEME
MIDTERM

8

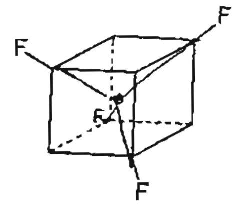
1. **What are the point group symmetries of the following molecules?**

(a.)cyclopropene

C_{2v}

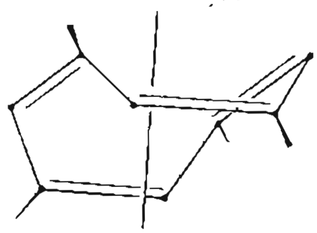


(b.) tetrafluorocubane



T_d

(c.)1,3,5,7-tetramethylcyclooctatetraene



S_4

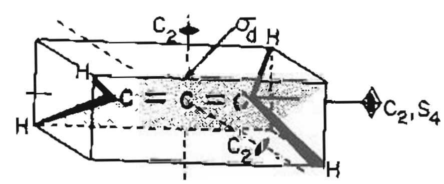
(d.) allene

D_{2d}

1,3,5,7-Tetramethylcyclooctatetraene

3. There is an S_4 axis. There are no additional independent symmetry elements; the set of methyl groups destroys all the vertical planes and horizontal C_2 axes that exist in C_8H_8 itself. The group is therefore S_4.

It may be noted that this molecule contains no center of symmetry or any plane of symmetry and yet it is *not* dissymmetric. It thus provides an excellent illustration of the rule developed in Section 3.10.



Allene.

D. 1. Allene (Fig. 1-37) does not belong to any of the special point grc
2. There are three C_2 axes.
3. There are two vertical mirror planes colinear with one of the axes. One is shown in Fig. 1-37 and the other includes the t C atoms and the two H atoms not in the plane shown in the draw
4. Three perpendicular C_2 axes must put us in the D point groups.
5. There is no horizontal mirror plane (which, by definition, wc be perpendicular to one of the C_2 axes).
6. The vertical mirror planes already noted must put us in the group L

If you had missed the two perpendicular C_2 axes of allene, you m have concluded that the point group was C_{2v}. The S_4 axis should tell y that something is wrong, though, since the C_{2v} point group doesn't h an S_4 operation. This should lead you to look for more symmetry in molecule. There is no substitute for experience in finding all of the symme elements present in a molecule.

2. $\ldots -3, -2, -1, 0, 1, 2, 3, \ldots$ + as combining operation

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j, k, l integers in set

Closure ✓ $j+k$ = another integer in set ✓

Associative ✓ $j+(k+l) = (j+k)+l$ ✓

Identity ✓ $j+0 = j$ ✓ 0, identity

Reciprocal ✓ $j+(-j) = 0$ ✓

Abelian ✓ $k+j = j+k$ ✓

3. D_{2d}

8

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
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)

$A_2 \otimes B_1$ 1 −1 1 −1 1 ✓

$= B_2$ 1 −1 1 −1 1 ✓ (irreducible)

$E \otimes E$ 4 0 4 0 0 ✓ ✓ (reducible)

$a_{A_1} = \frac{1}{8}[(1)(4)(1) + (1)(0)(2) + (1)(4)(1) + 0 + 0] = \frac{1}{8}(8) = 1$ ✓

$a_{A_2} = \frac{1}{8}[(1)(4)(1) + (1)(0)(0) + (1)(4)(1) + 0 + 0] = \frac{1}{8}(8) = 1$ ✓

$a_{B_1} = \frac{1}{8}[(1)(4)(1) + 0 + (1)(4)(1) + 0 + 0] = \frac{1}{8}(8) = 1$ ✓

$a_{B_2} = \frac{1}{8}[(1)(4)(1) + 0 + (1)(4)(1) + 0 + 0] = \frac{1}{8}(8) = 1$ ✓

$\boxed{a_E = \frac{1}{8}[(2)(4) - (2)(4)] = \frac{1}{8}(0) = 0}$

$E \otimes E = A_1 + A_2 + B_1 + B_2$

4.

	E	A	B	C
E	E	A	B	C
A	A	E	C	B
B	B	C	E	A
C	C	B	A	E

6

order of group 4 ✓

$AB = BA = C$

$AC = CA = B$ ✓

$BC = CB = A$ ✓

Abelian

each element E, A, B, C in a class by itself ✓

nontrivial subgroups

	E	A
E	E	A
A	A	E

	E	B
E	E	B
B	B	E

	E	C
E	E	C
C	C	E

✓

order 2 ✓