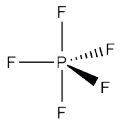
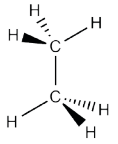
Symmetry and Group Theory – Exercise Set 2, Solutions

2.1) Identify the symmetry elements and determine the point groups of the following molecules.

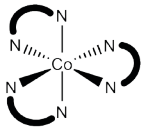
HCl



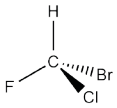
PF_5



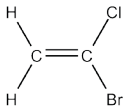
H_3CCH_3



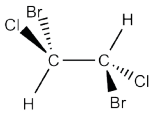
$[Co(en)_3]^{3+}$



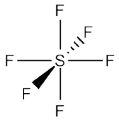
CHFClBr



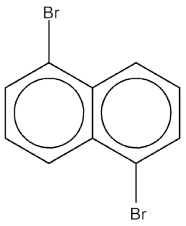
$H_2CCClBr$



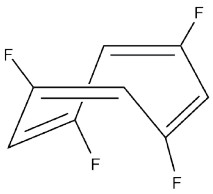
HClBrCCHClBr



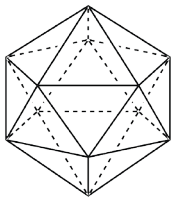
SF_6



1,5-dibromonaphthalene



1,3,5,7-tetrafluorocyclo-octatetraene


$B_{12}H_{12}^{2-}$
dodecahydro-closo-dodecaborate(2–) ion
(every corner represents one BH unit)

en = ethylenediamine

Molecule	***C_n***	***σ***	***i***	***S_n***	**Point group**
HCl	C_∞	σ_v	-	-	$C_{\infty v}$
PF_5	C_3, $3C_2$	σ_h, $3\sigma_v$	-	S_3	D_{3h}
H_3CCH_3	C_3, $3C_2$	$3\sigma_d$	i	S_6	D_{3d}
$Co(en)_3$	C_3, $3C_2$	-	-	-	D_3
CHFClBr	-	-	-	-	C_1
$H_2CCClBr$	-	σ	-	-	C_s
HClBrCCHClBr	-	-	i	-	C_i
SF_6	$3C_4$, $4C_3$, $6C_2$	$3\sigma_h$, $3\sigma_d$	i	$4S_6$, $3S_4$	O_h
$C_{10}H_6Br_2$	C_2	σ_h	i	-	C_{2h}
$C_8H_4F_4$	C_2	-	-	S_4	S_4
$B_{12}H_{12}$	$6C_5$, $10C_3$, $15C_2$	$15\ \sigma$	i	$6S_{10}$, $10S_6$	I_h

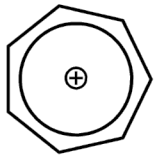
2.2) Determine the point groups of the following objects.

Pair of glasses	C_s
Erlenmeyer flask (no label)	$C_{\infty v}$
Screw	C_1
The number “96”	C_{2h}
Spoon	C_s

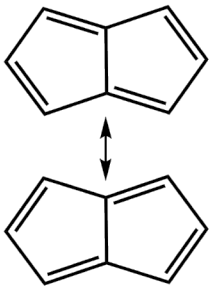
Tennis ball	D_{2d}
A printed page of paper	C_1
The outside of a car	C_s
The inside of a car	C_1

2.3) For the following hydrocarbons, determine

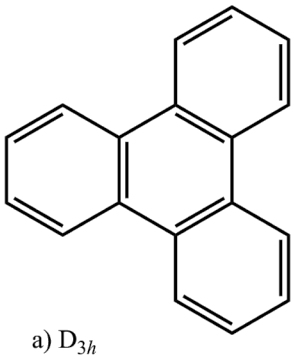
a) the point group,
b) the symmetry elements,
b) the number of chemically distinct carbon atoms,
c) the number of peaks in the ^{1}H NMR spectrum (neglect coupling).



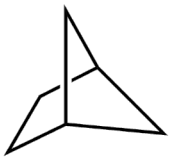
a) D_{7h}
b) {E, C_7, S_7, $7C_2$, σ_h, $7\sigma_v$}
c) 1
d) 1



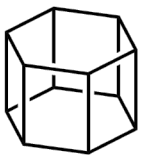
a) D_{2h}
b) {E, C_2, C'_2, C''_2, i, 3σ}
c) 3
d) 2



a) D_{3h}
b) {E, C_3, S_3, $3C_2$, σ_h, $3\sigma_v$}
c) 3
d) 2



a) C_{2v}
b) {E, C_2, $2\sigma_v$}
c) 3
d) 4

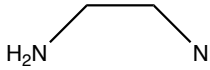


a) D_{6h}
b) {E, C_6, S_6, C_3, i, S_3, $C_6^3 \equiv C_2$, $3C'_2$, $3C''_2$, $3\sigma_d$, $3\sigma_v$, σ_h}
c) 1
d) 1

Homework

2.4) Determine the point groups of the following molecules and objects. Which of these molecules and objects can have a permanent dipole moment and which are chiral?

		Permanent dipole moment	**Chrial**
A	D_{2d}	✗	✗
B	C_{3v}	✓	✗
C	C_2	✓	✓
D	C_2	✓	✓
E	D_3	✗	✓
F	D_{2h}	✗	✗
G	D_{3h}	✗	✗
H	$C_{\infty v}$	✓	✗

2.5) The reaction scheme below shows a rearrangement reaction of an $M(en)_3$ complex, where 'en' is the bidentate ligand 

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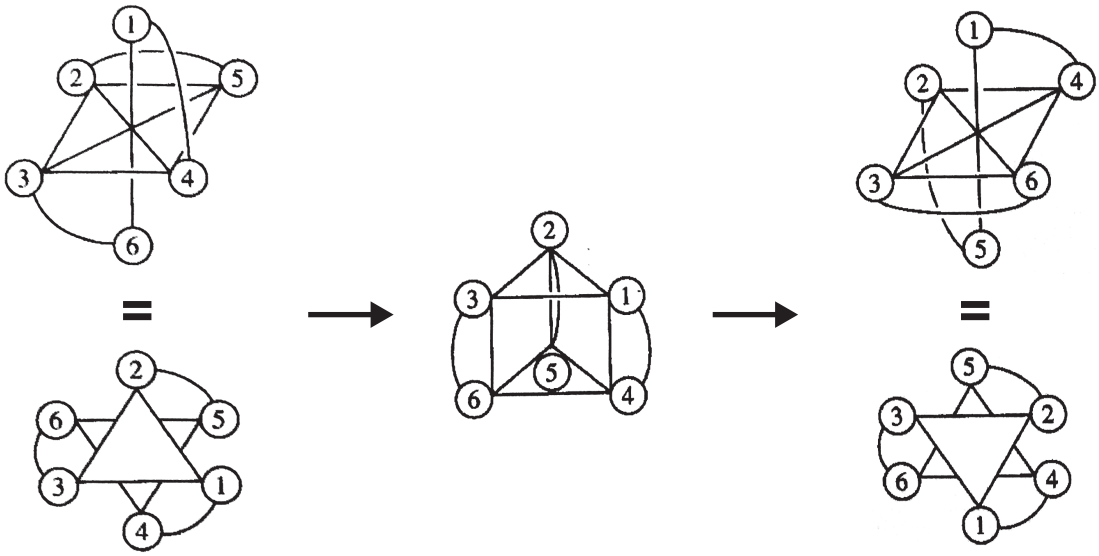
Both the reactant and product are shown in two different projections. The rearrangement is thought to be concerted, meaning all atoms move simultaneously.



a) Determine the point groups of the reactant, the transition state and the product. What is the point group of the complex while it undergoes rearrangement from the reactant to the transition state, and while it undergoes rearrangement from the transition state to the product?
b) What is the relationship between the point groups of reactant, product, and transition state?
c) How are the reactant and product related?

a) Both reactant and product have D_3 symmetry, the transition state has D_{3h} symmetry. During the rearrangement, the complex maintains D_3 symmetry.
b) D_3 is a subgroup of D_{3h}.
c) Reactant and product are enantiomers.