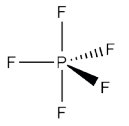
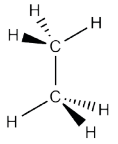
Symmetry and Group Theory – Exercise Set 2

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

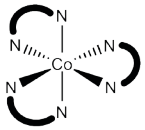
HCl



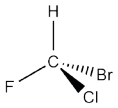
PF_5



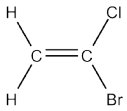
H_3CCH_3



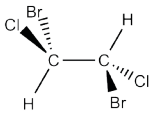
$[Co(en)_3]^{3+}$



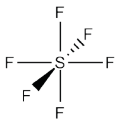
CHFClBr



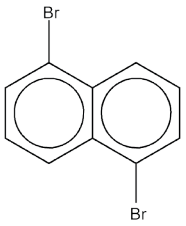
$H_2CCClBr$



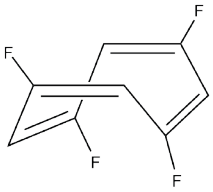
HClBrCCHClBr



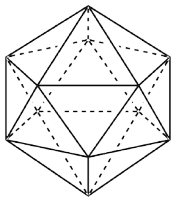
SF_6



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)

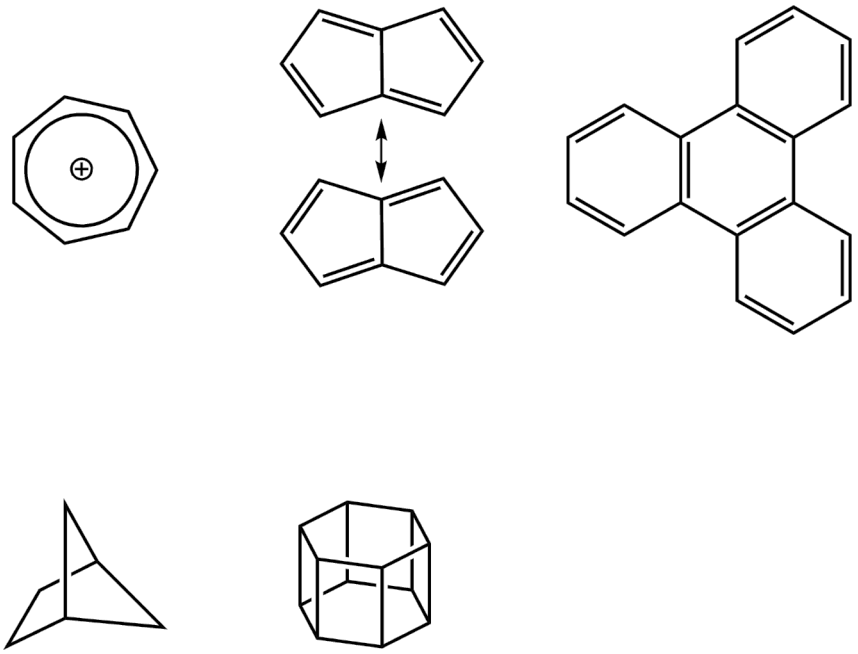
en = ethylenediamine

2.2) Determine the point groups of the following objects.

Pair of glasses
Erlenmeyer flask (no label)
Screw
The number “96”
Spoon
Tennis ball
A printed page of paper
The outside of a car
The inside of a car

2.3) For the following hydrocarbons, determine

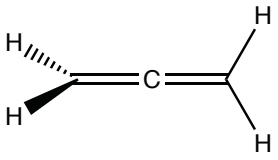
a) the point group,
b) the symmetry elements,
b) the number of chemically distinct carbon atoms,
c) the number of peaks in the ^{1}H NMR spectrum (neglect coupling).



Homework

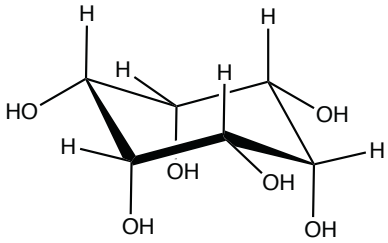
2.4) Determine the point groups of the following molecules and objects. Which of these molecules and objects can have a permanent dipole moment and which are chiral?

A



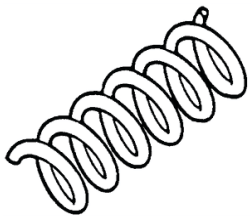
Allene

B



cis-Inositol

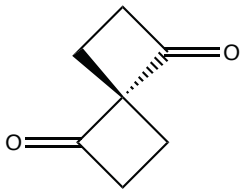
C



a helix

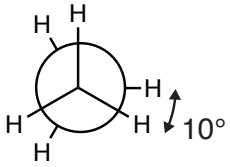
(assume perfect symmetry)

D

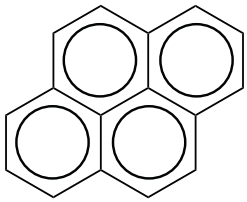


E

ethane in the configuration below

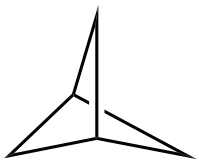


F

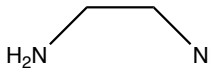


Pyrene

G



H

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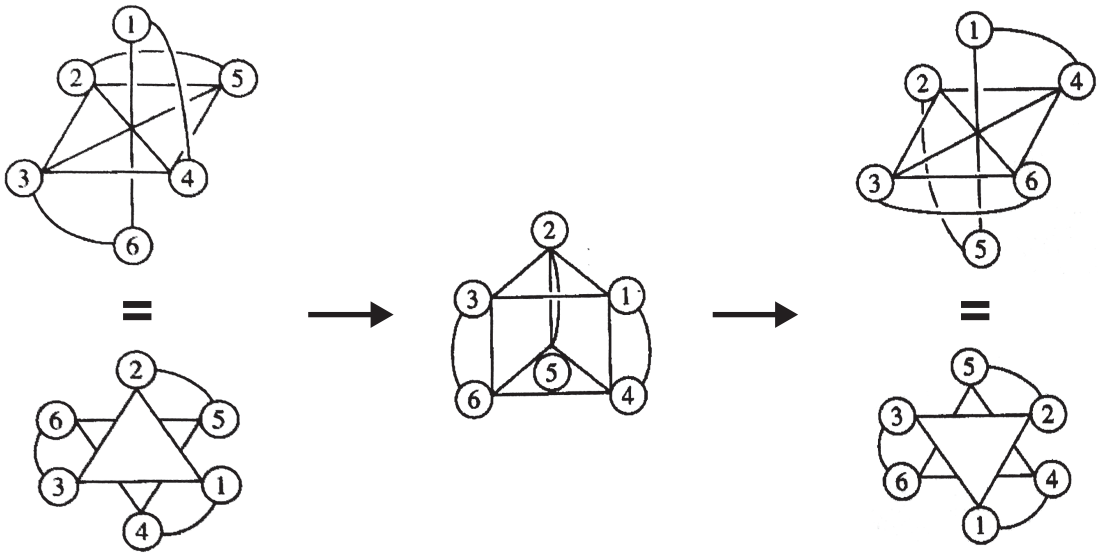
Both the reactant and product are shown in two different projections. The rearrangement is thought to be concerted, meaning all atoms move simultaneously.



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?