Symmetry and Group Theory – Exercise Set 1

1.1) Identify the symmetry elements (σ, i, C_n, S_n) of the following molecules.

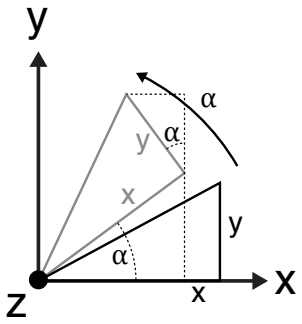
NH_3, $B(OH)_3$, CO, CO_2, CH_4, $W(CO)_6$, phenylalanine, $FeCp_2$ (Cp rings are staggered)

1.2) What are the matrix representations of σ_{xy} and σ_{xz} for the reflection of a point $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$?

1.3) Show that the rotation matrix

$$C_n = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with $\alpha = 2\pi/n$ performs a rotation around the z axis; the sketch below may be helpful. What matrices give a rotation around the other axes?



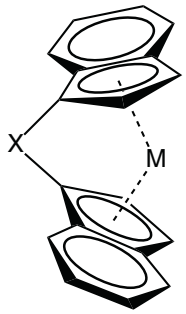
1.4) Show that $\sigma_{yz}\sigma_{xy} = C_2(y)$ for the transformation of a point $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$.

1.5) Determine the point group of the molecules in exercise 1.

Homework

1.6) Determine the point groups of the following molecules and objects.

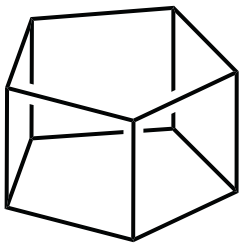
A



B

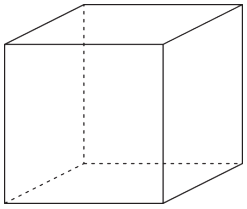
3 dz^2 orbital

C



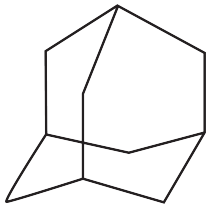
Uniform pentagonal prism

D



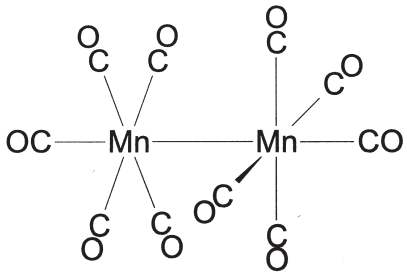
Cube

E

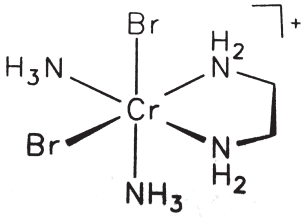


Adamantane ($C_{10}H_{16}$)

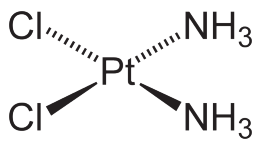
F



G



H



Cisplatin
(planar, consider NH_3 ligands as spheres)