Class Assignment 02/25/2021

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Questions (20 pts):

Q1. Determine the point groups for a-p

a. Ethane, CH₃-CH₃, (staggered conformation)

D3d: It has a principal C3 axis, a perpendicular C2 axis, and multiple vertical mirror planes within the C3 axis

b. Ethane (eclipsed conformation)

D3h: It has a principal C3 axis, a perpendicular C2 axis, and a horizontal plane perpendicular to the C3 axis

c. Chloroethane (staggered conformation)

Cs: Only one mirror plane, no rotational axis

d. 1,2-Dichloroethane (staggered *anti* conformation)

The point group is C_{2n}. Has C_2 rotational axes passing through the mid point of the C-C bond and perpendicular to the Cl-C-Cl plane. It has one diamond h plane perpendicular to the C_2 rotational axis.

e. Ethylene

Belongs to D_{2h} point group. Has 3 C_2 rotation axes and 3σ planes of symmetry

f. Acetylene

Acetylene is a linear molecule. It has C infinite rotational axis along the molecule axis. The principle axis is C infinite and it has an infinite number of C_2 rotational

axes perpendicular to the principal axis. It also has σh perpendicular to the principal axis. The point group is $D_{\infty h}$.

g. Naphthalene

Principal axis is C_2 2 perpendicular axes - D group Horizontal mirror plane - D_{nh} C_2 so -> D_{2h}

h. 1,8-dichloronaphthalene

Principal axis is C_2 No perpendicular axis - C group No horizontal mirror plane, but has mirror plane that contains principal axis-> C_{2v}

i. 1,5-dichloronaphthalene

Principal axis is C_2 No perpendicular C_2 axes so C group Has a horizontal mirror plane -> \mathbf{C}_{2h}

j. 1,2-Dichloronaphthalene

No rotational axis, only one mirror plane of molecule \rightarrow Cs

k. Cyclohexane (in chair conformation)

C₃ is the principal axis with 3 C₂ axes perpendicular to the C₃ axis. Also has mirror plane containing principle axis \rightarrow **D**_{3d}

I. 1,1' - Dichloroferrocene

C₂ is the principal axis, and a horizontal plane is present that is perpendicular to the C₂ axis. Also, no C₂ axis perpendicular to the principal axis. Thus, its point group --> C₂h.

m. Cis-[PtCl₂(NH₃)₂]

C₂ rotation axis and two vertical planes

C_{2v} molecule

n. Trans- $[PtCl_2(NH_3)_2]$

C₂ rotation axis, three vertical planes, and inversion center

D_{2h} molecule

o. Diborane

Three perpendicular $\mathbf{C}_{\mathbf{2}}$ axes and three perpendicular mirror planes

\mathbf{D}_{2h} molecule

p. Dibenzenechromium (eclipsed conformation)

 $\mathrm{C_6}$, $\mathrm{C_3}$, $\mathrm{C_2}$ perpendicular axes to the rings, six perpendicular $\mathrm{C_2}$ axes, horizontal plane

D_{6h} molecule