3.3: Determining the Point Group for a Molecule- the Schoenflies notation

The first step in determining the point group for a molecule is to determine the structure of the molecule. Once this is done, identify all of the symmetry elements the molecular structure possesses. Once this has been accomplished, you can use the preceding flowchart to determine the correct point group using the **Scheonflies notation** system.

Example 3.3.1

Determine the point group for a methane molecule.

Solution

A methane molecules has tetrahedral symmetry. It contains the following symmetry elements: E, 4 C_3 (one each along a C-H bond) axes, 6 σ planes (one each containing the carbon and a pair of hydrogen atoms), 3 C_2 axes (each on bisecting an HCH bond angle.) It also has 3 S_4 axes (each one co-linear with a C_2 axis.) The molecule belongs to the point group T_d, as can be discerned from the following analysis.

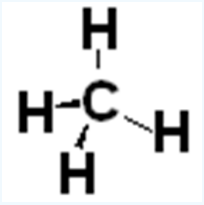

Figure 3.3.1

1. Is the molecular Linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? Yes
3. Does the molecule have a $C_{n\geq 4}$ axis? No
4. Does the molecule have any σ planes? Yes
5. Does the molecule have an inversion center? No

The molecule belongs to the T_d Point Group.

Example 3.3.2

Determine the point group for CH_3Cl.

Solution

Chloromethane has the same tetrahedral shape as methane, but belongs to the point group C_{3v}. The molecule has the following symmetry elements: E, C_3 (along the C-Cl bond axis) and 3 σ_v planes (each containing the chlorine and carbon atoms plus one hydrogen atom. The classification of the molecule goes as follows:

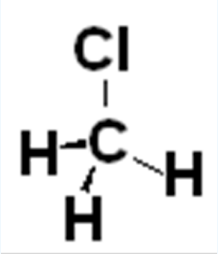

Figure 3.3.2

1. Is the molecule linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? No
3. Does the molecule have a C_n axis? Yes
4. Are there n C_2 axes perpendicular to the principle axis? No
5. Does the molecule have a σ_h plane? No
6. Does it have n σ_v planes? Yes

The molecule belongs to the C_{3v} point group.

Example 3.3.3

Determine the point group for benzene.

Solution

Benzene has a planar geometry and belongs to the point group D_{6h}. The molecule possesses the following symmetry elements: E, C_6, 6 C_2, 6 σ_v, σ_h and i. The classification of the molecule goes as follows:

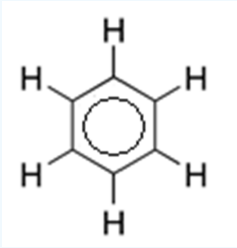

Figure 3.3.3

1. Is the molecule linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? No
3. Does the molecule have a C_n axis? (n = 6 for benzene) Yes
4. Are there n C_2 axes perpendicular to the principle axis? Yes
5. Does the molecule have a σ_h plane? Yes

The molecule belongs to the point group D_{6h}

Example 3.3.4

Classify ethane by its point group.

Solution

Ethene has a planar geometry. The molecule possesses the following symmetry elements: E, 3 C_2, 3 σ, and i. The classification of the molecule goes as follows:

1. Is the molecule linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? No
3. Does the molecule have a C_n axis? Yes ($n = 2$)
4. Are there n C_2 axes perpendicular to the principle axis? Yes
5. Does the molecule have a σ_h plane? Yes

The molecule belongs to the D_{2h} point group.

Example 3.3.5

Classify the isomers of dichloroethene by their point groups.

Solution

Dichloroethene has three isomers. All of them have a planar geometry. The cis- and gem- isomers have the following symmetry elements: E, C_2, and $2\sigma_v$. (The 1,1- (or gem-) isomer has the same elements as the cis- isomer.) The classification of the molecule goes as follows:

1. Is the molecule linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? No
3. Does the molecule have a C_n axis? Yes ($n = 2$)
4. Are there nC_2 axes perpendicular to the principle axis? No
5. Does the molecule have a σ_h plane? No

6. Does the molecule have $n\sigma_v$ planes? Yes

The cis-isomer belongs to the C_{2v} point group.

The trans-isomer has the following symmetry elements: E, C_2, σ_h, and i. The classification of the molecule goes as follows:

1. Is the molecule linear? No
2. Does the molecule have two or more $C_{n\geq 3}$ axes? No
3. Does the molecule have a C_n axis? Yes ($n = 2$)
4. Are there nC_2 axes perpendicular to the principle axis? No
5. Does the molecule have a σ_h plane? Yes

The trans-isomer belongs to the C_{2h} point group.
