Point Groups

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Outline

Four Defining Properties of a Group

1. The product of any two elements in the group and the square of each element must be an element in the group
2. One element in the group must commute with all others and leave them unchanged
3. The associative law of multiplication must hold
4. Every element must have a reciprocal, which is also an element of the group

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Molecular Symmetry Groups

- By inspection, make a complete list of the symmetry elements possessed by a given molecule
- Then, make a complete list of the symmetry *operations* generated by each of these elements
- Recognize that this complete list of symmetry operations satisfies the four criteria of a mathematical group
- Recognize that all molecules having this same list of symmetry elements belong to the same symmetry or “Point Group”

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Nonaxial Groups

Groups and their Operations

- C_1: E
- C_s: E, σ_h
- C_i: E, i
- Note that each Point Group is referred to by its label, e.g. C_s

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Groups with a Single Principal Rotation Axis

The C_n Groups

- C_2: E, C_2
- An example is HOOH in its equilibrium conformation
- C_3: E, C_3, ${C_3}^2$
- An example is a particular conformation of $B(OH)_3$
- The C_n groups other than C_1 have only the identity and a single principal rotation axis as elements of symmetry
- The C_n groups correspond to n-bladed propellor shapes lacking top-bottom symmetry

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D_n Groups

These have a principal n-fold rotation axis and $n \perp C_2$ axes

D_n Groups have no mirror planes or inversion centers

- D_2: E, $C_2(z)$, $C_2(y)$, $C_2(x)$,
- D_3: E, C_3, ${C_3}^2$, $3C_2$
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C_{nv} Groups

These have a principal n-fold rotation axis and n mirror planes that contain it

C_{nv} Groups have no inversion center or $\perp$ C_2 axes

- C_{2v}: E, $C_2(z)$, $\sigma_v(xz)$, $\sigma_v'(yz)$,
- C_{3v}: E, C_3, $C_3{}^2$, $3\sigma_v$
- The water and ammonia molecules are respective examples of C_{2v} and C_{3v} symmetry

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C_{nh} Groups

These have a principal *n*-fold rotation axis and a ⊥ mirror plane

C_{nh} Groups may have an inversion center or improper rotation axes

- C_{2h}: E, C_2, i, σ_h,
- *trans*-2-butene is an example of C_{2h} symmetry

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C_{nh} Groups may have an inversion center or improper rotation axes

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- *trans*-2-butene is an example of C_{2h} symmetry

Other Important Point Groups

- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- Molecules with multiple higher-order rotation axes, the cubic groups T, T_h, T_d, O, O_h

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Symmetry and Point Group Tutorial

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