Lecture 4: Point Groups

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UCIRVINE

http://ffgroup.chem.uci.edu

Definition

Point groups are groups of symmetry operations that keep at least one point in Euclidean space fixed.
Symmetry element of point groups:

(i) Identity E

(ii) n-fold rotation or symmetry axes C_n

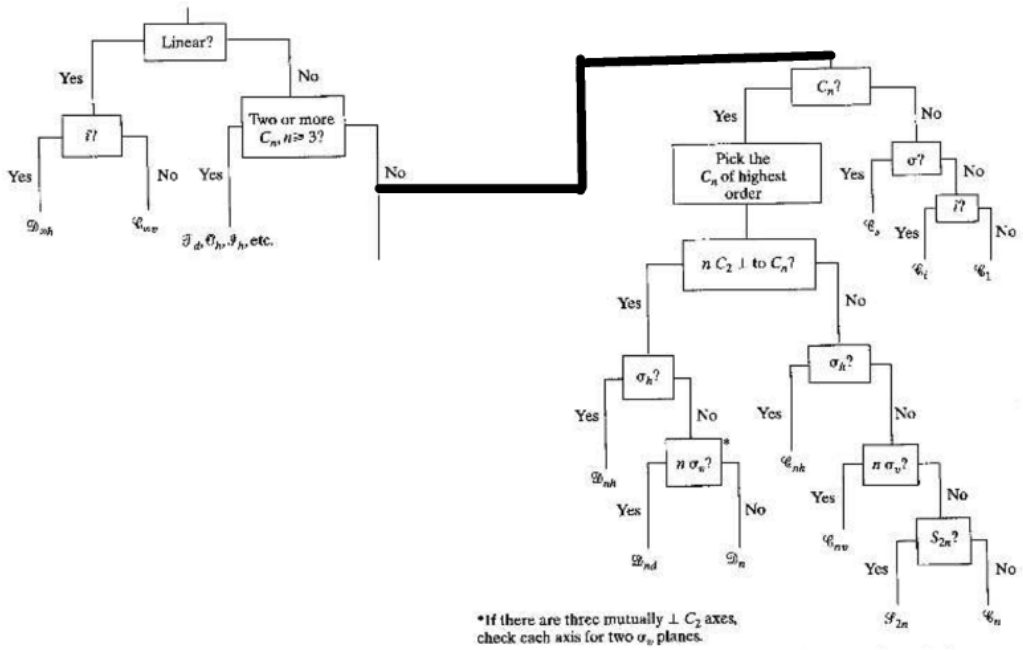
(iii) Reflection or symmetry or mirror planes σ

(iv) n-fold rotation-reflection axis S_n (includes $i \equiv S_2$)

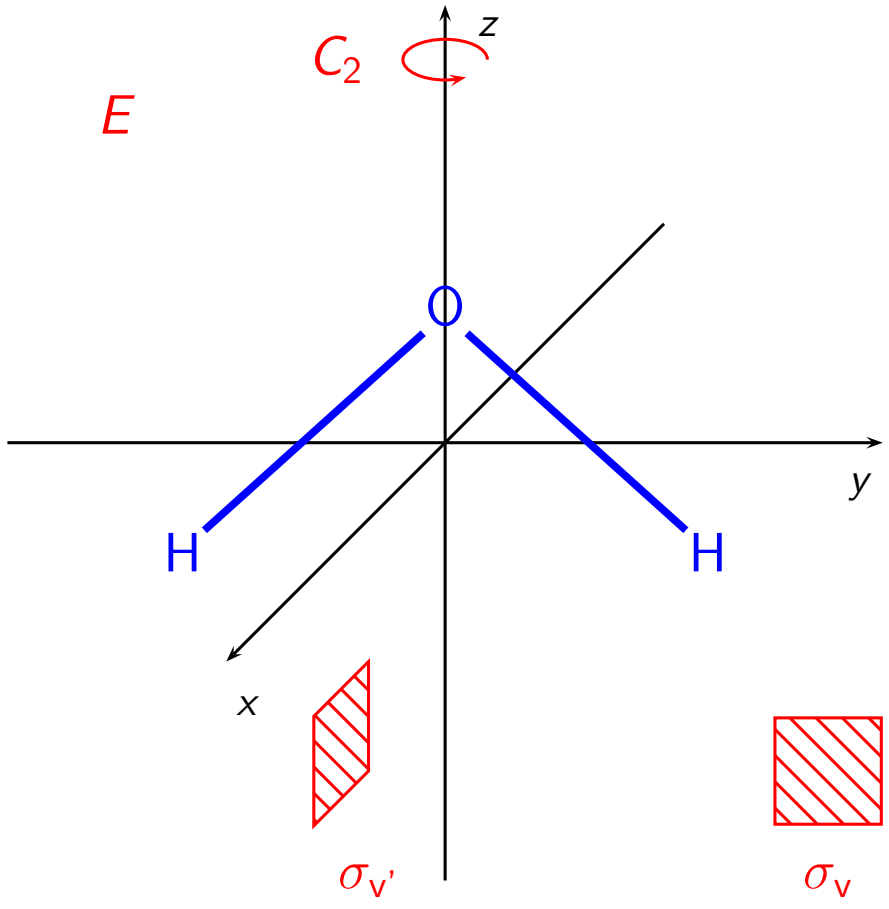
- All point groups are subroups of orthogonal group $O(N)$ (N is dimension)
- Molecular point groups: $N = 3$
  - 7 axial group families: C_n, S_{2n}, C_{nh}, C_{nv}, D_n, D_{nd}, D_{nh}
  - 7 polyhedradal group families: T, T_d, T_h, O, O_h, I, I_h

Determining Point Group Symmetry

1. Visualize the molecule (e.g. using a simple web-based renderer)
2. Determine *all* symmetry elements
3. Follow the flow chart:



Water Molecule



- Symmetry elements of water: $\{E, C_2, \sigma_v, \sigma_{v'}\}$
- Point group C_{2v}

Group Multiplication Table

- Product of two symmetry operations $c = a \cdot b$: Apply b followed by a
- C_{2v} group (multiplication) table:

a / b	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2	E	σ_v'	σ_v
σ_v	σ_v	σ_v'	E	C_2
σ_v'	σ_v'	σ_v	C_2	E

Web Resources

- Otterbein Symmetry: Visualize symmetry operations in 3D
- Achim Gelessus' Website: Character tables for chemically important point groups