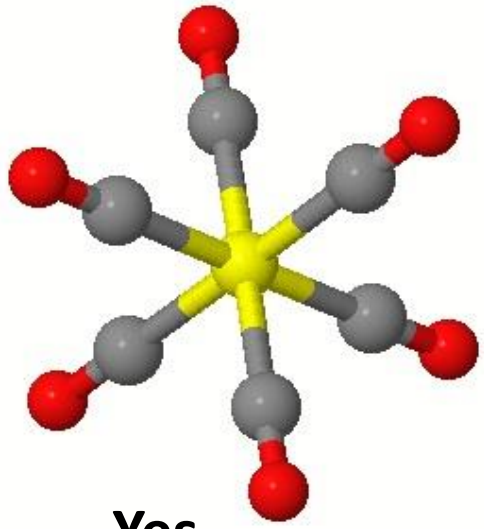
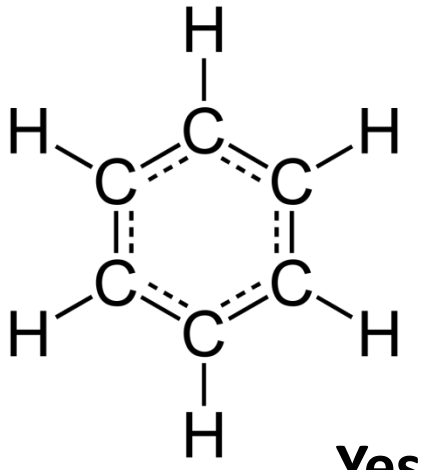
Lecture 8 Sept. 15, 2020

- ***Symmetry in Nature and in Molecules***
- ***Symmetry Operations***
- ***Symmetry Elements***
- ***Point Groups and Assignments***

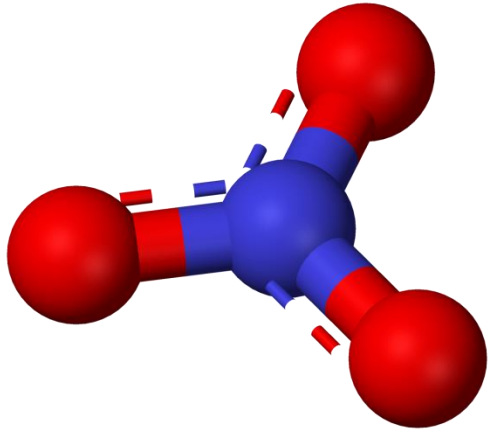
(Proper) Rotation in Molecules?



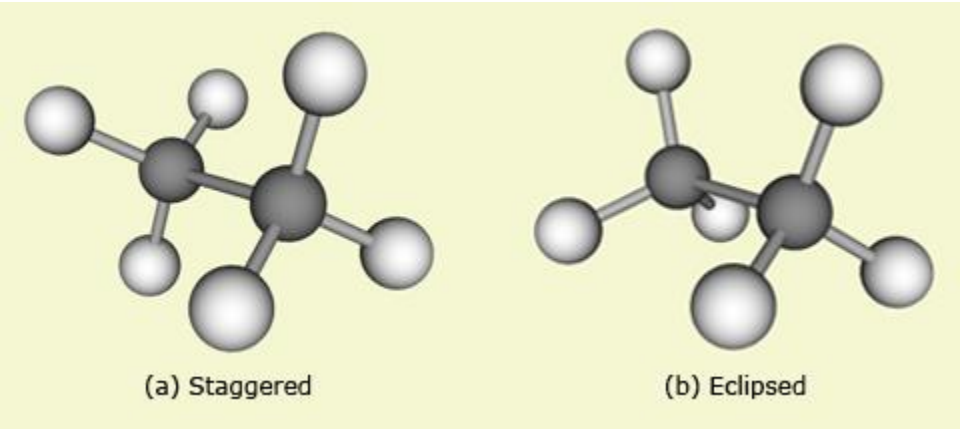
Yes



Yes

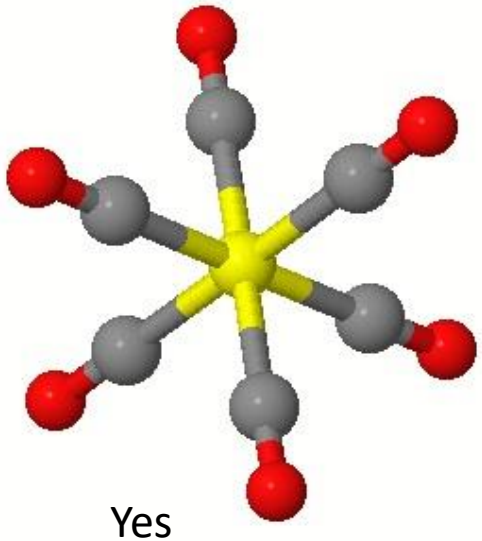


Yes

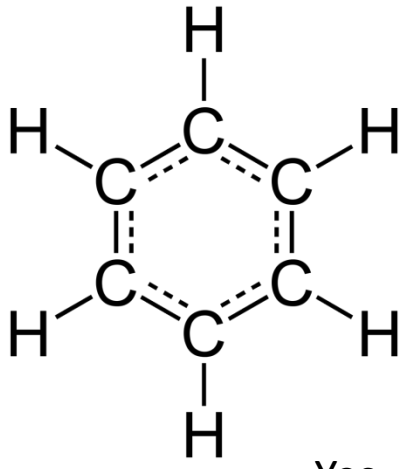


Yes **Yes**

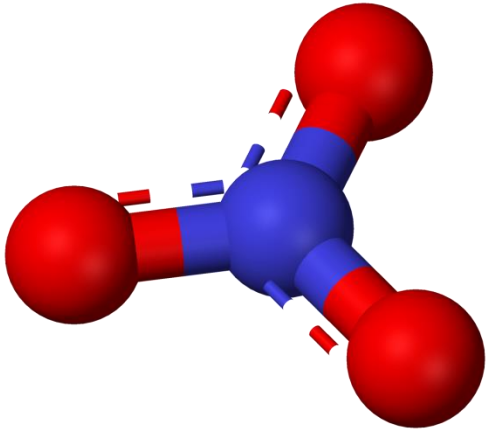
Reflection in a Plane in Molecules



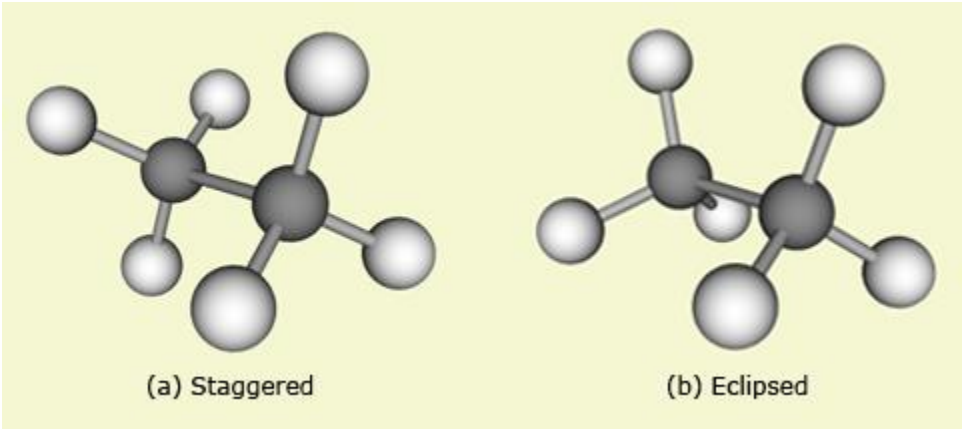
Yes



Yes



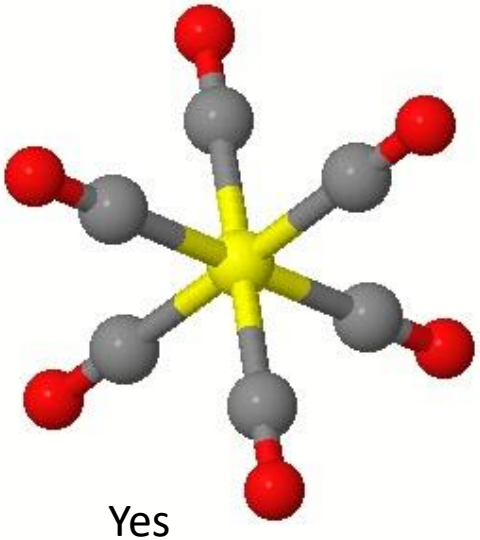
Yes



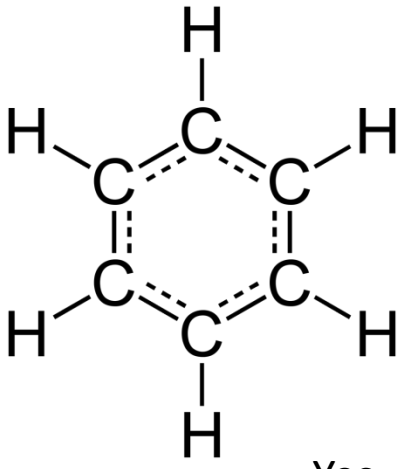
Yes

Yes

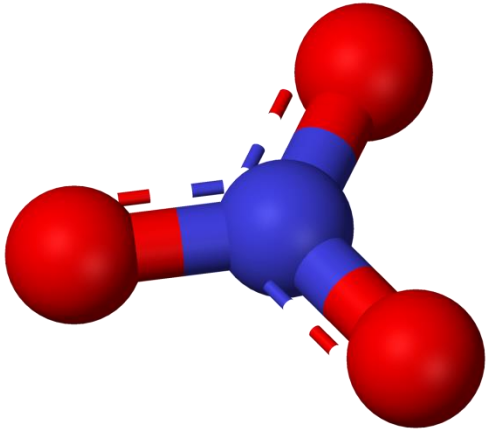
Reflection in a Plane that is perpendicular to the principal rotation axis?



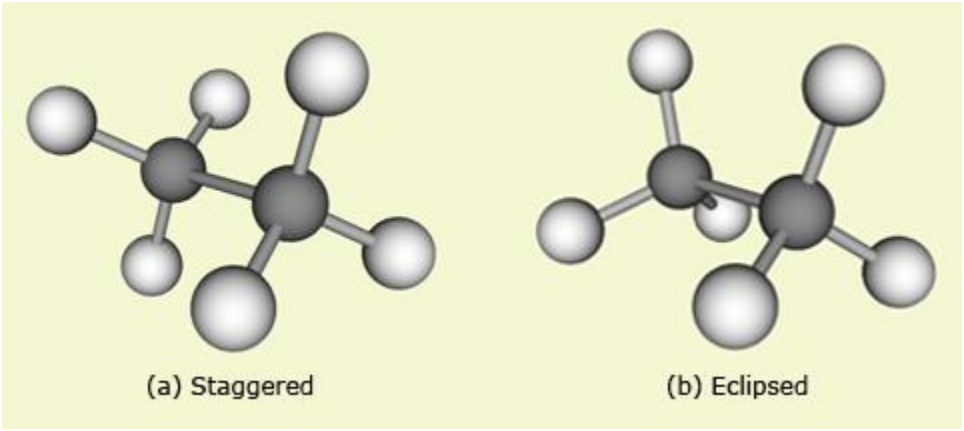
Yes



Yes



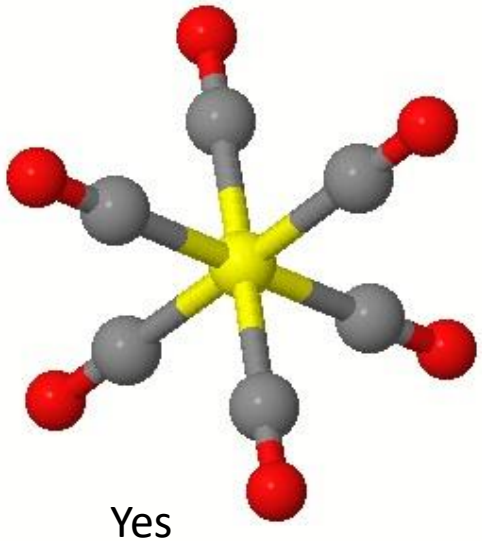
Yes



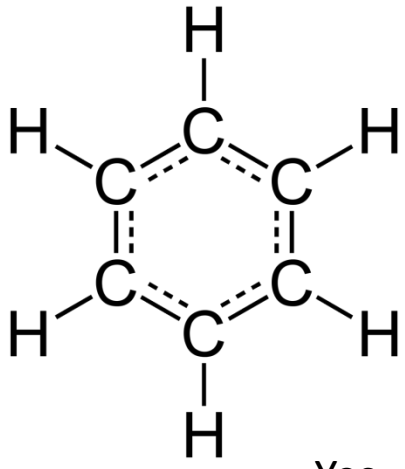
NO

Yes

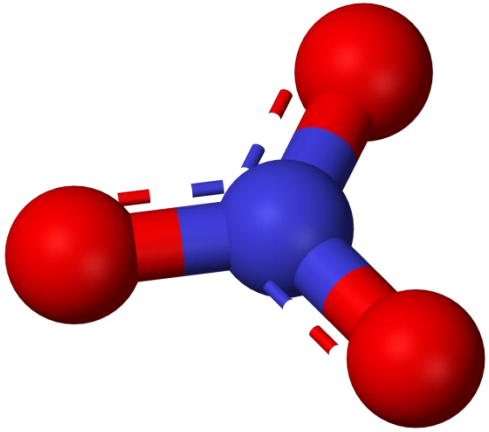
Center of Inversion in Molecules: x,y,z -> -x, -y, -z



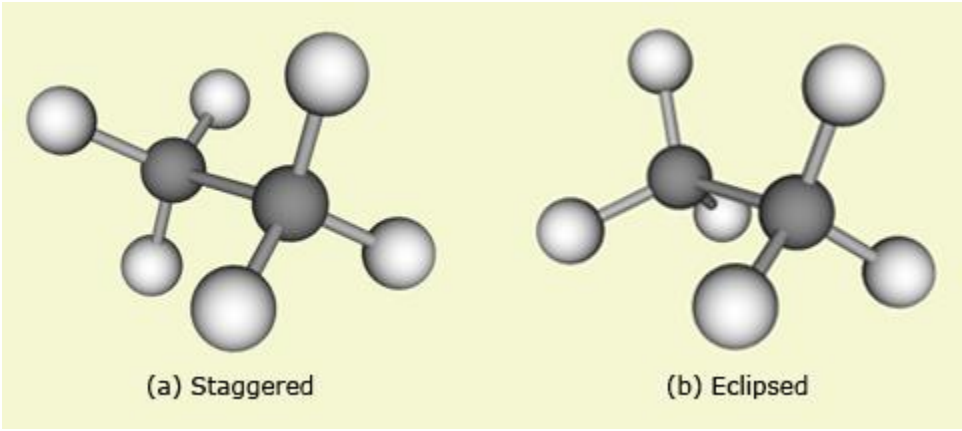
Yes



Yes



No



Yes

No

Let’s look for symmetry elements and operations in molecules

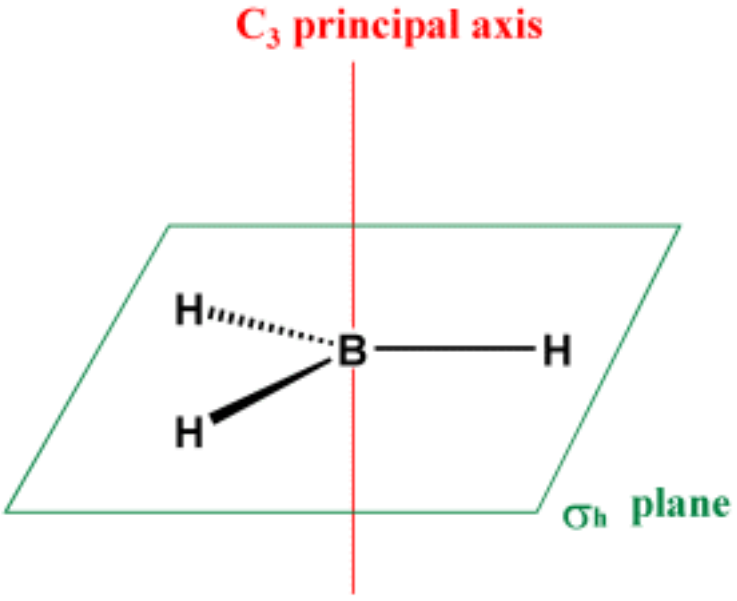
What is a point group?

A collection of symmetry elements for a specific symmetry, intersecting at a specific point for molecules, and displayed in a character table.

Symmetry elements/operations can be manipulated by
Group Theory, Representations and Character Tables

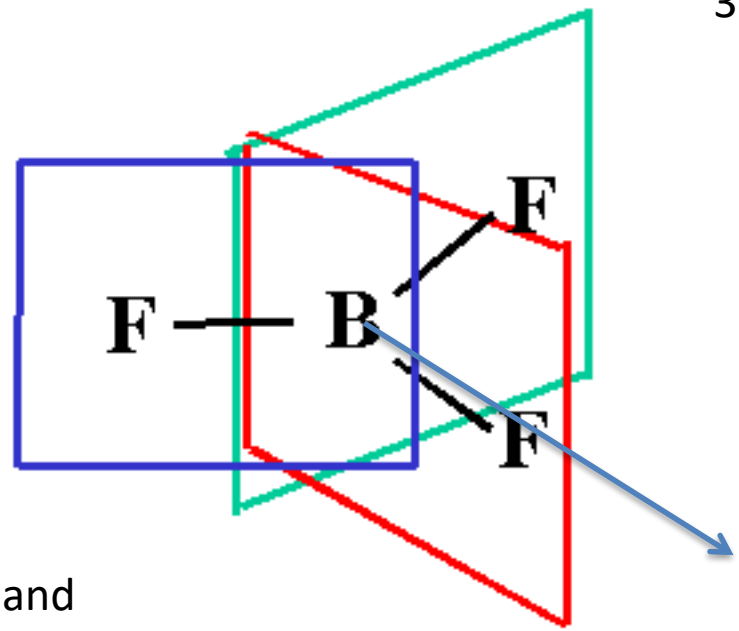
So, What IS a group?

And, What is a Character???



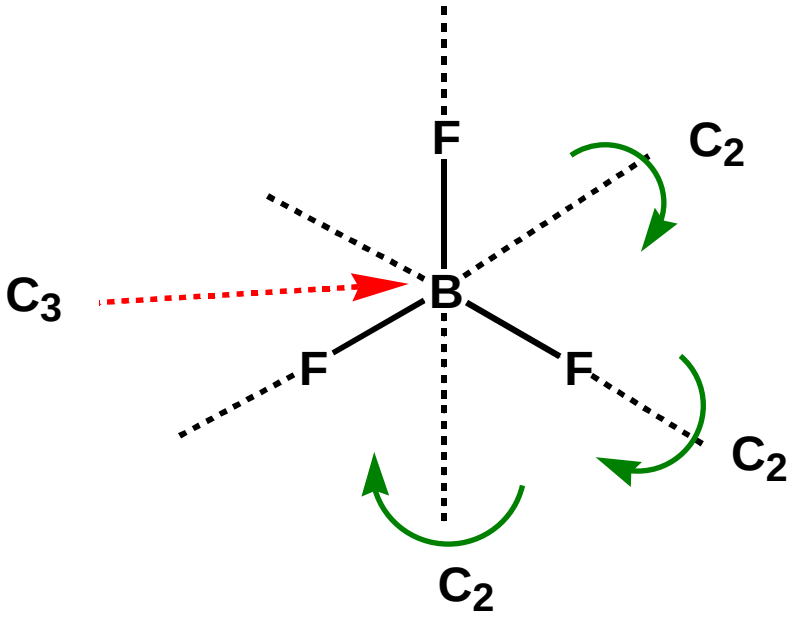
Altogether there are ? Symmetry operations for planar BH_3 or BF_3?

3 σ_v collinear with C_3



3 C_2 along the B-F bonds and perpendicular to C_3

Molecules can possess several distinct axes, e.g. BF_3:



Three C_2 axes, one along each B-F bond, perpendicular to C_3

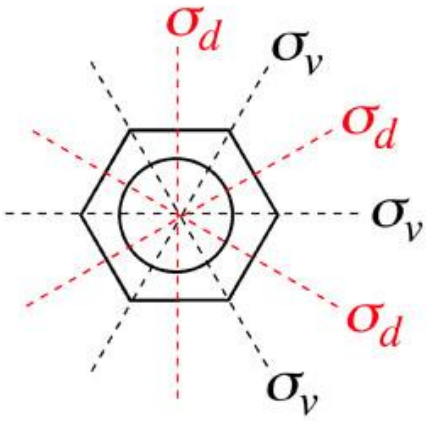
A Certain Class of point groups: D_{nh}

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

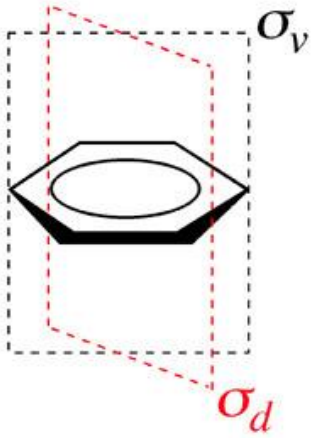
Vertical and Dihedral (σ_v that bisects C_2 axes) Mirror Planes

Benzene, C_6H_6 : 3 σ_d mirror planes and 3 σ_v mirror planes

top view, all 3 σ_v and all 3 σ_d shown



side view, one of each type shown

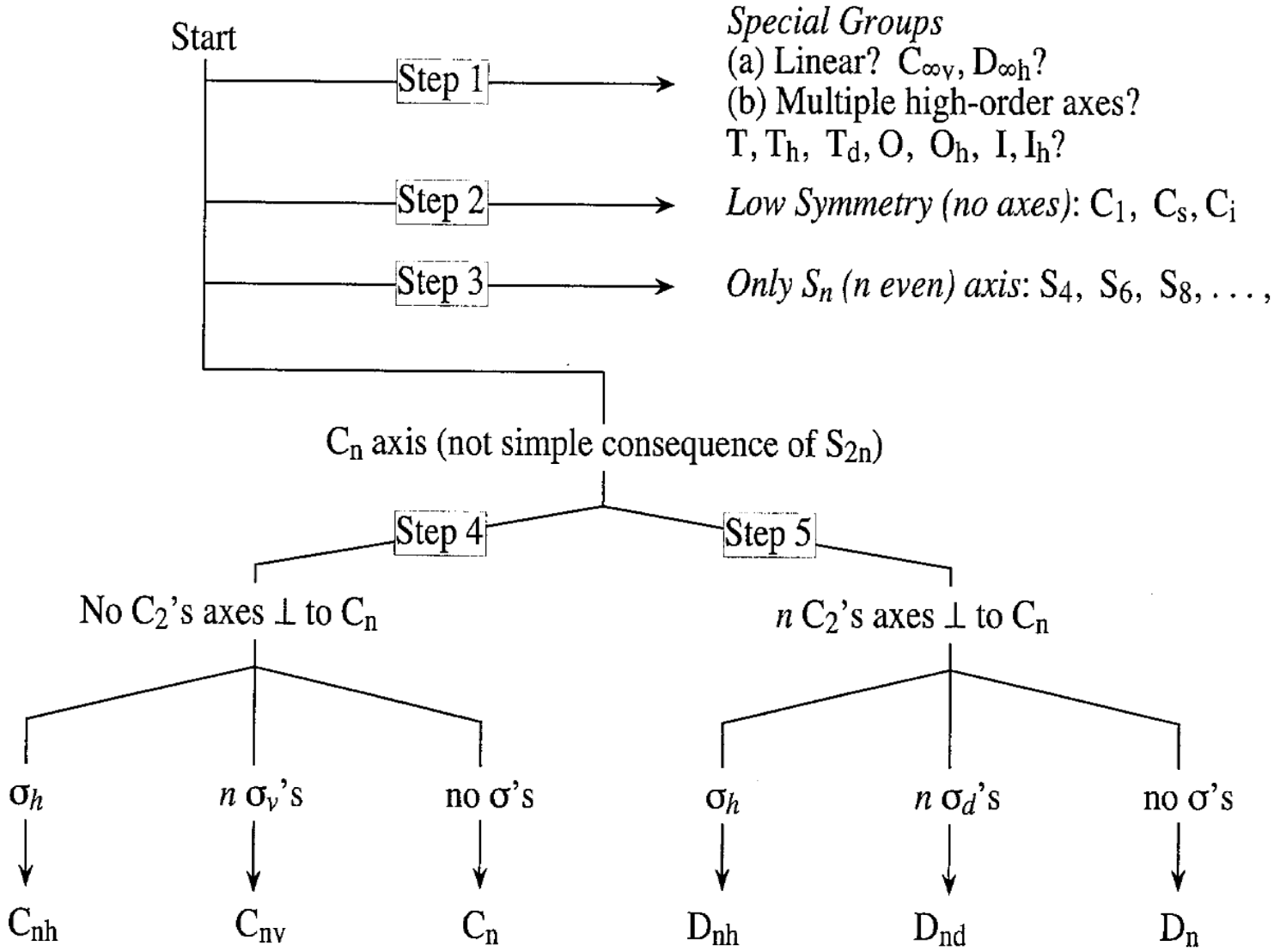


In a molecule that has **both** σ_v and σ_d mirror planes, the σ_v planes bisect as many atoms as possible and the σ_d planes bisect as many bonds as possible.

Symmetry Point Group Assignments

An object may be classified with respect to its symmetry elements or lack thereof. This is done by assigning a symmetry point group, reflecting the combination of symmetry elements present in the structure. For example, bromochlorofluoromethane has no symmetry element other than C1 and is assigned to that point group. All C1 group objects are chiral. Other low symmetry point groups are Cs (only a single plane of symmetry) and Ci (only a point of symmetry). Objects in either of these point groups are achiral.
Some objects are highly symmetric and incorporate many symmetry elements. Methane is an example of a high symmetry molecule, having 4 C3 axes, 3 C2 axes and 6 σ (planes); it belongs to the tetrahedral point group Td.
When combinations of rotational axes and planes are present, their relationship is designated by a v (vertical), h (horizontal) or d (diagonal). Thus, a plane containing the principle rotation axis is σv, a plane perpendicular to the principle rotation axis is σh, and a plane parallel to the principle rotation axis but bisecting the angle between two C2 axes is σd. By this notation, the six planes of the methane tetrahedron are all σd.

A Simple Approach to Point Group Assignments



The process used to assign a molecule to a point group is straightforward with a few exceptions. Use this schematic to guide you.

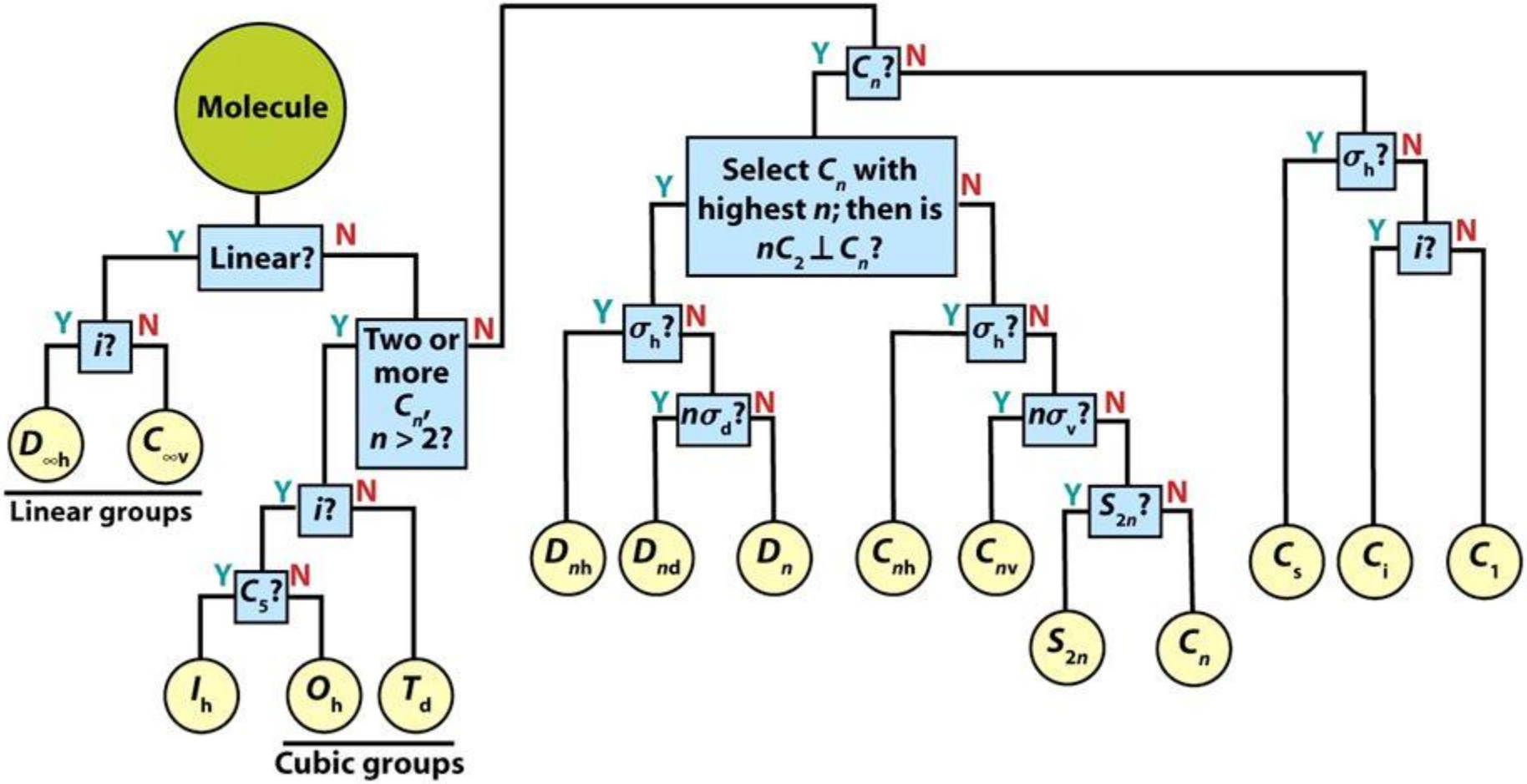
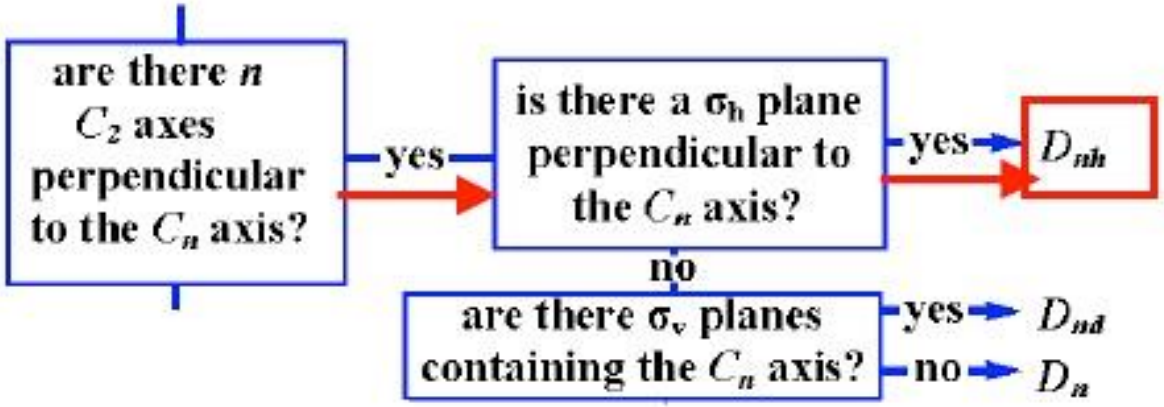
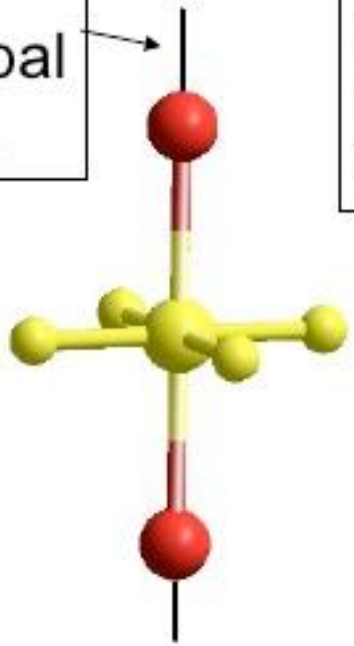


Figure 7-9
Shriver & Atkins Inorganic Chemistry, Fourth Edition

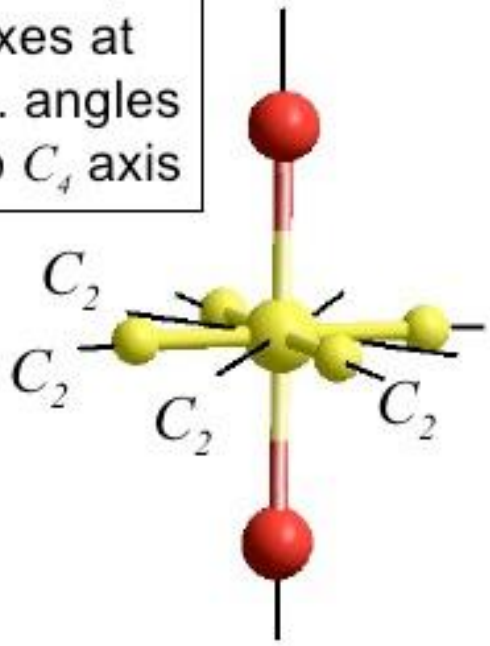
The D_{nh} point groups:



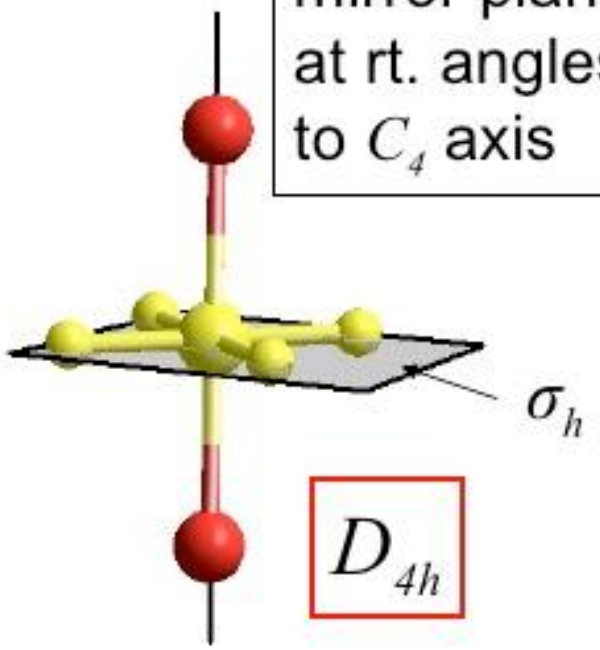
C_4 principal axis



four C_2 axes at rt. angles to C_4 axis



mirror plane at rt. angles to C_4 axis



D_{4h}