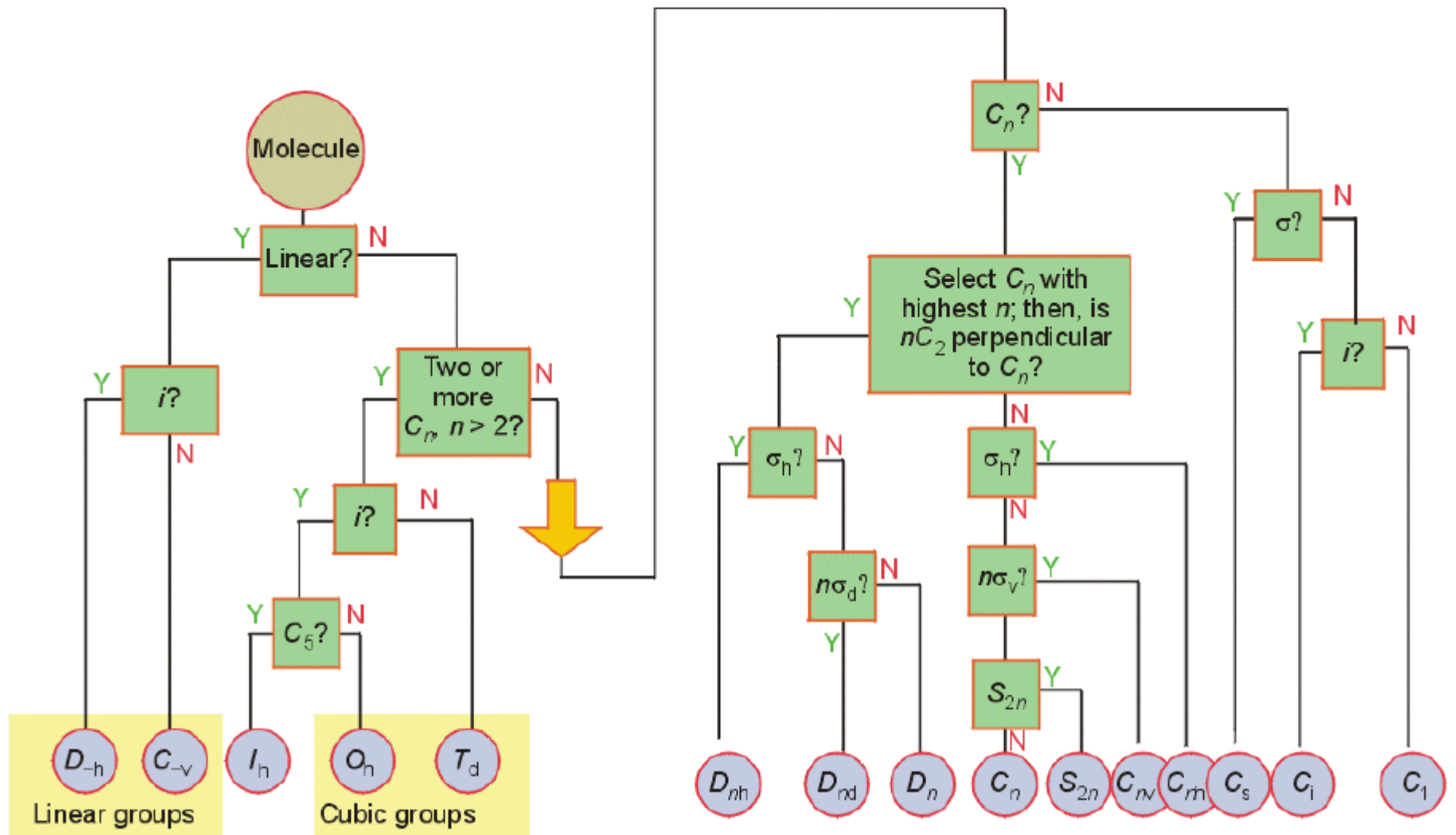


POINT GROUPS

Identifying point groups

1. Determine the symmetry is special (e.g. octahedral).
2. Determine if there is a principal rotation axis.
3. Determine if there are rotation axes perpendicular to the principal axis.
4. Determine if there are mirror planes.
5. Assign point group.

Identifying point groups



Point Groups

- Simpler chart: Molecule

Any Special Groups?

High or very low symmetry groups?

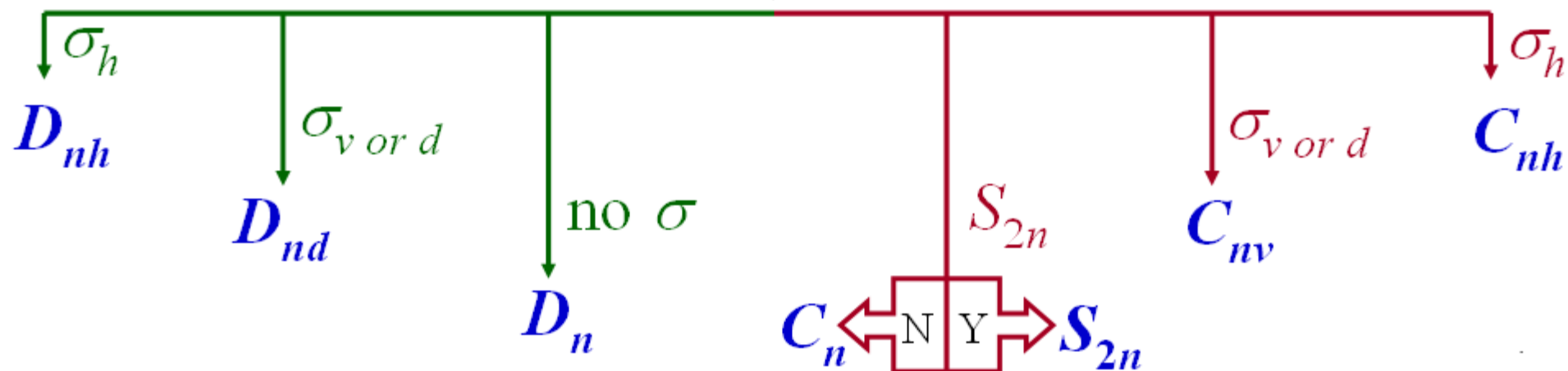
No

Any C_n ?

$C_2 \perp C_n$

YES

NO



Groups of Low and High Symmetry

- Very low symmetry:
 - C_1 : only E
 - C_s : only σ
 - C_i : only i
- High symmetry:
 - $C_{\infty v}$: linear \rightarrow no i , ∞C_n , $\infty \sigma$
 - $D_{\infty h}$: linear \rightarrow i , ∞C_n , $\infty \sigma$ (also $C_2 \perp C_\infty$ and $\sigma \perp C_\infty$)
 - T_d : tetrahedral
 - O_h : octahedral
 - I_h : icosahedral

Chirality and Polarity

- Molecules that are not superimposable to their mirror image are called “**chiral**” or “**dissymmetric**”.
 - Hands, propellers, copper wires *etc.*
- Chiral molecules can rotate the plane of polarized light, that is called “**optically active**”.
- Chiral molecule + mirror image → **enantiomers**
- Enantiomers rotate the polarized light 50%-50%.
 - Clockwise → dextrorotatory
 - Counterclockwise → levorotatory
- d- and l- may be measured experimentally!

Chirality and Polarity

- A molecule is not chiral if:
 - it has S_n (improper rotation axis)
 - it belongs to groups D_{nh}, D_{nd}
 - it is a cubic group (tetrahedral, octahedral, *etc.*)
- A “polar” molecule has a permanent electric dipole moment.
- A molecule can not be polar if it belongs to a group:
 - which has i (center of inversion)
 - of D and derivatives (mirror plane)
 - of cubic groups

Chirality and Polarity

- For a molecule to be chiral it must not have a S_n symmetry element:
 - mirror planes (S_1)
 - inversion centers (S_2)
- **Chiral groups:** C_1, C_n, D_n
- For a molecule to be polar:
 - it must not have an inversion center
 - or more than one rotation axis
 - or a mirror plane that does not include the principle rotation axis
- **Polar groups:** C_1, C_s, C_n, C_{nv}