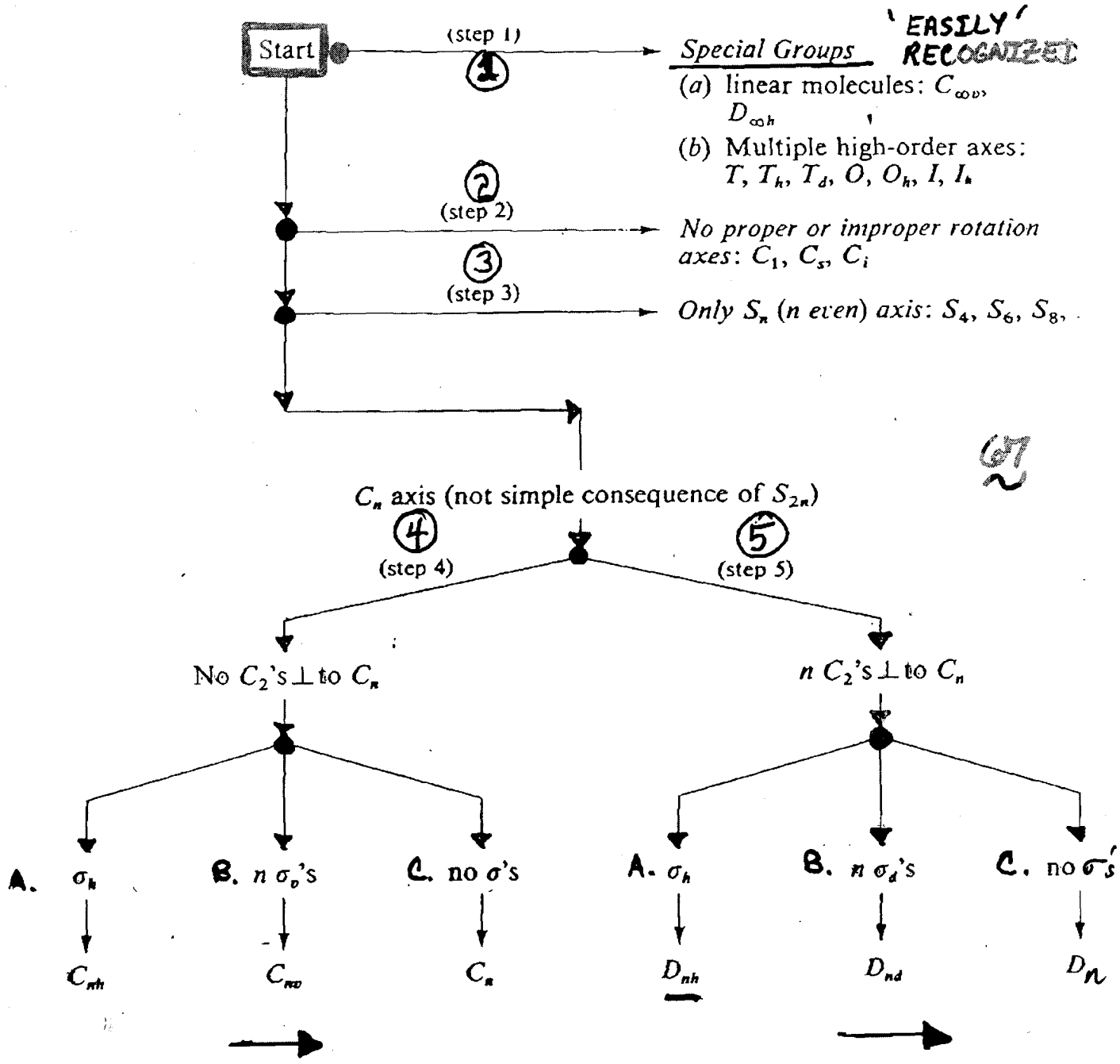
CYL 601 Handout 2

SYSTEMATIC CLASSIFICATION OF POINT GROUP SYMMETRY.



FLOWCHART

Point Groups

Revision Notes

The set of symmetry operations of any geometrical shape forms a mathematical group, which obeys four rules:

i. The product of two members of the group, and the square of any member, is also a member of the group.
ii. There must be an identity element.
iii. Combination must be associative, i.e. (AB)C = A(BC)
iv. Every member must have an inverse, i.e. if A is a member, then A^{-1} must also be a member, where $AA^{-1} = E$.

Symmetry operations do not necessarily commute, i.e. AB does not always equal BA.

A molecule can be assigned to its point group by a method which does not require the listing of all symmetry operations of the molecule; the method merely involves looking for certain key symmetry elements. The symbol for most molecular symmetry groups is in three parts e.g.

C_{4v} C_{2h} D_{3h} D_{6d}

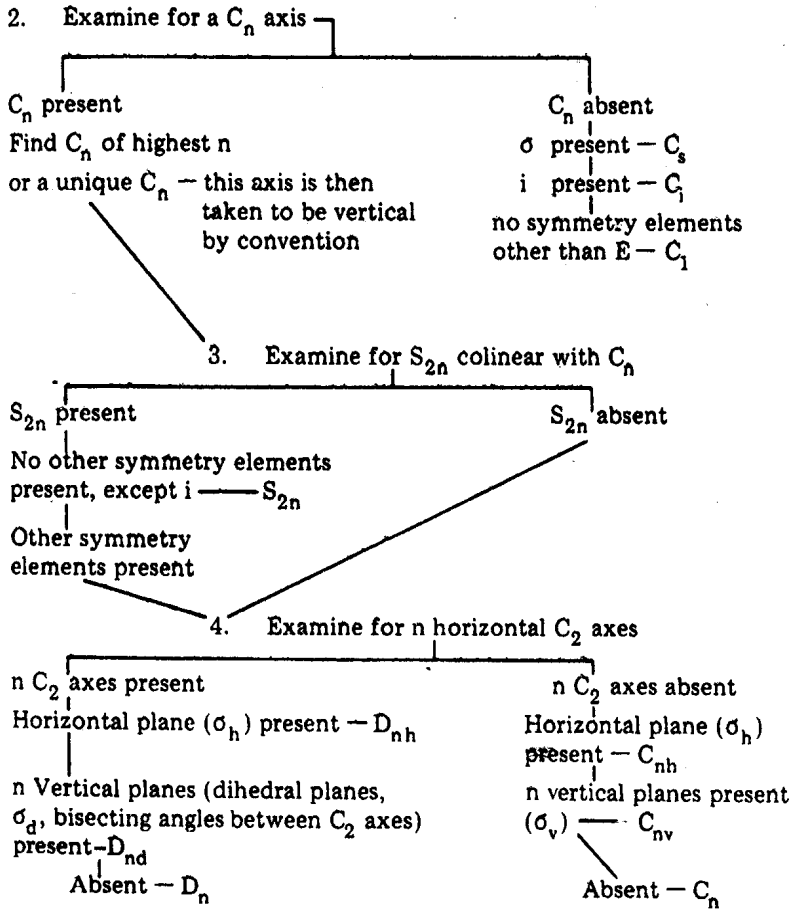
These have the following meanings:

i. The number indicates the order of the principal (highest order) axis. This axis conventionally defines the vertical direction.
ii. The capital letter is D if an n-fold principal axis is accompanied by n two-fold axes at right angles to it; otherwise the letter is C.
iii. The small letter is h if a horizontal plane is present. If n vertical planes are present, the letter is v for a C group but d (= dihedral) for a D group. (N.B. h takes precedence over v or d.) If no vertical or horizontal planes are present, the small letter is omitted.

Systematic Classification of Molecules into Point Groups

C = rotation axis
S = improper axis (alternating axis)
i = inversion centre
σ = plane of symmetry

1. Examine for special groups
   a. Linear, no σ perpendicular to molecular axis — $C_{\infty v}$
   b. Linear, σ perpendicular to molecular axis — $D_{\infty h}$
   c. Tetrahedral — T_d
   d. Octahedral — O_h
   e. Dodecahedral or icosahedral — I_h



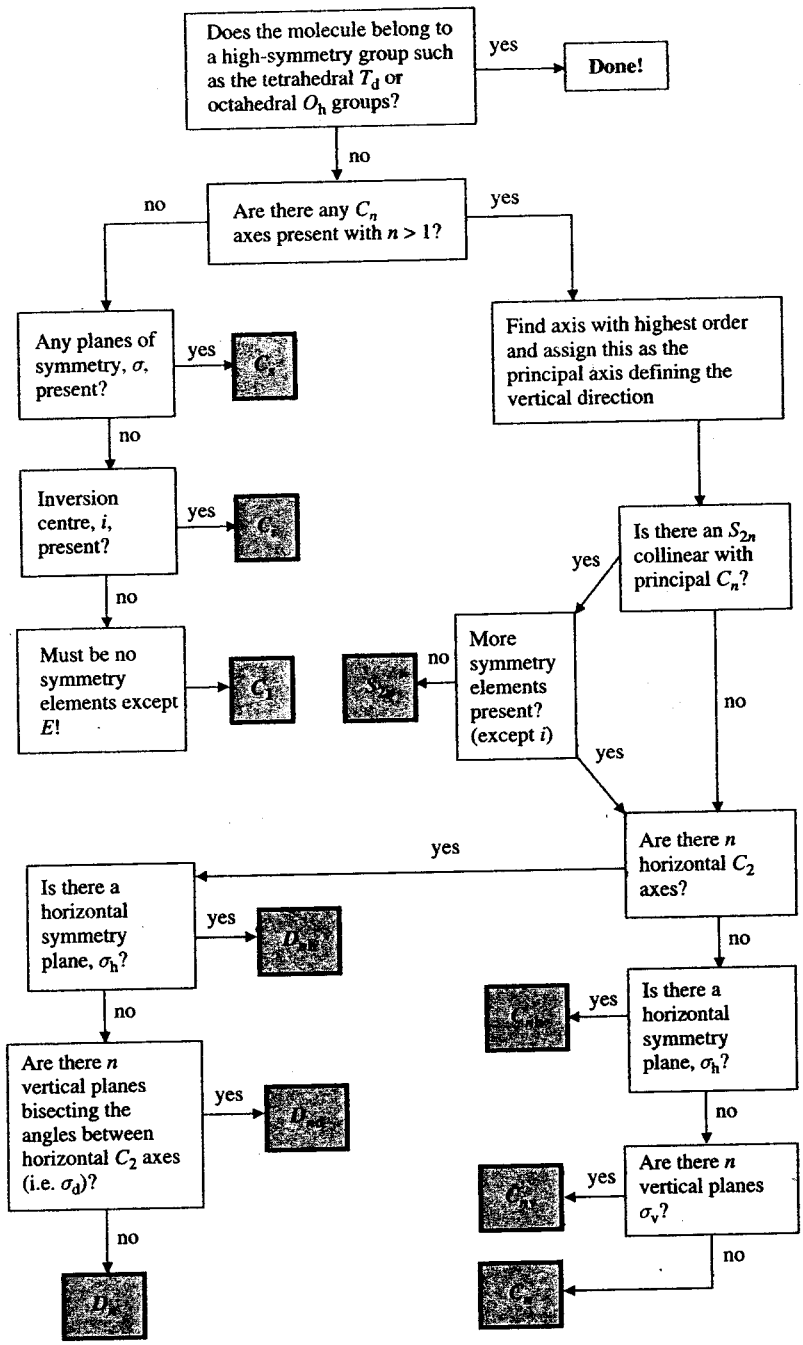


Figure 3.29 *Flow diagram for point group assignment.*