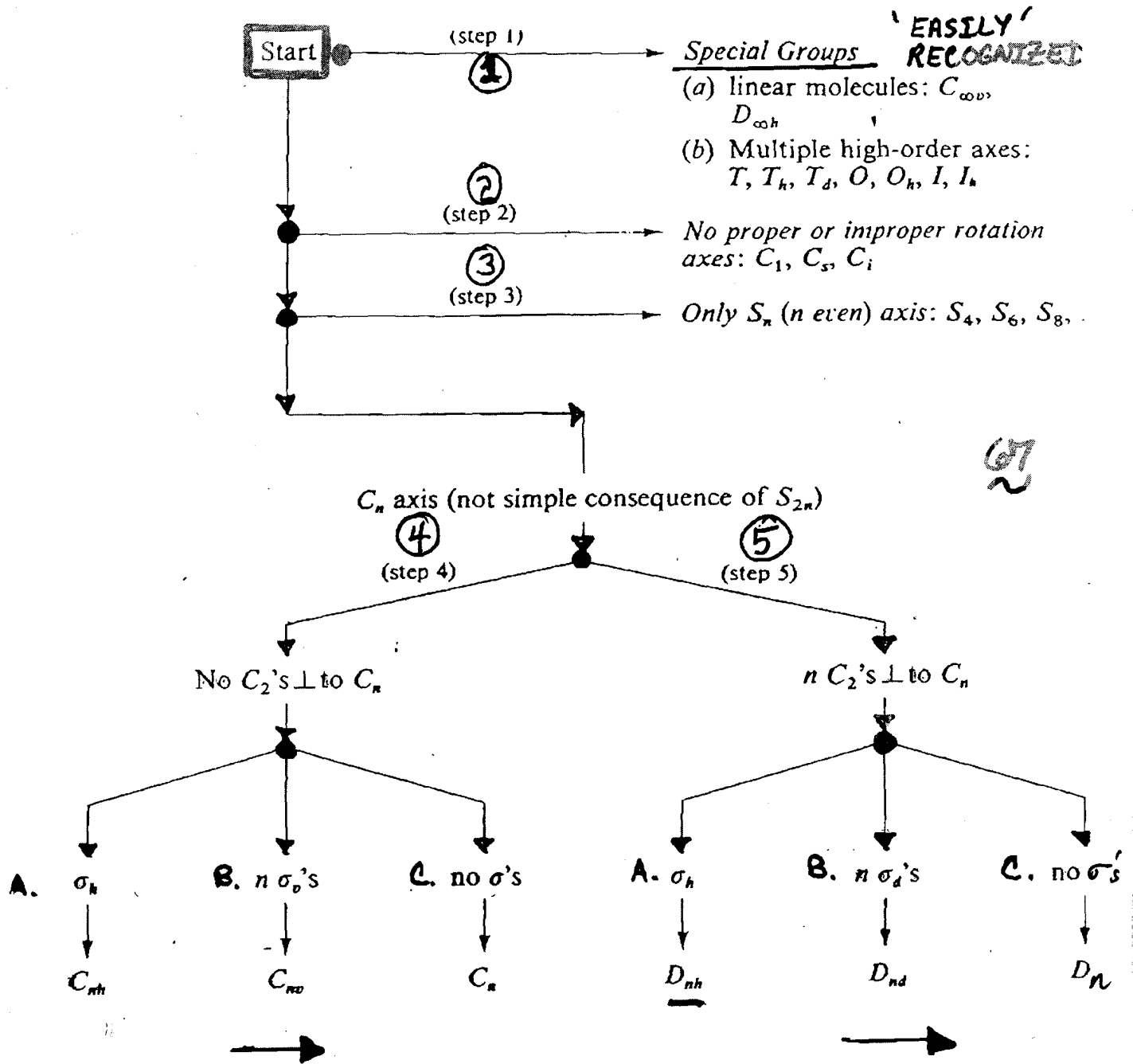


SYSTEMATIC CLASSIFICATION OF POINT GROUP SYMMETRY.



FLOWCHART

Point Groups

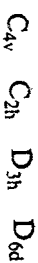
Revision Notes

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

- The product of two members of the group, and the square of any member, is also a member of the group.
- There must be an identity element.
- Combination must be associative, i.e. $(AB)C = A(BC)$
- 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.



These have the following meanings:

- The number indicates the order of the principal (highest order) axis. This axis conventionally defines the vertical direction.
- 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.
- 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

- Linear, no σ perpendicular to molecular axis — $C_{\infty v}$
- Linear, σ perpendicular to molecular axis — $D_{\infty h}$
- Tetrahedral — T_d
- Octahedral — O_h
- Dodecahedral or icosahedral — I_h

2. Examine for a C_n axis

C_n present
Find C_n of highest n
or a unique C_n — this axis is then taken to be vertical by convention

C_n absent
σ present — C_s
i present — C_i
no symmetry elements other than E — C_1

3. Examine for S_{2n} collinear with C_n

S_{2n} present
No other symmetry elements present, except i — S_{2n}

Other symmetry elements present

4. Examine for n horizontal C_2 axes

$n C_2$ axes present
Horizontal plane (σ_h) present — D_{nh}

n Vertical planes (dihedral planes, σ_d , bisecting angles between C_2 axes)
present — D_{nd}
Absent — D_n

$n C_2$ axes absent
Horizontal plane (σ_h) present — C_{nh}

n vertical planes present (σ_v) — C_{nv}
Absent — C_n

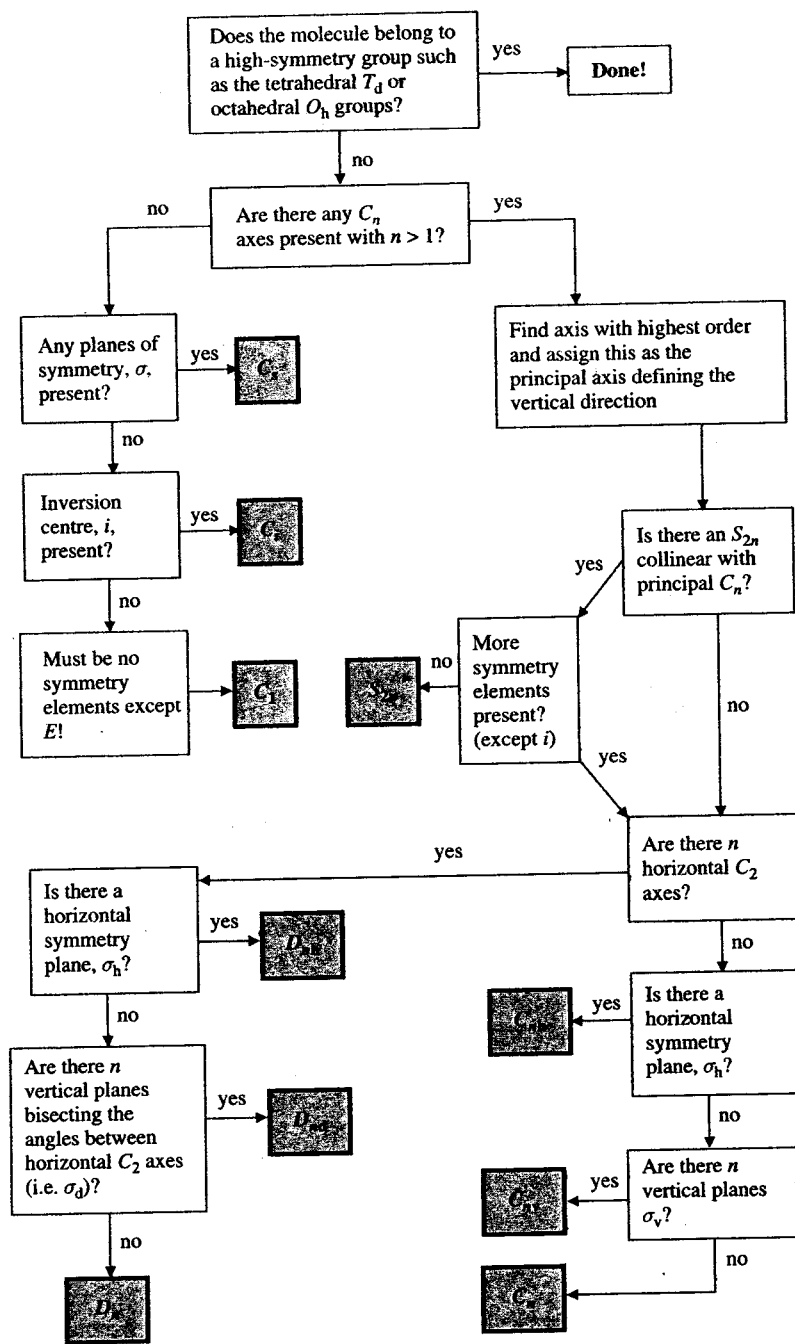


Figure 3.29 Flow diagram for point group assignment.

Figure 3.30 and-stick model of a molecule with a C_3 axis.

alternative point group, in the case of a C_6 axis, for example, in the case of a C_6 axis, Figure 3.30 shows the flow diagram. It is clear that a C_6 axis is present. However, the average of the symmetry operations C_6^2 and C_6^4 is C_3 . This S_6 axis is present around the C_6 axis, other than the C_6 axis itself. The horizontal D point group, which contains a C_6 axis, and so are not possible.

Another point group, Figure 3.31, is accessible.

Figure 3.31 (b) side view.