TABLE 4.2 Groups of Low Symmetry

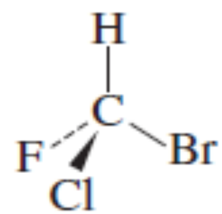
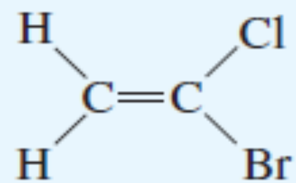
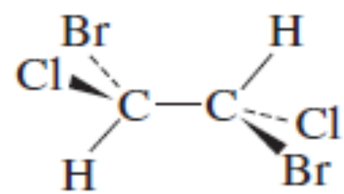
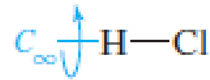
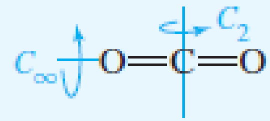
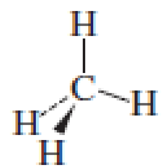
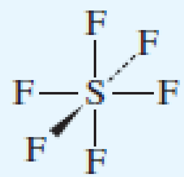
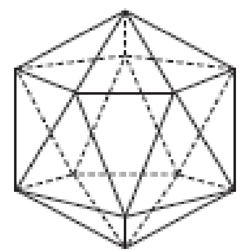
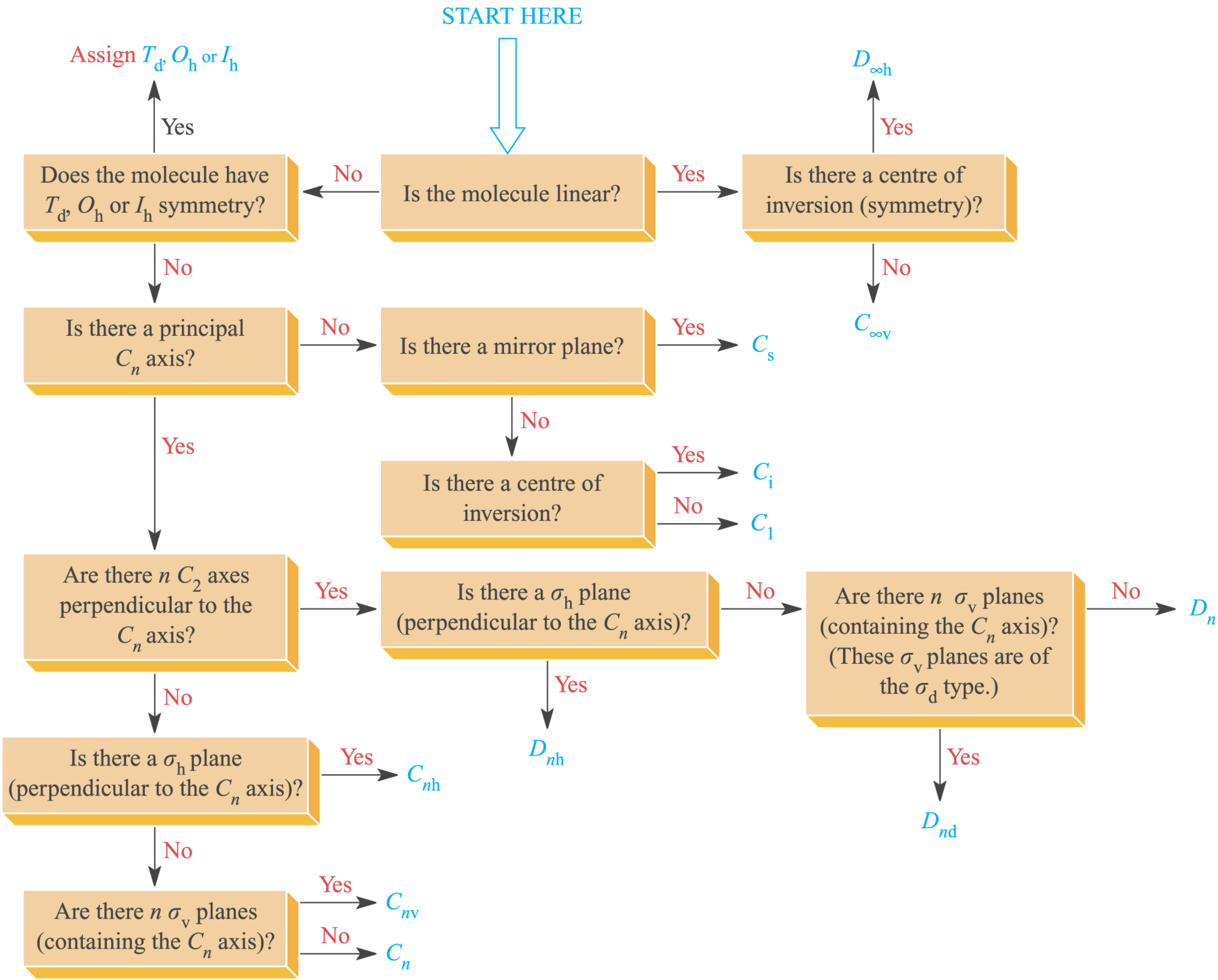
Group	Symmetry	Examples	
C_1	No symmetry other than the identity operation	CHFClBr	
C_s	Only one mirror plane	$H_2C{=}CClBr$	
C_i	Only an inversion center; few molecular examples	HClBrC—CHClBr (staggered conformation)	

TABLE 4.3 Groups of High Symmetry

Group	Description	Examples
$C_{\infty v}$	These molecules are linear, with an infinite number of rotations and an infinite number of reflection planes containing the rotation axis. They do not have a center of inversion.	
$D_{\infty h}$	These molecules are linear, with an infinite number of rotations and an infinite number of reflection planes containing the rotation axis. They also have perpendicular C_2 axes, a perpendicular reflection plane, and an inversion center.	
T_d	Most (but not all) molecules in this point group have the familiar tetrahedral geometry. They have four C_3 axes, three C_2 axes, three S_4 axes, and six σ_d planes. They have no C_4 axes.	
O_h	These molecules include those of octahedral structure, although some other geometrical forms, such as the cube, share the same set of symmetry operations. Among their 48 symmetry operations are four C_3 rotations, three C_4 rotations, and an inversion.	
I_h	Icosahedral structures are best recognized by their six C_5 axes, as well as many other symmetry operations—120 in all.	 $B_{12}H_{12}^{2-}$ with BH at each vertex of an icosahedron

In addition, there are four other groups, T, T_h, O, and I, which are rarely seen in nature. These groups are discussed at the end of this section.



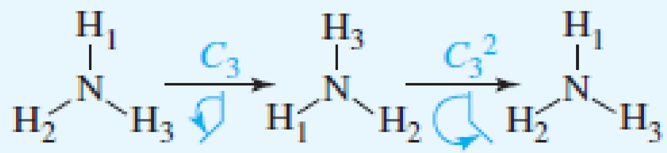
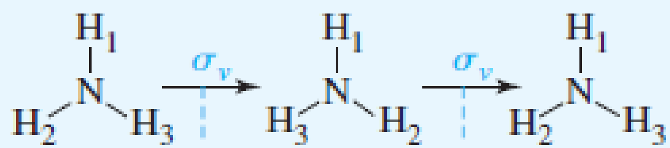
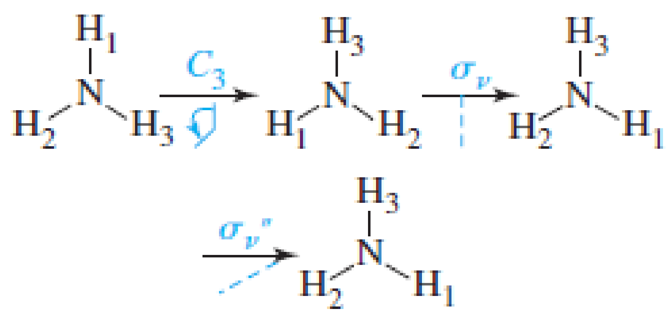
START HERE
Is the molecule linear?
Yes
Is there a centre of inversion (symmetry)?
Yes
$D_{\infty h}$
No
$C_{\infty v}$
No
Does the molecule have T_d, O_h or I_h symmetry?
Yes
Assign T_d, O_h or I_h
No
Is there a principal C_n axis?
No
Is there a mirror plane?
Yes
C_s
No
Is there a centre of inversion?
Yes
C_i
No
C_1
Yes
Are there n C_2 axes perpendicular to the C_n axis?
Yes
Is there a σ_h plane (perpendicular to the C_n axis)?
Yes
D_{nh}
No
Are there n σ_v planes (containing the C_n axis)? (These σ_v planes are of the σ_d type.)
Yes
D_{nd}
No
D_n
No
Is there a σ_h plane (perpendicular to the C_n axis)?
Yes
C_{nh}
No
Are there n σ_v planes (containing the C_n axis)?
Yes
C_{nv}
No
C_n

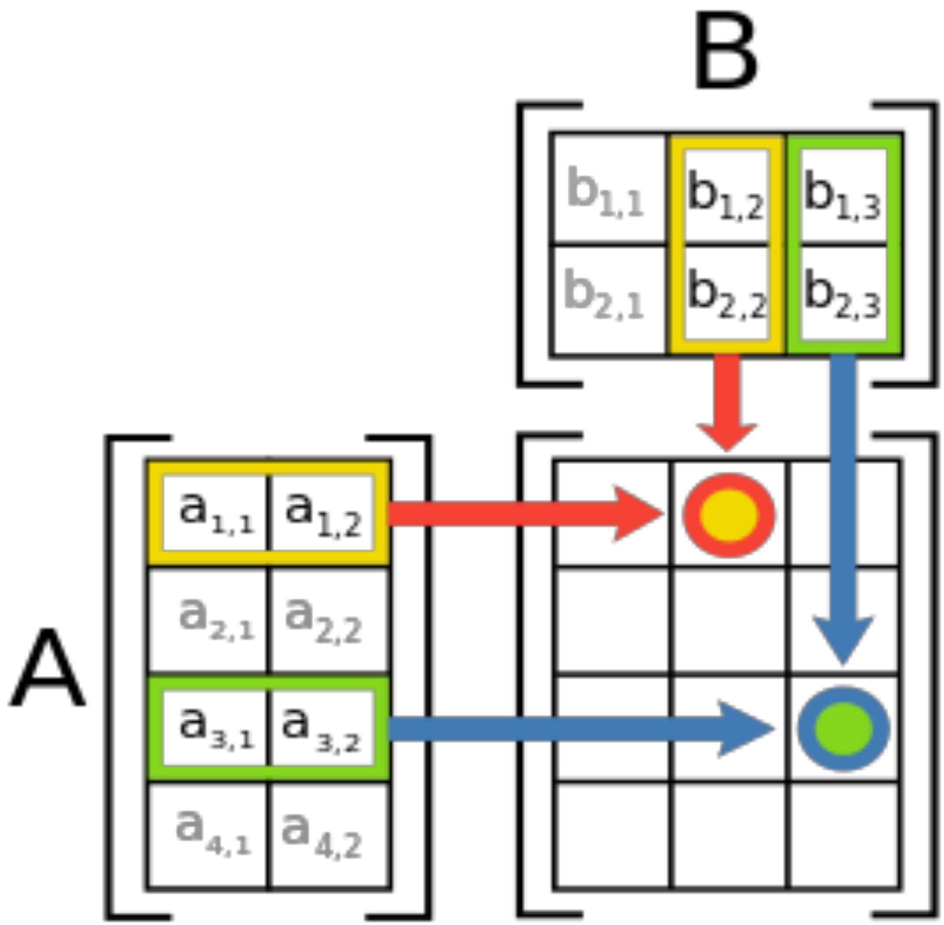
Point group	Characteristic symmetry elements	Comments
C_s	E, one σ plane	
C_i	E, inversion centre	
C_n	E, one (principal) n-fold axis	
C_{nv}	E, one (principal) n-fold axis, n σ_v planes	
C_{nh}	E, one (principal) n-fold axis, one σ_h plane, one S_n-fold axis which is coincident with the C_n axis	The S_n axis necessarily follows from the C_n axis and σ_h plane For $n = 2$, 4 or 6, there is also an inversion centre
D_{nh}	E, one (principal) n-fold axis, n C_2 axes, one σ_h plane, n σ_v planes, one S_n-fold axis	The S_n axis necessarily follows from the C_n axis and σ_h plane For $n = 2$, 4 or 6, there is also an inversion centre
D_{nd}	E, one (principal) n-fold axis, n C_2 axes, n σ_v planes, one S_{2n}-fold axis	For $n = 3$ or 5, there is also an inversion centre
T_d		Tetrahedral
O_h		Octahedral
I_h		Icosahedral

http://symmetry.otterbein.edu/tutorial/pointgroups.html

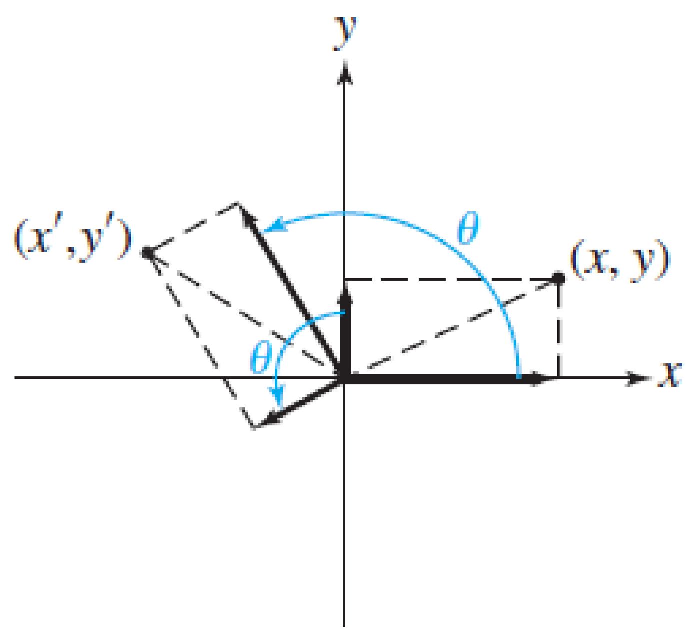
http://www.reciprocalnet.org/edumodules/symmetry/pointgroups/index.html

TABLE 4.6 Properties of a Group

Property of Group	Examples from Point Group
1. Each group must contain an **identity** operation that commutes (in other words, $EA = AE$) with all other members of the group and leaves them unchanged ($EA = AE = A$).	C_{3v} molecules (and *all* molecules) contain the identity operation E.
2. Each operation must have an **inverse** that, when combined with the operation, yields the identity operation (sometimes a symmetry operation may be its own inverse). *Note*: By convention, we perform sequential symmetry operations *from right to left* as written.	 $C_3^2C_3 = E$ (C_3 and C_3^2 are inverses of each other)  $\sigma_v\sigma_v = E$ (mirror planes are shown as dashed lines; σ_v is its own inverse)
3. The product of any two group operations must also be a member of the group. This includes the product of any operation with itself.	 $\sigma_v C_3$ has the same overall effect as σ_v'', therefore we write $\sigma_v C_3 = \sigma_v''$. It can be shown that the products of any two operations in C_{3v} are also members of C_{3v}.
4. The associative property of combination must hold. In other words, $A(BC) = (AB)C$.	$C_3(\sigma_v\sigma_v') = (C_3\sigma_v)\sigma_v'$



B
b1,1
b1,2
b1,3
b2,1
b2,2
b2,3
A
a1,1
a1,2
a2,1
a2,2
a3,1
a3,2
a4,1
a4,2



General case: $x' = x\cos\theta - y\sin\theta$

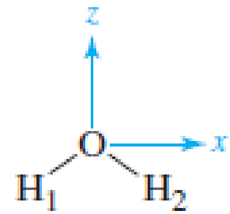
$y' = x\sin\theta + y\cos\theta$

For C_3: $\theta = 2\pi/3 = 120°$

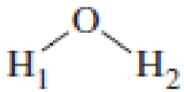
General Transformation Matrix for rotation by $\theta°$ about z axis:

$$\begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

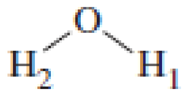
TABLE 4.8 Representation Flowchart: $H_2O(C_{2v})$



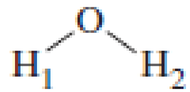
Symmetry Operations



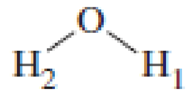
after E



after C_2



after $\sigma_v(xz)$



after $\sigma_v'(yz)$

Reducible Matrix Representations

$$E: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad C_2: \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \sigma_v(xz): \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \sigma_v'(yz): \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Characters of Matrix Representations

3	–1	1	1

Block Diagonalized Matrices

$$\begin{bmatrix} [1] & 0 & 0 \\ 0 & [1] & 0 \\ 0 & 0 & [1] \end{bmatrix} \quad \begin{bmatrix} [-1] & 0 & 0 \\ 0 & [-1] & 0 \\ 0 & 0 & [1] \end{bmatrix} \quad \begin{bmatrix} [1] & 0 & 0 \\ 0 & [-1] & 0 \\ 0 & 0 & [1] \end{bmatrix} \quad \begin{bmatrix} [-1] & 0 & 0 \\ 0 & [1] & 0 \\ 0 & 0 & [1] \end{bmatrix}$$

E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$
3	−1	1	1

	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$	*Coordinate Used*
	1	−1	1	−1	x
	1	−1	−1	1	y
	1	1	1	1	z
Γ	3	−1	1	1	

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	−1	1	1	−1	R_z	
E_g	2	−1	0	2	−1	0	(R_x, R_y)	$(x^2 - y^2, xy)$ (xz, yz)
A_{1u}	1	1	1	−1	−1	−1		
A_{2u}	1	1	−1	−1	−1	1	z	
E_u	2	−1	0	−2	1	0	(x, y)	

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)

TABLE 4.9 Properties of the Characters for the C_{3v} Point Group

Property	C_{3v} Example
1. Order	6 (6 symmetry operations)
2. Classes	3 classes: E $2C_3\ (= C_3, C_3^2)$ $3\sigma_v\ (= \sigma_v, \sigma_v', \sigma_v'')$
3. Number of irreducible representations	3 (A_1, A_2, E)
4. Sum of squares of dimensions equals the order of the group	$1^2 + 1^2 + 2^2 = 6$
5. Sum of squares of characters multiplied by the number of operations in each class equals the order of the group	$E \quad 2C_3 \quad 3\sigma_v$ A_1: $1^2 + 2(1)^2 + 3(1)^2 = 6$ A_2: $1^2 + 2(1)^2 + 3(-1)^2 = 6$ E: $2^2 + 2(-1)^2 + 3(0)^2 = 6$ (Multiply the squares by the number of symmetry operations in each class.)
6. Orthogonal representations	The sum of the products of any two representations multiplied by the number of operations in each class equals 0. Example of $A_2 \times E$: $(1)(2) + 2(1)(-1) + 3(-1)(0) = 0$
7. Totally symmetric representation	A_1, with all characters $= 1$

Complex	Point group
$M(CO)_6$	
$M(CO)_5X$	
trans-$M(CO)_4X_2$	
cis-$M(CO)_4X_2$	
fac-$M(CO)_3X_3$	
mer-$M(CO)_3X_3$	

Complex	Point group
$M(CO)_6$	O_h
$M(CO)_5X$	C_{4v}
trans-$M(CO)_4X_2$	D_{4h}
cis-$M(CO)_4X_2$	C_{2v}
fac-$M(CO)_3X_3$	C_{3v}
mer-$M(CO)_3X_3$	C_{2v}