CHAPTER 4: SYMMETRY AND GROUP THEORY

4.1 a. Ethane in the staggered conformation has 2 C_3 axes (the C–C line), 3 perpendicular C_2 axes bisecting the C–C line, in the plane of the two C's and the H's on opposite sides of the two C's. No σ_h, $3\sigma_d$, i, S_6. Overall, a $\boldsymbol{D_{3d}}$ molecule.

b. Ethane in eclipsed conformation has two C_3 axes (the C–C line), three perpendicular C_2 axes bisecting the C–C line, in the plane of the two C's and the H's on the same side of the two C's. Mirror planes include σ_h and $3\sigma_d$. Overall, a $\boldsymbol{D_{3h}}$ molecule.

c. Chloroethane in the staggered conformation has only one mirror plane, through both C's, the Cl, and the opposite H on the other C. Overall, a $\boldsymbol{C_s}$ molecule.

d. 1,2-dichloroethane in the *trans* conformation has a C_2 axis perpendicular to the C–C bond and perpendicular to the plane of both Cl's and both C's, a σ_h plane through both Cl's and both C's, and an inversion center. Overall, a $\boldsymbol{C_{2h}}$ molecule.

4.2 a. Ethylene is a planar molecule, with C_2 axes through the C's and perpendicular to the C–C bond both in the plane of the molecule and perpendicular to it. It also has a σ_h plane and two σ_d planes (arbitrarily assigned). Overall, a $\boldsymbol{D_{2h}}$ molecule.

b. Chloroethylene is also a planar molecule, with the only symmetry element the mirror plane of the molecule. Therefore, a $\boldsymbol{C_s}$ molecule.

c. 1,1-dichloroethylene has a C_2 axis coincident with the C–C bond, and two mirror planes, one the plane of the molecule and one perpendicular to the plane of the molecule through both C's. Overall, a $\boldsymbol{C_{2v}}$ molecule.

cis-1,2-dichloroethylene has a C_2 axis perpendicular to the C–C bond and in the plane of the molecule, two mirror planes (one in the plane of the molecule and one perpendicular to the plane of the molecule and perpendicular to the C–C bond). Overall a $\boldsymbol{C_{2v}}$ molecule.

trans-1,2-dichloroethylene has a C_2 axis perpendicular to the C–C bond and perpendicular to the plane of the molecule, a mirror plane in the plane of the molecule, and an inversion center. Overall, a $\boldsymbol{C_{2h}}$ molecule.

4.3 a. Acetylene has a C_∞ axis through all four atoms, an infinite number of perpendicular C_2 axes, a σ_h plane, and an infinite number of σ_d planes through all four atoms. Overall, a $\boldsymbol{D_{\infty h}}$ molecule.

b. Fluoroacetylene has only the C_∞ axis through all four atoms and an infinite number of mirror planes, also through all four atoms. Overall a $\boldsymbol{C_{\infty v}}$ molecule.

c. Methylacetylene has a C_3 axis through the carbons and three σ_v planes, each including one hydrogen and all three C's. Overall, a $\boldsymbol{C_{3v}}$ molecule.

d. 3-Chloropropene (assuming a rigid molecule, no rotation around the C–C bond) has no rotation axes and only one mirror plane through Cl and all three C atoms. Overall, a $\boldsymbol{C_s}$ molecule.

e. Phenylacetylene (again assuming no internal rotation) has a C_2 axis down the long axis of the molecule and two mirror planes, one the plane of the benzene ring and the other perpendicular to it. The point group is $\boldsymbol{C_{2v}}$.

4.4 a. Napthalene has three perpendicular C_2 axes, and a horizontal mirror plane (regardless of which C_2 is taken as the principal axis), making it a $\boldsymbol{D_{2h}}$ molecule.

b. 1,8-dichloronaphthalene has only one C_2 axis, the C–C bond joining the two rings, and two mirror planes, making it a $\boldsymbol{C_{2v}}$ molecule.

c. 1,5-dichloronaphthalene has one C_2 axis perpendicular to the plane of the molecule, a horizontal mirror plane, and an inversion center; overall, $\boldsymbol{C_{2h}}$.

d. 1,2-dichloronaphthalene has only the mirror plane of the molecule, and is a $\boldsymbol{C_s}$ molecule.

4.5 a. 1,1′-dichloroferrocene has a C_2 axis parallel to the rings, perpendicular to the Cl–Fe–Cl σ_h mirror plane. It also has an inversion center; overall, $\boldsymbol{C_{2h}}$.

b. Dibenzenechromium has collinear C_6, C_3, and C_2 axes perpendicular to the rings, six perpendicular C_2 axes and a σ_h plane, making it a $\boldsymbol{D_{6h}}$ molecule. It also has three σ_v and three σ_d planes, S_3 and S_6 axes, and an inversion center.

c. Benzenebiphenylchromium has a mirror plane through the Cr and the biphenyl bridge bond. It has no other symmetry elements, so it is a $\boldsymbol{C_s}$ molecule.

d. H_3O^+ has the same symmetry as NH_3: a C_3 axis, and three σ_v planes for a $\boldsymbol{C_{3v}}$ molecule.

e. O_2F_2 has a C_2 axis perpendicular to the O–O bond and perpendicular to a line connecting the fluorines. With no other symmetry elements, it is a $\boldsymbol{C_2}$ molecule.

f. Formaldehyde has a C_2 axis collinear with the C=O bond, a mirror plane including all the atoms, and another perpendicular to the first and including the C and O atoms. Overall, $\boldsymbol{C_{2v}}$.

g. S_8 has C_4 and C_2 axes perpendicular to the average plane of the ring, four C_2 axes through opposite bonds, and four mirror planes perpendicular to the ring, each including two S atoms. Overall, $\boldsymbol{D_{4d}}$.

h. Borazine has a C_3 axis perpendicular to the plane of the ring, three perpendicular C_2 axes, and a horizontal mirror plane. Overall, $\boldsymbol{D_{3h}}$.

i. Tris(oxalato)chromate(III) has a C_3 axis and three perpendicular C_2 axes, each splitting a C–C bond and passing through the Cr. Overall, $\boldsymbol{D_3}$.

j. A tennis ball has three perpendicular C_2 axes (one through the narrow portions of each segment, the others through the seams) and two mirror planes including the first rotation axis. Overall, $\boldsymbol{D_{2d}}$.

4.6 a. Cyclohexane in the chair conformation has a C_3 axis perpendicular to the average plane of the ring, three perpendicular C_2 axes between the carbons, and three σ_v planes, each including the C_3 axis and one of the C_2 axes. Overall, $\boldsymbol{D_{3d}}$.

b. Tetrachloroallene has three perpendicular C_2 axes, one collinear with the double bonds, and the other two at 45° to the Cl—C—Cl planes. It also has two σ_v planes, one defined by each of the Cl–C–Cl groups. Overall, $\boldsymbol{D_{2d}}$. (Note that the ends of tetrachlorallene are staggered.)

c. The sulfate ion is tetrahedral. $\boldsymbol{T_d}$.

d. Most snowflakes have hexagonal symmetry (Figure 4.2), and have collinear C_6, C_3 and C_2 axes, six perpendicular C_2 axes, and a horizontal mirror plane. Overall, $\boldsymbol{D_{6h}}$. (For high quality images of snowflakes, including some that have different shapes, see K. G. Libbrecht, *Snowflakes*, Voyageur Press, Minneapolis, MN, 2008.)

e. Diborane has three perpendicular C_2 axes and three perpendicular mirror planes. $\boldsymbol{D_{2h}}$.

f. 1,3,5-tribromobenzene has a C_3 axis perpendicular to the plane of the ring, three perpendicular C_2 axes, and a horizontal mirror plane. $\boldsymbol{D_{3h}}$.

1,2,3-tribromobenzene has a C_2 axis through the middle Br and two perpendicular mirror planes which include this axis. $\boldsymbol{C_{2v}}$.

1,2,4-tribromobenzene has only the plane of the ring as a mirror plane. $\boldsymbol{C_s}$.

g. A tetrahedron inscribed in a cube has $\boldsymbol{T_d}$ symmetry (see Figure 4.6).

h. The left and right ends of B_3H_8 are staggered with respect to each other. There is a C_2 axis through the borons. In addition, there are two planes of symmetry, each containing four H atoms, and two C_2 axes between these planes and perpendicular to the original C_2. The point group is $\boldsymbol{D_{2d}}$.

4.7 a. A sheet of typing paper has three perpendicular C_2 axes and three perpendicular mirror planes. Overall, $\boldsymbol{D_{2h}}$.

b. An Erlenmeyer flask has an infinite-fold rotation axis and an infinite number of σ_v planes. $\boldsymbol{C_{\infty v}}$.

c. A screw has no symmetry operations other than the identity, for a $\boldsymbol{C_1}$ classification.

d. The number 96 (with the correct type font) has a C_2 axis perpendicular to the plane of the paper, making it $\boldsymbol{C_{2h}}$.

e. Your choice—the list is too long to attempt to answer it here.

f. A pair of eyeglasses has only a vertical mirror plane. $\boldsymbol{C_s}$.

g. A 5-pointed star has a C_5 axis, five perpendicular C_2 axes, one horizontal and five vertical mirror planes. $\boldsymbol{D_{5h}}$.

h. A fork has only a mirror plane. C_s.

i. Captain Hook has no symmetry operation other than the identity. $\boldsymbol{C_1}$.

j. A metal washer has a C_∞ axis, an infinite number of perpendicular C_2 axes, an infinite number of σ_v mirror planes, and a horizontal mirror plane. Overall, $\boldsymbol{D_{\infty h}}$.

4.8

a. D_{2h}

b. D_{4h} (note the four knobs)

c. C_s

d. C_{2v}

e. C_{6v}

f. C_3

g. C_{2h}

h. C_{8v}

i. $D_{\infty h}$

j. C_{3v}

4.9

a. D_{3h}

b. D_{4h}

c. C_s

d. C_3

e. C_{2v}

f. C_s (note holes)

g. $C_{\infty v}$ (ignoring decorations)

h. C_{3v}

i. $D_{\infty h}$

j. C_1

4.10 Hands (of identical twins): C_2 Baseball: D_{2d} Atomium: C_{3v}

Eiffel Tower: C_{4v} Dominoes: 6×6: C_{2v} 3×3: C_2 5×4: C_s

Bicycle wheel: The wheel shown has 32 spokes. The point group assignment depends on how the pairs of spokes (attached to both the front and back of the hub) connect with the rim. If the pairs alternate with respect to their side of attachment, the point group is D_{8d}. Other arrangements are possible, and different ways in which the spokes cross can affect the point group assignment; observing an actual bicycle wheel is recommended. (If the crooked valve is included, there is no symmetry, and the point group is a much less interesting C_1.)

4.11 **a.** Problem 3.34:

a. $VOCl_3$: C_{3v}

b. PCl_3: C_{3v}

c. SOF_4: C_{2v}

d. SO_3: D_{3h}

e. ICl_3: C_{2v}

f. SF_6: O_h

g. IF_7: D_{5h}

h. XeO_2F_4: D_{4h}

i. CF_2Cl_2: C_{2v}

j. P_4O_6: T_d

b. Problem 3.35:

a. PH_3: C_{3v}
b. H_2Se: C_{2v}
c. SeF_4: C_{2v}
d. PF_5: D_{3h}
e. IF_5: C_{4v}
f. XeO_3: C_{3v}
g. BF_2Cl: C_{2v}
h. $SnCl_2$: C_{2v}
i. KrF_2: $D_{\infty h}$
j. $IO_2F_5^{2-}$: D_{5h}

4.12 **a.** Figure 3.8:

a. CO_2: $D_{\infty h}$
b. SO_3: D_{3h}
c. CH_4: T_d
d. PCl_5: D_{3h}
e. SF_6: O_h
f. IF_7: D_{5h}
g. TaF_8^{3-}: D_{4d}

b. Figure 3.15:

a. CO_2: $D_{\infty h}$
b. COF_2: C_{2v}
c. NO_2^-: C_{2v}
d. SO_3: D_{3h}
e. SNF_3: C_{3v}
f. SO_2Cl_2: C_{2v}
g. XeO_3: C_{3v}
h. SO_4^{2-}: T_d
i. SOF_4: C_{2v}
j. ClO_2F_3: C_{2v}
k. XeO_3F_2: D_{3h}
l. IOF_5: C_{4v}

4.13 **a.** p_x has $C_{\infty v}$ symmetry. (Ignoring the difference in sign between the two lobes, the point group would be $D_{\infty h}$.)

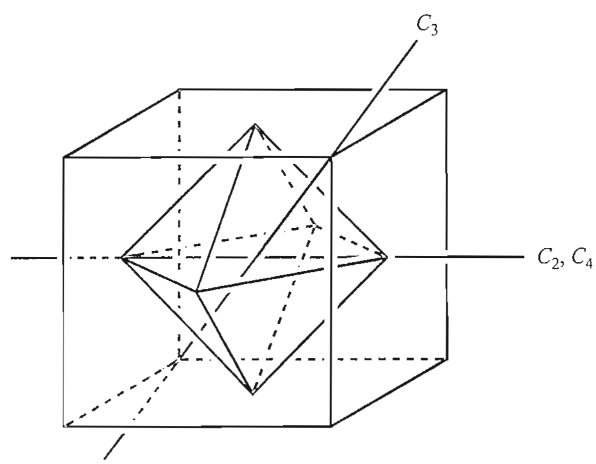
b. d_{xy} has D_{2h} symmetry. (Ignoring the signs, the point group would be D_{4h}.)

c. $d_{x^2-y^2}$ has D_{2h} symmetry. (Ignoring the signs, the point group would be D_{4h}.)

d. d_{z^2} has $D_{\infty h}$ symmetry.

e. f_{xyz} has T_d symmetry.

4.14 **a.** The superimposed octahedron and cube show the matching symmetry elements.



The descriptions below are for the elements of a cube; each element also applies to the octahedron.

E Every object has an identity operation.

$8\ C_3$ Diagonals through opposite corners of the cube are C_3 axes.

$6\ C_2$ Lines bisecting opposite edges are C_2 axes.

$6\ C_4$ Lines through the centers of opposite faces are C_4 axes. Although there are only three such lines, there are six axes, counting the C_4^3 operations.

$3\,C_2$ $(=C_4^2)$ The lines through the centers of opposite faces are C_4 axes as well as C_2 axes.

i The center of the cube is the inversion center.

$6S_4$ The C_4 axes are also S_4 axes.

$8S_6$ The C_3 axes are also S_6 axes.

$3\sigma_h$ These mirror planes are parallel to the faces of the cube.

$6\sigma_d$ These mirror planes are through two opposite edges.

b. O_h

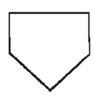
c. O

4.15 **a.** on-deck circle $D_{\infty h}$

b. batter's box D_{2h}

c. cap C_s

d. bat $C_{\infty v}$

e. home plate C_{2v} 

f. baseball D_{2d} (see Figure 4.1)

g. pitcher C_1

4.16

a. D_{2h}

b. C_{2v}

c. C_{2v}

d. D_{4h}

e. C_{5h}

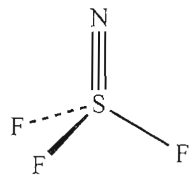
f. C_{2v}

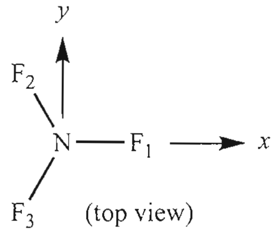
g. D_{2h}

h. D_{4h}

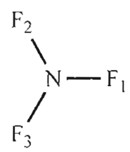
i. C_{2h}

4.17 SNF_3

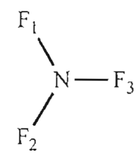




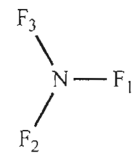
Symmetry Operations



after E



after C_3



after $\sigma_v(xz)$

Matrix Representations (reducible)

$$E: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad C_3: \begin{bmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \sigma_v(xz): \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Characters of Matrix Representations

3	0	1

Block Diagonalized Matrices

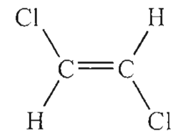
$$\begin{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & [1] \end{bmatrix} \qquad \begin{bmatrix} \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & [1] \end{bmatrix} \qquad \begin{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & [1] \end{bmatrix}$$

Irreducible Representations

E	$2\,C_3$	$3\,\sigma_v$	Coordinates used
2	–1	0	(x, y)
1	1	1	z

Character Table

C_{3v}	E	$2\,C_3$	$3\,\sigma_v$	Matching Functions	
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	–1	R_z	
E	2	–1	0	$(x, y), (R_x, R_y)$	$(x^2-y^2, xy)(xz, yz)$



4.18 a. C_{2h} molecules have E, C_2, i, and σ_h operations.

b.

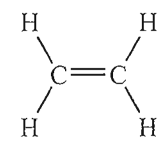
$$E: \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \quad C_2: \begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{matrix} \quad i: \begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{matrix} \quad \sigma_v: \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{matrix}$$

c. These matrices can be block diagonalized into three 1×1 matrices, with the representations shown in the table.

	$\chi(E)$	$\chi(C_2)$	$\chi(i)$	$\chi(\sigma_h)$	
B_u	1	−1	−1	1	from the x and y coefficients
A_u	1	1	−1	−1	from the z coefficients

The total is $\Gamma = 2B_u + A_u$.

d. Multiplying B_u and A_u:
$1 \times 1 + (-1) \times 1 + (-1) \times (-1) + 1 \times (-1) = 0$, proving they are orthogonal



4.19 a. D_{2h} molecules have E, $C_2(z)$, $C_2(y)$, $C_2(x)$, i, $\sigma(xy)$, $\sigma(xz)$, and $\sigma(yz)$ operations.

b.

$$E: \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad C_2(z): \begin{vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad C_2(y): \begin{vmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{vmatrix}$$

$$C_2(x): \begin{vmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{vmatrix} \quad i: \begin{vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{vmatrix} \quad \sigma(xy): \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{vmatrix}$$

$$\sigma(xz): \begin{vmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad \sigma(yz): \begin{vmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

c.

	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$
χ	3	−1	−1	−1	−3	1	1	1

d.

Γ_1	1	−1	−1	1	−1	1	1	−1	matching B_{3u}
Γ_2	1	−1	1	−1	−1	1	−1	1	matching B_{2u}
Γ_3	1	1	−1	−1	−1	−1	1	1	matching B_{1u}

e. $\Gamma_1 \times \Gamma_2 = 1 \times 1 + (-1) \times (-1) + (-1) \times 1 + 1 \times (-1) + (-1) \times (-1) + 1 \times 1$
$+ 1 \times (-1) + (-1) \times 1 = 0$

$\Gamma_1 \times \Gamma_3 = 1 \times 1 + (-1) \times 1 + (-1) \times (-1) + 1 \times (-1) + (-1) \times (-1) + 1 \times (-1)$
$+ 1 \times 1 + (-1) \times 1 = 0$

$\Gamma_2 \times \Gamma_3 = 1 \times 1 + (-1) \times 1 + 1 \times (-1) + (-1) \times (-1) + (-1) \times (-1) + 1 \times (-1)$
$+ (-1) \times 1 + 1 \times 1 = 0$

4.20 **a.** $h = 8$ (the total number of symmetry operations)

b. $A_1 \times E = 1 \times 2 + 2 \times 1 \times 0 + 1 \times (-2) + 2 \times 1 \times 0 + 2 \times 1 \times 0 = 0$
$A_2 \times E = 1 \times 2 + 2 \times 1 \times 0 + 1 \times (-2) + 2 \times (-1) \times 0 + 2 \times (-1) \times 0 = 0$
$B_1 \times E = 1 \times 2 + 2 \times (-1) \times 0 + 1 \times (-2) + 2 \times 1 \times 0 + 2 \times (-1) \times 0 = 0$
$B_2 \times E = 1 \times 2 + 2 \times (-1) \times 0 + 1 \times (-2) + 2 \times (-1) \times 0 + 2 \times 1 \times 0 = 0$

c. E: $4 + 2 \times 0 + 4 + 2 \times 0 + 2 \times 0 = 8$
A_1: $1 + 2 \times 1 + 1 + 2 \times 1 + 2 \times 1 = 8$
A_2: $1 + 2 \times 1 + 1 + 2 \times 1 + 2 \times 1 = 8$
B_1: $1 + 2 \times 1 + 1 + 2 \times 1 + 2 \times 1 = 8$
B_2: $1 + 2 \times 1 + 1 + 2 \times 1 + 2 \times 1 = 8$

d. $\Gamma_1 = 2A_1 + B_1 + B_2 + E$:
A_1: $1/8[1 \times 6 + 2 \times 1 \times 0 + 1 \times 2 + 2 \times 1 \times 2 + 2 \times 1 \times 2] = 2$
A_2: $1/8[1 \times 6 + 2 \times 1 \times 0 + 1 \times 2 + 2 \times (-1) \times 2 + 2 \times (-1) \times 2] = 0$
B_1: $1/8[1 \times 6 + 2 \times (-1) \times 0 + 1 \times 2 + 2 \times 1 \times 2 + 2 \times (-1) \times 2] = 1$
B_2: $1/8[1 \times 6 + 2 \times (-1) \times 0 + 1 \times 2 + 2 \times (-1) \times 2 + 2 \times 1 \times 2] = 1$
E: $1/8[2 \times 6 + 2 \times 0 \times 0 + (-2) \times 2 + 2 \times 0 \times 2 + 2 \times 0 \times 2] = 1$

$\Gamma_2 = 3\,A_1 + 2A_2 + B_1$:
A_1: $1/8[1 \times 6 + 2 \times 1 \times 4 + 1 \times 6 + 2 \times 1 \times 2 + 2 \times 1 \times 0] = 3$
A_2: $1/8[1 \times 6 + 2 \times 1 \times 4 + 1 \times 6 + 2 \times (-1) \times 2 + 2 \times (-1) \times 0] = 2$
B_1: $1/8[1 \times 6 + 2 \times (-1) \times 4 + 1 \times 6 + 2 \times 1 \times 2 + 2 \times (-1) \times 0] = 1$
B_2: $1/8[1 \times 6 + 2 \times (-1) \times 4 + 1 \times 6 + 2 \times (-1) \times 2 + 2 \times 1 \times 0] = 0$
E: $1/8[2 \times 6 + 2 \times 0 \times 4 + (-2) \times 6 + 2 \times 0 \times 2 + 2 \times 0 \times 0] = 0$

4.21 C_{3v}
$\Gamma_1 = 3A_1 + A_2 + E$:
A_1: $1/6[1 \times 6 + 2 \times 1 \times 3 + 3 \times 1 \times 2] = 3$
A_2: $1/6[1 \times 6 + 2 \times 1 \times 3 + 3 \times (-1) \times 2] = 1$
E: $1/6[2 \times 6 + 2 \times (-1) \times 3 + 3 \times 0 \times 2] = 1$

$\Gamma_2 = A_2 + E$:
A_1: $1/6[1 \times 5 + 2 \times 1 \times (-1) + 3 \times 1 \times (-1)] = 0$
A_2: $1/6[1 \times 5 + 2 \times 1 \times (-1) + 3 \times (-1) \times (-1)] = 1$
E: $1/6[2 \times 5 + 2 \times (-1) \times (-1) + 3 \times 0 \times (-1)] = 2$

O_h

$\Gamma_3 = A_{1g} + E_g + T_{1u}$:

A_{1g}: $1/48[6 + 0 + 0 + 12 + 6 + 0 + 0 + 0 + 12 + 12] = 1$

A_{2g}: $1/48[6 + 0 + 0 - 12 + 6 + 0 + 0 + 0 + 12 - 12] = 0$

E_g: $1/48[12 + 0 + 0 + 0 + 12 + 0 + 0 + 0 + 24 + 0] = 1$

T_{1g}: $1/48[18 + 0 + 0 + 12 - 6 + 0 + 0 + 0 - 12 - 12] = 0$

T_{2g}: $1/48[18 + 0 + 0 - 12 - 6 + 0 + 0 + 0 - 12 + 12] = 0$

A_{1u}: $1/48[6 + 0 + 0 + 12 + 6 + 0 + 0 + 0 - 12 - 12] = 0$

A_{2u}: $1/48[6 + 0 + 0 - 12 + 6 + 0 + 0 + 0 - 12 + 12] = 0$

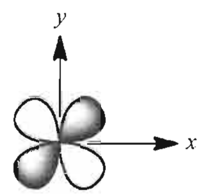
E_u: $1/48[12 + 0 + 0 + 0 + 12 + 0 + 0 + 0 - 24 + 0] = 0$

T_{1u}: $1/48[18 + 0 + 0 + 12 - 6 + 0 + 0 + 0 + 12 + 12] = 1$

T_{2u}: $1/48[18 + 0 + 0 - 12 - 6 + 0 + 0 + 0 + 12 - 12] = 0$

4.22

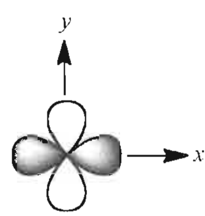
The d_{xy} characters match the characters in the B_{2g} representation.



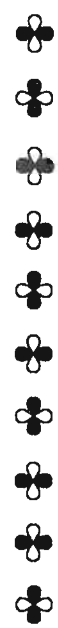
d_{xy}

	d_{xy}	χ
E		1
C_4		−1
C_2		1
C_2'		−1
C_2''		1
i		1
S_4		−1
σ_h		1
σ_v		−1
σ_d		1

The $d_{x^2-y^2}$ characters match those of the B_{1g} representation.



$d_{x^2-y^2}$



	$d_{x^2-y^2}$	χ
E		1
C_4		−1
C_2		1
C_2'		1
C_2''		−1
i		1
S_4		−1
σ_h		1
σ_v		1
σ_d		−1

4.23 Chiral: **4.5**: O_2F_2, $[Cr(C_2O_4)_3]^{3-}$ **4.6**: none **4.7**: screw, Captain Hook **4.8**: recycle symbol **4.9**: set of three wind turbine blades, coiled spring