

	Weight	Log		Weight	Log
(H ₂ O) _{1/2}	9.0075	0.954604	OCOCH ₃	59.044	1.771176
H ₂ O	18.015	1.255634	(OCOCH ₃) ₂	118.09	2.072206
(H ₂ O) _{1 1/2}	27.023	1.431725	(OCOCH ₃) ₃	177.13	2.248297
(H ₂ O) ₂	36.030	1.55666	(OCOCH ₃) ₄	236.18	2.373236
(H ₂ O) ₃	54.045	1.732756	(OCOCH ₃) ₅	295.22	2.470146
(H ₂ O) ₄	72.060	1.857694	(OCOCH ₃) ₆	354.26	2.549327
(H ₂ O) ₅	90.075	1.954604	(OCOCH ₃) ₇	413.31	2.616274
(H ₂ O) ₆	108.09	1.033786	(OCOCH ₃) ₈	472.35	2.674266
			(OCOCH ₃) ₉	531.40	2.725418
			(OCOCH ₃) ₁₀	590.44	2.771176
OCH ₃	31.034	1.491838			
(OCH ₃) ₂	62.068	1.792867	(CH ₃) ₃ Si	73.195	1.864481
(OCH ₃) ₃	93.102	1.968959	[(CH ₃) ₃ Si] ₂	146.39	2.165511
(OCH ₃) ₄	124.14	2.093897	[(CH ₃) ₃ Si] ₃	219.59	2.341603
(OCH ₃) ₅	155.17	2.190807	[(CH ₃) ₃ Si] ₄	292.78	2.466541
(OCH ₃) ₆	186.20	2.26999	[(CH ₃) ₃ Si] ₅	365.98	2.563451
(OCH ₃) ₇	217.24	2.336936	[(CH ₃) ₃ Si] ₆	439.17	2.642633
(OCH ₃) ₈	248.27	2.394928			
OC ₂ H ₅	45.061	1.653801	C ₆ H ₅	77.106	1.887088
(OC ₂ H ₅) ₂	90.122	1.954831	(C ₆ H ₅) ₂	154.21	2.188118
(OC ₂ H ₅) ₃	135.18	2.130922	(C ₆ H ₅) ₃	231.32	2.364209
(OC ₂ H ₅) ₄	180.24	2.255861	(C ₆ H ₅) ₄	308.42	2.489148
(OC ₂ H ₅) ₅	225.31	2.352771	(C ₆ H ₅) ₅	385.53	2.586058
			(C ₆ H ₅) ₆	462.64	2.665239
			(C ₆ H ₅) ₇	539.74	2.732186
			(C ₆ H ₅) ₈	616.85	2.790178

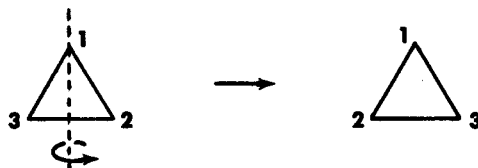
V. MOLECULAR SYMMETRY: DEFINITIONS AND COMMON SYSTEMS

This section is meant to serve as a guide to point group classification of molecules (objects). The symbols are those of the Schoenflies system. For more thorough treatment and special topics, the following bibliography is offered.

- F. A. Cotton, *Chemical Applications of Group Theory*, Interscience, New York, 1963 (2nd ed., 1971).
- H. Jaffé and M. Orchin, *Symmetry in Chemistry*, Wiley, New York, 1965.
- M. Orchin and H. Jaffé, *Symmetry, Point Groups and Character Tables*, *J. Chem. Educ.*, **47**, 246, 372, 510 (1970).
- R. L. Carter, *A Flow-Chart Approach to Point Group Classification*, *J. Chem. Educ.*, **45**, 44 (1968). See also J. Donohue, *ibid.*, **46**, 27 (1969).
- J. L. Carlos, Jr., *Molecular Symmetry and Optical Inactivity*, *J. Chem. Educ.*, **45**, 248 (1968).
- E. L. Muetterties, *Topological Representation of Stereoisomerism*, *J. Amer. Chem. Soc.*, **91**, 1936 (1969) [cf. *ibid.*, **91**, 3098 (1969)].
- K. Mislow and M. Raban, "Stereoisomeric Relationships of Groups in Molecules," in *Topics in Stereochemistry*, Vol. 1, Interscience, New York, 1967.

A. Definitions and Symbols

Symmetry operation--movement of a body in such a way, that after the movement has been performed every point of the body is coincident with an equivalent point (maybe the same point) in the original orientation. In other words, the body has been moved into a configuration indistinguishable from (but not necessarily identical to) the original. For example, rotation by 180° about the axis shown in an equilateral triangle produces a triangle indistinguishable from the original with respect to the viewer, but not strictly identical if the corners have an imaginary label:



Symmetry element--a line, plane, or point about which (with reference to which) one or more symmetry operations may be carried out.

Symmetry Element	Symbol	Symmetry Operation(s)
Identity	E	None.
n-Fold axis (proper axis)	C_n	Rotate object about such an axis through $2\pi/n$.
Mirror plane	σ	Reflect object in the plane.
Center of symmetry (center of inversion)	i	Inversion of all atoms or groups through the center.
n-Fold alternating axis (improper axis; rotation-reflection axis)	S_n	Rotate object by $2\pi/n$ about axis, followed by reflection in plane perpendicular to the axis.

B. Classification of Shapes

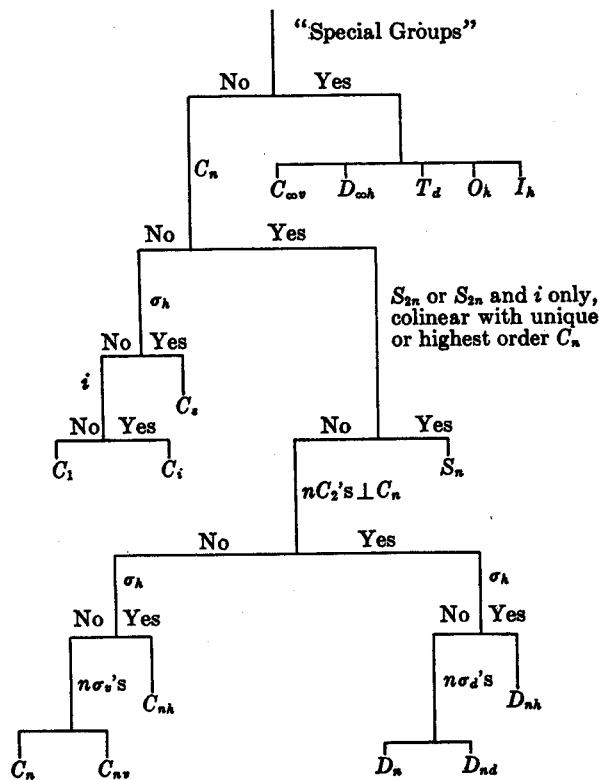
Objects are conveniently classified within the following scheme (K. Mislow, Introduction to Stereochemistry, Benjamin, New York, 1966).

1. No Reflection Symmetry: Dissymmetry (object and its mirror image are nonsuperimposable)
 - a. No C_n , therefore asymmetric--lacking any symmetry elements (except the trivial onefold axis; point group C_1).
 - b. One or more C_n (point groups \underline{C}_n and \underline{D}_n , therefore dissymmetric).
2. Reflection Symmetry
 - a. A σ but no C_n (in point group \underline{C}_s).
 - b. No σ (group \underline{S}_n).

c. Both σ and C_n (groups C_{nv} , C_{nh} , D_{nd} , D_{nh} , T_d , O_h , I_h , K_h). (The symbols stand for the following: \underline{C} = cylindrical; \underline{D} = dihedral; \underline{T} = tetrahedral; \underline{O} = octahedral; \underline{I} = icosahedral; \underline{K}_h = a sphere, which possesses all possible symmetry elements).

3. Flow Chart for Classifying Molecular Symmetry into Point Groups

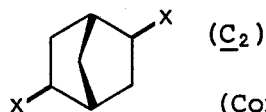
The following is reproduced from R. L. Carter, J. Chem. Educ., 45, 44 (1968) by permission of the Division of Chemical Education, ACS.



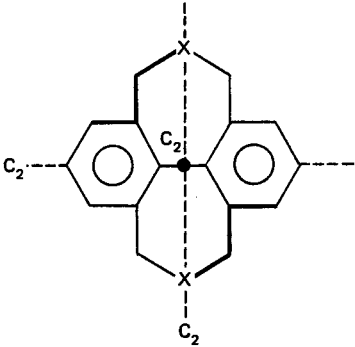
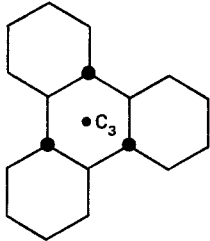
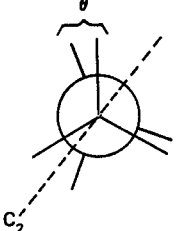
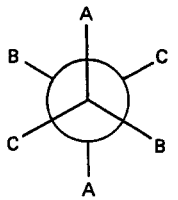
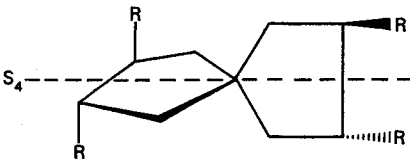
C. Examples of Common Point Groups

Not all symmetry elements may be identified in the illustrations.

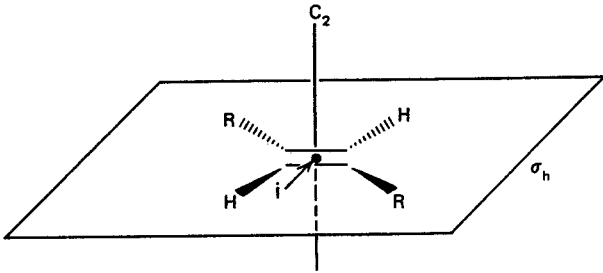
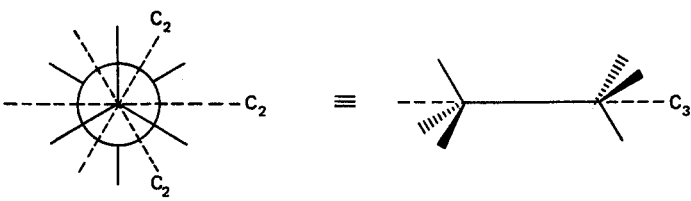
Group	Definition	Examples
\underline{C}_n	Has only a C_n (∴ dissymmetric)	A hand (C_1 , asymmetric); $XCH=C=CHX$ (\underline{C}_2); hexahelicene (\underline{C}_2);



(Continued)

Group	Definition	Examples
\underline{D}_n	Has one $C_n \perp$ which there are n - C_2 's : $\underline{D}_n \equiv C_n + nC_2$	(\underline{D}_2) (doubly bridged biphenyls)
		
	(\underline{D}_3)	 
\underline{C}_s	Has one σ but no C_n .	$CH_2=CHCl$; $CH_2=CBrCl$; bromocyclopropane; CH_3OH in skew or eclipsed conformation; 2-fluoronaphthalene.
\underline{S}_n	A rare group. Has <u>no</u> σ , but an S_n which passes through the molecule. S_2 is same as \underline{C}_i (center of inversion).	
		($\underline{S}_2 \equiv \underline{C}_i$)
		
		(\underline{S}_4)

(Continued)

Group	Definitions	Examples
\underline{C}_{nv}	One C_n plus n - σ containing the C_n : $\underline{C}_{nv} \equiv C_n + n\sigma$. \underline{C}_{1v} is same as \underline{C}_s and \underline{C}_{1h} (see below). A special case is $\underline{C}_{\infty v}$ which applies to linear molecules only and is referred to as conical symmetry; e.g., HBr, HCN, $\text{FC}\equiv\text{CH}$, CO.	$\text{H}_2\text{O}(\underline{C}_{2v})$; $\text{CH}_2=\text{CF}_2(\underline{C}_{2v})$; $\text{CH}_2\text{Cl}_2(\underline{C}_{2v})$; $\text{H}_2\text{CO}(\underline{C}_{2v})$; $\text{NH}_3(\underline{C}_{3v})$; $\text{CHCl}_3(\underline{C}_{3v})$; eclipsed $\text{CH}_3\text{CF}_3(\underline{C}_{3v})$; planar-cisoid 1,3-butadiene (\underline{C}_{2v}).
\underline{C}_{nh}	One C_n plus one "horizontal" plane $\perp C_n$: $\underline{C}_{nh} \equiv C_n + \sigma_n$. Note: all \underline{C}_{2h} objects also have i .	Planar-transoid 1,3-butadiene (\underline{C}_{2h}).
		
\underline{D}_{nd}	Has all symmetry elements of \underline{D}_n plus n -diagonal planes bisecting the angles between the n - C_2 's. $\underline{D}_{nd} \equiv (C_n + nC_2) + n\sigma_d$.	Cyclo-octatetraene (tub-shaped) (\underline{D}_{2d}); allene (\underline{D}_{2d}); chair cyclohexane (\underline{D}_{3d}); staggered ferrocene (\underline{D}_{5d}). Staggered ethane (\underline{D}_{3d}):
		
\underline{D}_{nh}	Has all symmetry elements of \underline{D}_n and \underline{C}_{nv} plus one $\sigma \perp C_n$: $\underline{D}_{nh} \equiv (C_n + nC_2) + n\sigma_v + \sigma_h$. A special case is $\underline{D}_{\infty h}$ (referred to as cylindrical symmetry), containing a C_∞ , ∞ - σ_v 's, and one σ_h ; e.g., acetylene, CO_2 , OCCCO (carbon suboxide). Note: $\underline{D}_{\infty h}$ molecules also contain ∞ - C_2 's perpendicular to the molecular axis.	Naphthalene (\underline{D}_{2h}); benzene (\underline{D}_{6h}); CH_2CH_2 (\underline{D}_{2h}); eclipsed ethane (\underline{D}_{3h}); planar CH_3^+ (\underline{D}_{3h}); cyclopropane (\underline{D}_{3h}); planar cyclopentane (\underline{D}_{5h}); eclipsed ferrocene (\underline{D}_{5h}).

(Continued)

Group	Definitions	Examples
T_d	Has 3 mutually perpendicular C_2 's + 4 C_3 's + 6 σ 's. (The C_2 's coincide with 3 S_4 's).	Methane; adamantane; $SiCl_4$.
O_h	Has 6 C_4 's + 8 C_3 's + 9 C_2 's (3 of which are coincident with C_4) + i + 9 σ .	Regular octahedron, as in $Fe(CN)_6^-$; $Cr(CO)_6$.

VI. CHARACTER TABLES FOR COMMON SYMMETRY GROUPS

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz

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

C_{3v}	E	$2C_3$	$3\sigma_v$		
A ₁	1	1	1	z	$x^2 + y^2, z^2$
A ₂	1	1	-1	R	
E	2	-1	0	(x, y) (R_x, R_y)	$(x^2 - y^2, xy)$ (xz, yz)

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A ₁	1	1	1	1	1	z	$x^2 + y^2, z^2$
A ₂	1	1	1	-1	-1	R_z	
B ₁	1	-1	1	1	-1		$x^2 - y^2$
B ₂	1	-1	1	-1	1		xy
E	2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)

$C_{\infty v}$	E	$2C_{\infty \phi}$...	$\infty \sigma_v$		
$A_1 \equiv \Sigma^+$	1	1	...	1	z R_z (x, y); (R_x, R_y)	$x^2 + y^2, z^2$ (xz, yz) ($x^2 - y^2, xy$)
$A_2 \equiv \Sigma^-$	1	1	...	-1		
$E_1 \equiv \Pi$	2	$2 \cos \phi$...	0		
$E_2 \equiv \Delta$	2	$2 \cos 2\phi$...	0		
$E_3 \equiv \Phi$	2	$2 \cos 3\phi$...	0		
...		

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z R_x, R_y z x, y	x^2, y^2, z^2, xy xz, yz
B_g	1	-1	1	-1		
A_u	1	1	-1	-1		
B_u	1	-1	-1	1		

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	
A_g	1	1	1	1	1	1	1	1	x^2, y^2, z^2 xy xz yz z y x
B_{1g}	1	1	-1	-1	1	1	-1	-1	
B_{2g}	1	-1	1	-1	1	-1	1	-1	
B_{3g}	1	-1	-1	1	1	-1	-1	1	
A_u	1	1	1	1	-1	-1	-1	-1	
B_{1u}	1	1	-1	-1	-1	-1	1	1	
B_{2u}	1	-1	1	-1	-1	1	-1	1	
B_{3u}	1	-1	-1	1	-1	1	1	-1	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	R_z (x, y)	$x^2 + y^2, z^2$ ($x^2 - y^2, xy$)
A_2'	1	1	-1	1	1	-1		
E'	2	-1	0	2	-1	0		
A_1''	1	1	1	-1	-1	-1	z (R_x, R_y)	(xz, yz)
A_2''	1	1	-1	-1	-1	1		
E''	2	-1	0	-2	1	0		

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		$x^2 - y^2$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	(R_x, R_y)	xy
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		(xz, yz)
E_g	2	0	-2	0	0	2	0	-2	0	0	z	
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1		
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1	(x, y)	
E_u	2	0	-2	0	0	-2	0	2	0	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1		xz, yz
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	(R_x, R_y)	(xz, yz)
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		$(x^2 - y^2, xy)$
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0	z	
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0		
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1		
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	(x, y)	
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1		
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0		
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0		

$D_{\infty h}$	E	$2C_{\infty}^{\phi}$...	$\infty\sigma_v$	i	$2S_{\infty}^{\phi}$...	∞C_2		
Σ_g^+	1	1	...	1	1	1	...	1	R_z	$x^2 + y^2, z^2$
Σ_g^-	1	1	...	-1	1	1	...	-1		(R_x, R_y)
Π_g	2	$2 \cos \phi$...	0	2	$-2 \cos \phi$...	0	(R_x, R_y)	(xz, yz)
Δ_g	2	$2 \cos 2\phi$...	0	2	$2 \cos \phi$...	0		$(x^2 - y^2, xy)$
...		
Σ_u^+	1	1	...	1	-1	-1	...	-1	z	
Σ_u^-	1	1	...	-1	-1	-1	...	1		
Π_u	2	$2 \cos \phi$...	0	-2	$2 \cos \phi$...	0	(x, y)	
Δ_u	2	$2 \cos 2\phi$...	0	-2	$-2 \cos 2\phi$...	0		
...		

D _{2d}	E	2S ₄	C ₂	2C ₂ '	2σ _d	
A ₁	1	1	1	1	1	R _z x ² + y ² , z ²
A ₂	1	1	1	-1	-1	
B ₁	1	-1	1	1	-1	x ² - y ²
B ₂	1	-1	1	-1	1	xy
E	2	0	-2	0	0	(x, y); (xz, yz) (R _x , R _y)

D _{3d}	E	2C ₃	3C ₂	i	2S ₆	3σ _d	
A _{1g}	1	1	1	1	1	1	R _z x ² + y ² , z ²
A _{2g}	1	1	-1	1	1	-1	
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	z (x, y)
A _{2u}	1	1	-1	-1	-1	1	
E _u	2	-1	0	-2	1	0	

D _{4d}	E	2S ₈	2C ₄	2S ₈ ³	C ₂	4C ₂ '	4σ _d	
A ₁	1	1	1	1	1	1	1	R _z x ² + y ² , z ²
A ₂	1	1	1	1	1	-1	-1	
B ₁	1	-1	1	-1	1	1	-1	z (x, y)
B ₂	1	-1	1	-1	1	-1	1	
E ₁	2	√2	0	-√2	-2	0	0	(R _x , R _y) (x ² - y ² , xy) (xz, yz)
E ₂	2	0	-2	0	2	0	0	
E ₃	2	-√2	0	√2	-2	0	0	

T _d	E	8C ₃	3C ₂ ^{''}	6S ₄ [*]	6σ _d	
A ₁	1	1	1	1	1	x ² + y ² + z ²
A ₂	1	1	1	-1	-1	
E	2	-1	2	0	0	(2z ² - x ² - y ² , x ² - y ²)
T ₁	3	0	-1	1	-1	(R _x , R _y , R _z) (x, y, z)
T ₂	3	0	-1	-1	1	

*The x-, y-, and z-axes.

O _h	E	8C ₃	6C ₂	6C ₄ *	3C ₂ " (≡3C ₄ ²)	i	6S ₄	8S ₆	3σ _h	6σ _d	
A _{1g}	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
A _{2g}	1	1	-1	-1	1	1	-1	1	1	-1	
E _g	2	-1	0	0	2	2	0	-1	2	0	$(2z^2 - x^2 - y^2, x^2 - y^2)$
T _{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)
T _{2g}	3	0	1	-1	-1	3	-1	0	-1	1	(xz, yz, xy)
A _{1u}	1	1	1	1	1	-1	-1	-1	-1	-1	
A _{2u}	1	1	-1	-1	1	-1	1	-1	-1	1	
E _u	2	-1	0	0	2	-2	0	1	-2	0	
T _{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)
T _{2u}	3	0	1	-1	-1	-3	1	0	1	-1	

*For x-, y-, and z-axes.

VII. COMPUTER PROGRAMS

The increasing use of computers in all areas of chemistry has made necessary the establishment of libraries of computer programs. The largest of these and the one containing the widest selection of programs is the Quantum Chemistry Program Exchange, Chemistry Department, Room 204, Indiana University, Bloomington, Ind. 47401. A membership fee and a charge for each program requested is required; however, in cases where no funds are available the charges may be waived. Programs in the following categories are available from QCPE:

- Matrix, algebraic, and arithmetic utility
- Expansions and special functions
- Quantum mechanical integrals
- Eigenvalues and eigenvectors
- Symmetry analysis and allied numerical quantities
- Self-consistent field programs
- Other programs based on electronic energy
- Other treatments of chemical systems (spectral and rate data, etc.)
- Miscellaneous programs (sort, etc.)

Listings of several computer programs of general interest can be found in the series, Computer Programs for Chemistry, D. F. DeTar, Ed., Vols. 1-3, Benjamin, New York, 1968-1969. These programs are also available on tape from Benjamin.

A large number of computer programs can be obtained, often without charge, directly from their authors. Many of these can be found by checking the notes in the Journal of Chemical Education. The ones mentioned in this source are oriented toward educational usage but many have direct research application.

A library of programs for X-ray crystallography can be found in I U Cr World List of Crystallographic Computer Programs, 2nd ed., D. P. Shoemaker, Ed., 1966, available from Polycrystal Book Service, P. O. Box 11567, Pittsburgh, Pa. 15238, or A. Oosterhoek's Vitgevers Mij. N. U., Domstraat 11-13, Utrecht, Netherlands. Another source of programs for X-ray crystallography is the University of Maryland Computer Science Center. For further information, contact Dr. James M. Stewart in care of the University, College Park, Md. 20742.