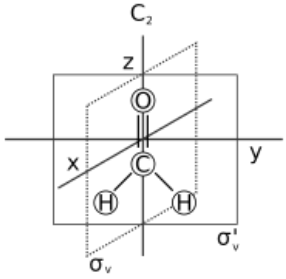
Molecular symmetry

Molecular symmetry in chemistry describes the symmetry present in molecules and the classification of molecules according to their symmetry. Molecular symmetry is a fundamental concept in chemistry, as it can be used to predict or explain many of a molecule's chemical properties, such as its dipole moment and its allowed spectroscopic transitions.To do this it is necessary to classify the states of the molecule using the irreducible representations from the character table of the symmetry group of the molecule. Many university level textbooks on physical chemistry, quantum chemistry, spectroscopy and inorganic chemistry devote a chapter to symmetry.[1][2][3][4][5][6]

The framework for the study of molecular symmetry is provided by group theory, and in particular irreducible representation theory. Symmetry is useful in the study of molecular orbitals, with applications such as the Hückel method, ligand field theory, and the Woodward-Hoffmann rules. Another framework on a larger scale is the use of crystal systems to describe crystallographic symmetry in bulk materials.

Many techniques for the practical assessment of molecular symmetry exist, including X-ray crystallography and various forms of spectroscopy. Spectroscopic notation is based on symmetry considerations.



Symmetry elements of formaldehyde. C_2 is a two-fold rotation axis. σ_v and σ_v' are two non-equivalent reflection planes.

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Symmetry concepts

The study of symmetry in molecules makes use of group theory.

Elements

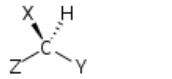
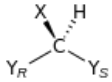
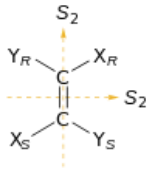
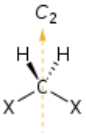
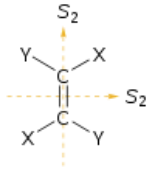
The point group symmetry of a molecule can be described by 5 types of symmetry element.

- **Symmetry axis**: an axis around which a rotation by $\frac{360^\circ}{n}$ results in a molecule indistinguishable from the original. This is also called an *n*-fold **rotational axis** and abbreviated C_n. Examples are the C_2 axis in water and the C_3 axis in ammonia. A molecule can have more than one symmetry axis; the one with the highest *n* is called the **principal axis**, and by convention is aligned with the z-axis in a Cartesian coordinate system.
- **Plane of symmetry**: a plane of reflection through which an identical copy of the original molecule is generated. This is also called a mirror plane and abbreviated σ (sigma = Greek "s", from the German 'Spiegel' meaning mirror).[7] Water has two of them: one in the plane of the molecule itself and one perpendicular to it. A symmetry plane parallel with the principal axis is dubbed *vertical* (σ_v) and one perpendicular to it *horizontal* (σ_h). A third type of symmetry plane exists: If a vertical symmetry plane additionally bisects the angle between two 2-fold rotation axes perpendicular to the principal axis, the plane is dubbed dihedral (σ_d). A symmetry plane can also be identified by its Cartesian orientation, e.g., (xz) or (yz).
- **Center of symmetry** or **inversion center**, abbreviated *i*. A molecule has a center of symmetry when, for any atom in the molecule, an identical atom exists diametrically opposite this center an equal distance from it. In other words, a molecule has

a center of symmetry when the points (x,y,z) and (−x,−y, −z) correspond to identical objects. For example, if there is an oxygen atom in some point (x,y,z), then there is an oxygen atom in the point (−x,−y,−z). There may or may not be an atom at the inversion center itself. Examples are xenon tetrafluoride where the inversion center is at the Xe atom, and benzene (C_6H_6) where the inversion center is at the center of the ring.

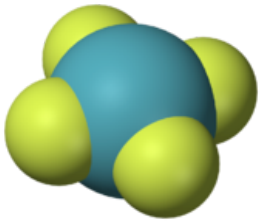
- **Rotation-reflection axis**: an axis around which a rotation by $\frac{360°}{n}$, followed by a reflection in a plane perpendicular to it, leaves the molecule unchanged. Also called an *n*-fold **improper rotation axis**, it is abbreviated S_n. Examples are present in tetrahedral silicon tetrafluoride, with three S_4 axes, and the staggered conformation of ethane with one S_6 axis. An S_1 axis corresponds to a mirror plane σ and an S_2 axis is an inversion center *i*. A molecule which has no S_n axis for any value of n is a chiral molecule.
- **Identity**, abbreviated to E, from the German 'Einheit' meaning unity.[8] This symmetry element simply consists of no change: every molecule has this element. While this element seems physically trivial, it must be included in the list of symmetry elements so that they form a mathematical group, whose definition requires inclusion of the identity element. It is so called because it is analogous to multiplying by one (unity). In other words, E is a property that any object needs to have regardless of its symmetry properties.[9]

Examples of the relationship between chirality and symmetry

Rotational axis (C_n)	**Improper rotational elements (S_n)**		
	Chiral no S_n	**Achiral** mirror plane $S_1 = \sigma$	**Achiral** inversion centre $S_2 = i$
C_1			
C_2			

Operations

The five symmetry elements have associated with them five types of **symmetry operation**, which leave the molecule in a state indistinguishable from the starting state. They are sometimes distinguished from symmetry elements by a caret or circumflex. Thus, $\hat{C}_n$ is the rotation of a molecule around an axis and $\hat{E}$ is the identity operation. A symmetry element can have more than one symmetry operation associated with it. For example, the C_4 axis of the square xenon tetrafluoride (XeF_4) molecule is associated with two $\hat{C}_4$ rotations (90°) in opposite directions and a $\hat{C}_2$ rotation (180°). Since $\hat{C}_1$ is equivalent to $\hat{E}$, $\hat{S}_1$ to σ and $\hat{S}_2$ to $\hat{\imath}$, all symmetry operations can be classified as either proper or improper rotations.



XeF_4, with square planar geometry, has 1 C_4 axis and 4 C_2 axes orthogonal to C_4. These five axes plus the mirror plane perpendicular to the C_4 axis define the D_{4h} symmetry group of the molecule.

For linear molecules, either clockwise or counterclockwise rotation about the molecular axis by any angle Φ is a symmetry operation.

Symmetry groups

Groups

The symmetry operations of a molecule (or other object) form a group. In mathematics, a group is a set with a binary operation that satisfies the four properties listed below.

In a **symmetry group**, the group elements are the symmetry operations (not the symmetry elements), and the binary combination consists of applying first one symmetry operation and then the other. An example is the sequence of a C_4 rotation about the z-axis and a reflection in the xy-plane, denoted $\sigma(xy)C_4$. By convention the order of operations is from right to left.

A symmetry group obeys the defining properties of any group.

(1) *closure* property:
For every pair of elements *x* and *y* in *G*, the *product* *x**y* is also in *G*.
(in symbols, for every two elements *x*, *y*∈*G*, *x***y* is also in *G*).
This means that the group is *closed* so that combining two elements produces no new elements. Symmetry operations have this property because a sequence of two operations will produce a third state indistinguishable from the second and therefore from the first, so that the net effect on the molecule is still a symmetry operation.
(2) *Associative property*:
For every *x* and *y* and *z* in *G*, both (*x***y*)**z* and *x**(*y***z*) result with the same element in *G*.
(in symbols, (*x***y*)**z* = *x**(*y***z*) for every *x*, *y*, and *z* ∈ *G*)
(3) *existence of identity* property:
There must be an element (say *e*) in *G* such that product any element of *G* with *e* make no change to the element.
(in symbols, *x***e*=*e***x*= *x* for every *x*∈ *G*)

(4) *existence of inverse element*:

For each element (*x*) in *G*, there must be an element *y* in *G* such that product of *x* and *y* is the identity element *e*.

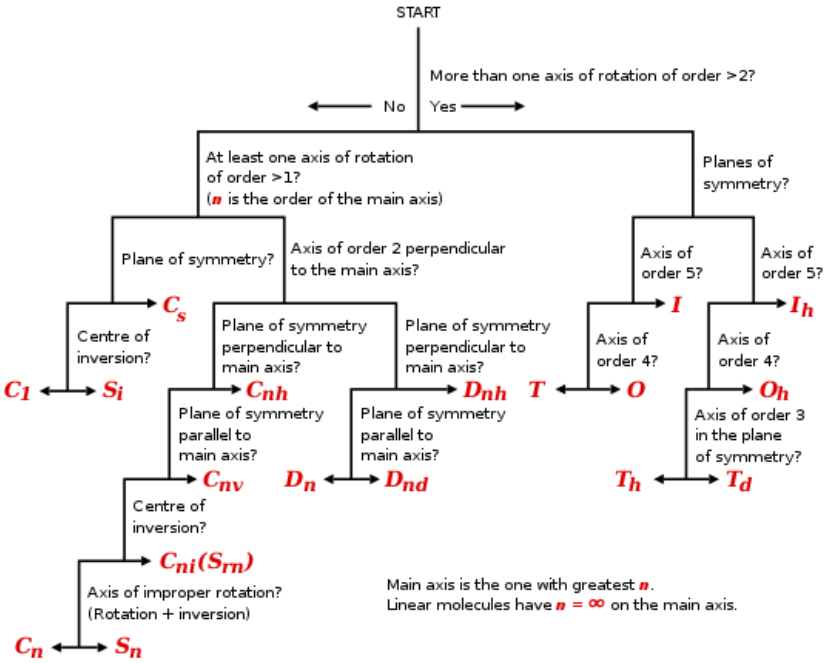
(in symbols, for each $x \in G$ there is a $y \in G$ such that $x*y=y*x= e$ for every $x \in G$)

The *order* of a group is the number of elements in the group. For groups of small orders, the group properties can be easily verified by considering its composition table, a table whose rows and columns correspond to elements of the group and whose entries correspond to their products.

Point groups and permutation-inversion groups

The successive application (or *composition*) of one or more symmetry operations of a molecule has an effect equivalent to that of some single symmetry operation of the molecule. For example, a C_2 rotation followed by a σ_v reflection is seen to be a σ_v' symmetry operation: $\sigma_v * C_2 = \sigma_v'$. ("Operation A followed by B to form C" is written BA = C).[9] Moreover, the set of all symmetry operations (including this composition operation) obeys all the properties of a group, given above. So (*S*,*) is a group, where *S* is the set of all symmetry operations of some molecule, and * denotes the composition (repeated application) of symmetry operations.

This group is called the point group of that molecule, because the set of symmetry operations leave at least one point fixed (though for some symmetries an entire axis or an entire plane remains fixed). In other words, a point group is a group that summarizes all symmetry operations that all molecules in that category have.[9] The symmetry of a crystal, by contrast, is described by a space group of symmetry operations, which includes translations in space.



Flowchart for determining the point group of a molecule

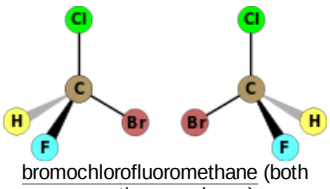
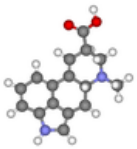
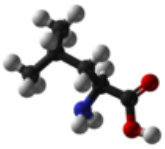
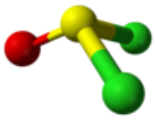
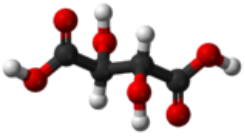
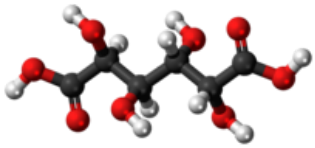
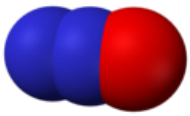
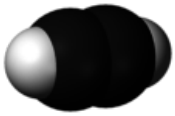
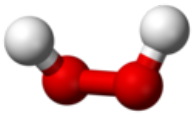
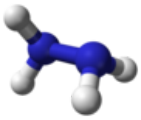
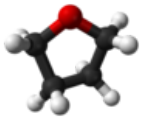
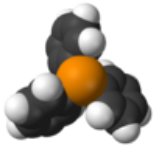
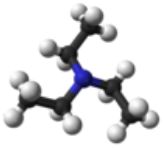
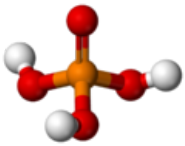
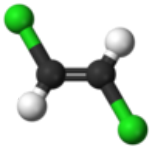
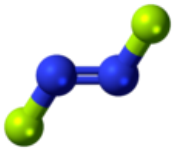
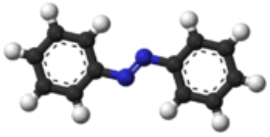
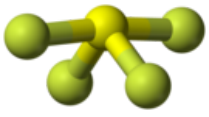
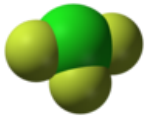
One can determine the symmetry operations of the point group for a particular molecule by considering the geometrical symmetry of its molecular model. However, when one USES a point group to classify molecular states, the operations in it are not to be interpreted in the same way. Instead the operations are interpreted as rotating and/or reflecting the vibronic (vibration-electronic) coordinates[10] and these operations commute with the vibronic Hamiltonian. They are "symmetry operations" for that vibronic Hamiltonian. The point group is used to classify by symmetry the vibronic eigenstates. The symmetry classification of the rotational levels, the eigenstates of the full (rotation-vibration-electronic) Hamiltonian, requires the use of the appropriate permutation-inversion group as introduced by Longuet-Higgins.[11]

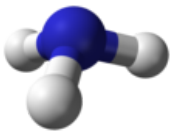
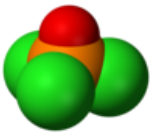
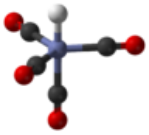
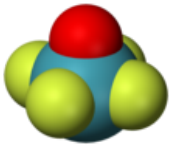
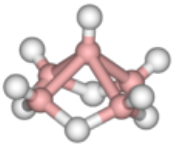
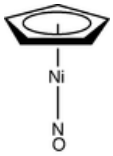
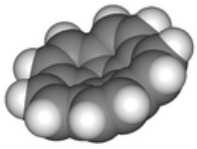
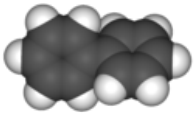
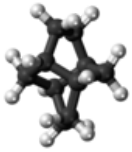
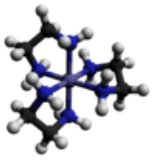
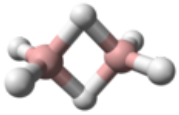
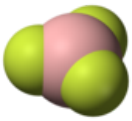
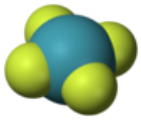
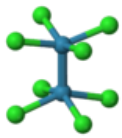
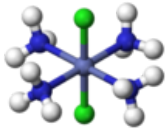
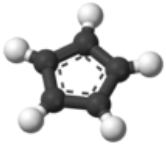
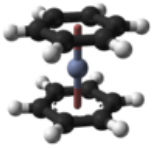
Examples of point groups

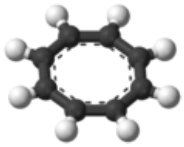
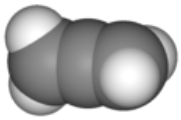
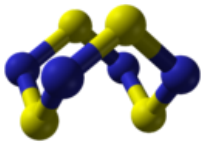
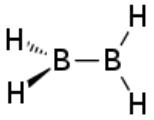
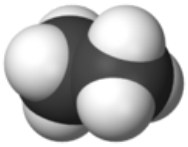
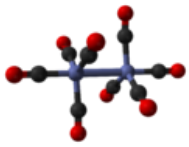
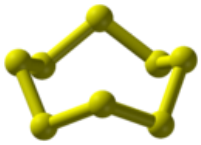
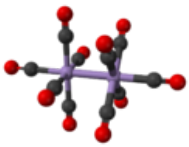
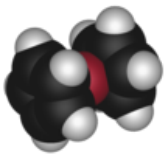
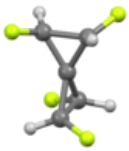
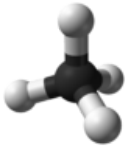
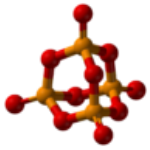
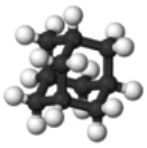
Assigning each molecule a point group classifies molecules into categories with similar symmetry properties. For example, PCl_3, POF_3, XeO_3, and NH_3 all share identical symmetry operations.[12] They all can undergo the identity operation E, two different C_3 rotation operations, and three different σ_v plane reflections without altering their identities, so they are placed in one point group, C_{3v}, with order 6.[13] Similarly, water (H_2O) and hydrogen sulfide (H_2S) also share identical symmetry operations. They both undergo the identity operation E, one C_2 rotation, and two σ_v reflections without altering their identities, so they are both placed in one point group, C_{2v}, with order 4.[14] This classification system helps scientists to study molecules more efficiently, since chemically related molecules in the same point group tend to exhibit similar bonding schemes, molecular bonding diagrams, and spectroscopic properties.[9]

Common point groups

The following table contains a list of point groups labelled using the Schoenflies notation, which is common in chemistry and molecular spectroscopy. The description of structure includes common shapes of molecules, which can be explained by the VSEPR model.

Point group	Symmetry operations[15]	Simple description of typical geometry	Example 1	Example 2	Example 3
C_1	E	no symmetry, chiral	 bromochlorofluoromethane (both enantiomers shown)	 lysergic acid	 L-leucine and most other α-amino acids except glycine
C_s	E σ_h	mirror plane, no other symmetry	 thionyl chloride	 hypochlorous acid	 chloroiodomethane
C_i	E *i*	inversion center	 *meso*-tartaric acid	 mucic acid (*meso*-galactaric acid)	(*S*,*R*) 1,2-dibromo-1,2-dichloroethane (*anti* conformer)
$C_{\infty v}$	E $2C_\infty^{\Phi}$ $\infty\sigma_v$	linear	 hydrogen fluoride (and all other heteronuclear diatomic molecules)	 nitrous oxide (dinitrogen monoxide)	 hydrocyanic acid (hydrogen cyanide)
$D_{\infty h}$	E $2C_\infty^{\Phi}$ $\infty\sigma_i$ *i* $2S_\infty^{\Phi}$ ∞C_2	linear with inversion center	 oxygen (and all other homonuclear diatomic molecules)	 carbon dioxide	 acetylene (ethyne)
C_2	E C_2	"open book geometry", chiral	 hydrogen peroxide	 hydrazine	 tetrahydrofuran (twist conformation)
C_3	E C_3	propeller, chiral	 triphenylphosphine	 triethylamine	 phosphoric acid
C_{2h}	E C_2 *i* σ_h	planar with inversion center, no vertical plane	 *trans*-1,2-dichloroethylene	 *trans*-dinitrogen difluoride	 *trans*-azobenzene
C_{3h}	E C_3 C_3^2 σ_h S_3 S_3^5	propeller	 boric acid	 phloroglucinol (1,3,5-trihydroxybenzene)	
C_{2v}	E C_2 $\sigma_v(xz)$ $\sigma_v'(yz)$	angular (H_2O) or see-saw (SF_4) or T-shape (ClF_3)	 water	 sulfur tetrafluoride	 chlorine trifluoride

C_{3v}	E $2C_3$ $3\sigma_v$	trigonal pyramidal	 non-inverting ammonia	 phosphorus oxychloride	 cobalt tetracarbonyl hydride, $HCo(CO)_4$
C_{4v}	E $2C_4$ C_2 $2\sigma_v$ $2\sigma_d$	square pyramidal	 xenon oxytetrafluoride	 pentaborane(9), B_5H_9	 nitroprusside anion $[Fe(CN)_5(NO)]^{2-}$
C_{5v}	E $2C_5$ $2C_5^2$ $5\sigma_v$	'milking stool' complex	 $Ni(C_5H_5)(NO)$	 corannulene	
D_2	E $C_2(x)$ $C_2(y)$ $C_2(z)$	twist, chiral	 biphenyl (skew conformation)	 twistane ($C_{10}H_{16}$)	cyclohexane twist conformation
D_3	E $C_3(z)$ $3C_2$	triple helix, chiral	 Tris(ethylenediamine)cobalt(III) cation	 tris(oxalato)iron(III) anion	
D_{2h}	E $C_2(z)$ $C_2(y)$ $C_2(x)$ *i* $\sigma(xy)$ $\sigma(xz)$ $\sigma(yz)$	planar with inversion center, vertical plane	 ethylene	 pyrazine	 diborane
D_{3h}	E $2C_3$ $3C_2$ σ_h $2S_3$ $3\sigma_v$	trigonal planar or trigonal bipyramidal	 boron trifluoride	 phosphorus pentachloride	 cyclopropane
D_{4h}	E $2C_4$ C_2 $2C_2'$ $2C_2''$ *i* $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$	square planar	 xenon tetrafluoride	 octachlorodimolybdate(II) anion	 *Trans*-$[Co^{III}(NH_3)_4Cl_2]^+$ (excluding H atoms)
D_{5h}	E $2C_5$ $2C_5^2$ $5C_2$ σ_h $2S_5$ $2S_5^3$ $5\sigma_v$	pentagonal	 cyclopentadienyl anion	 ruthenocene	 C_{70}
D_{6h}	E $2C_6$ $2C_3$ C_2 $3C_2'$ $3C_2''$ *i* $2S_3$ $2S_6$ σ_h $3\sigma_d$ $3\sigma_v$	hexagonal	 benzene	 bis(benzene)chromium	 coronene ($C_{24}H_{12}$)

D_{7h}	E C_7 S_7 $7C_2$ σ_h $7\sigma_v$	heptagonal	 tropylium ($C_7H_7^+$) cation		
D_{8h}	E C_8 C_4 C_2 S_8 *i* $8C_2$ σ_h $4\sigma_v$ $4\sigma_d$	octagonal	 cyclooctatetraenide ($C_8H_8^{2-}$) anion	 uranocene	
D_{2d}	E $2S_4$ C_2 $2C_2'$ $2\sigma_d$	90° twist	 allene	 tetrasulfur tetranitride	 diborane(4) (excited state)
D_{3d}	E $2C_3$ $3C_2$ *i* $2S_6$ $3\sigma_d$	60° twist	 ethane (staggered rotamer)	 dicobalt octacarbonyl (non-bridged isomer)	 cyclohexane chair conformation
D_{4d}	E $2S_8$ $2C_4$ $2S_8^3$ C_2 $4C_2'$ $4\sigma_d$	45° twist	 sulfur (crown conformation of S_8)	 dimanganese decacarbonyl (staggered rotamer)	 octafluoroxenate ion (idealized geometry)
D_{5d}	E $2C_5$ $2C_5^2$ $5C_2$ *i* $2S_{10}^3$ $2S_{10}$ $5\sigma_d$	36° twist	 ferrocene (staggered rotamer)		
S_4	E $2S_4$ C_2		 1,2,3,4-tetrafluorospiropentane[16]		
T_d	E $8C_3$ $3C_2$ $6S_4$ $6\sigma_d$	tetrahedral	 methane	 phosphorus pentoxide	 adamantane
T_h	E $4C_3$ $4C_3^2$ *i* $3C_2$ $4S_6$ $4S_6^5$ $3\sigma_h$	pyritohedron			
O_h	E $8C_3$ $6C_2$ $6C_4$ $3C_2$ *i* $6S_4$ $8S_6$ $3\sigma_h$ $6\sigma_d$	octahedral or cubic	 sulfur hexafluoride	 molybdenum hexacarbonyl	 cubane
I_h	E $12C_5$ $12C_5^2$ $20C_3$ $15C_2$ *i*	icosahedral or dodecahedral			

	$12S_{10}\ 12S_{10}^3$ $20S_6\ 15\sigma$		 Buckminsterfullerene	 dodecaborate anion	 dodecahedrane	

Representations

The symmetry operations can be represented in many ways. A convenient representation is by matrices. For any vector representing a point in Cartesian coordinates, left-multiplying it gives the new location of the point transformed by the symmetry operation. Composition of operations corresponds to matrix multiplication. Within a point group, a multiplication of the matrices of two symmetry operations leads to a matrix of another symmetry operation in the same point group.[9] For instance, in the C_{2v} example this is:

$$\underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{C_2} \times \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\sigma_v} = \underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\sigma_v'}$$

Although an infinite number of such representations exist, the irreducible representations (or "irreps") of the group are commonly used, as all other representations of the group can be described as a linear combination of the irreducible representations.

Character tables

For each point group, a **character table** summarizes information on its symmetry operations and on its irreducible representations. As there are always equal numbers of irreducible representations and classes of symmetry operations, the tables are square.

The table itself consists of **characters** that represent how a particular irreducible representation transforms when a particular symmetry operation is applied. Any symmetry operation in a molecule's point group acting on the molecule itself will leave it unchanged. But, for acting on a general entity, such as a vector or an orbital, this need not be the case. The vector could change sign or direction, and the orbital could change type. For simple point groups, the values are either 1 or −1: 1 means that the sign or phase (of the vector or orbital) is unchanged by the symmetry operation (*symmetric*) and −1 denotes a sign change (*asymmetric*).

The representations are labeled according to a set of conventions:

- A, when rotation around the principal axis is symmetrical
- B, when rotation around the principal axis is asymmetrical
- E and T are doubly and triply degenerate representations, respectively
- when the point group has an inversion center, the subscript g (German: *gerade* or even) signals no change in sign, and the subscript u (*ungerade* or uneven) a change in sign, with respect to inversion.
- with point groups $C_{\infty v}$ and $D_{\infty h}$ the symbols are borrowed from angular momentum description: Σ, Π, Δ.

The tables also capture information about how the Cartesian basis vectors, rotations about them, and quadratic functions of them transform by the symmetry operations of the group, by noting which irreducible representation transforms in the same way. These indications are conventionally on the righthand side of the tables. This information is useful because chemically important orbitals (in particular *p* and *d* orbitals) have the same symmetries as these entities.

The character table for the C_{2v} symmetry point group is given below:

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

Consider the example of water (H_2O), which has the C_{2v} symmetry described above. The $2p_x$ orbital of oxygen has B_1 symmetry as in the fourth row of the character table above, with x in the sixth column). It is oriented perpendicular to the plane of the molecule and switches sign with a C_2 and a $\sigma_v'(yz)$ operation, but remains unchanged with the other two operations (obviously, the character for the identity operation is always +1). This orbital's character set is thus {1, −1, 1, −1}, corresponding to the B_1 irreducible representation. Likewise, the $2p_z$ orbital is seen to have the symmetry of the A_1 irreducible representation (*i.e.*: none of the symmetry operations change it), $2p_y$ B_2, and the $3d_{xy}$ orbital A_2. These assignments and others are noted in the rightmost two columns of the table.

Historical background

Hans Bethe used characters of point group operations in his study of ligand field theory in 1929, and Eugene Wigner used group theory to explain the selection rules of atomic spectroscopy.[17] The first character tables were compiled by László Tisza (1933), in connection to vibrational spectra. Robert Mulliken was the first to publish character tables in English (1933), and E. Bright Wilson used them in 1934 to predict the symmetry of vibrational normal modes.[18] The complete set of 32 crystallographic point groups was published in 1936 by Rosenthal and Murphy.[19]

Molecular nonrigidity

As discussed above in the section **Point groups and permutation-inversion groups,** point groups are useful for classifying the vibronic states of *rigid* molecules (sometimes called *semi-rigid* molecules) which undergo only small oscillations about a single equilibrium geometry. Longuet-Higgins has introduced a more general type of symmetry group suitable not only for classifying the rovibronic states of rigid molecules but also for classifying the states of *non-rigid* (or *fluxional*) molecules that tunnel between equivalent geometries (called *versions*[20]) and which can also allow for the distorting effects of molecular rotation.[11] These groups are known as *permutation-inversion* groups, because the symmetry operations in them are energetically feasible permutations of identical nuclei, or inversion with respect to the center of mass (the parity operation), or a combination of the two.

For example, ethane (C_2H_6) has three equivalent staggered conformations. Tunneling between the conformations occurs at ordinary temperatures by internal rotation of one methyl group relative to the other. This is not a rotation of the entire molecule about the C_3 axis. Although each conformation has D_{3d} symmetry, as in the table above, description of the internal rotation and associated quantum states and energy levels requires the more complete permutation-inversion group G_{36}.

Similarly, ammonia (NH_3) has two equivalent pyramidal (C_{3v}) conformations which are interconverted by the process known as nitrogen inversion. This is not the point group inversion operation $\boldsymbol{i}$ used for centrosymmetric rigid molecules (i.e., the inversion of vibrational displacements and electronic coordinates in the nuclear center of mass) since NH_3 has no inversion center and is not centrosymmetric. Rather it the inversion of the nuclear and electronic coordinates in the molecular center of mass (sometimes called the parity operation), which happens to be energetically feasible for this molecule. The appropriate permutation-inversion group to be used in this situation is $D_{3h}(M)$ which is isomorphic with the point group D_{3h}.

Additionally, as examples, the methane (CH_4) and H_3^+ molecules have highly symmetric equilibrium structures with T_d and D_{3h} point group symmetries respectively; they lack permanent electric dipole moments but they do have very weak pure rotation spectra because of rotational centrifugal distortion.[21][22] The permutation-inversion groups required for the complete study of CH_4 and H_3^+ are $T_d(M)$ and $D_{3h}(M)$, respectively.

A second and less general approach to the symmetry of nonrigid molecules is due to Altmann.[23][24] In this approach the symmetry groups are known as *Schrödinger supergroups* and consist of two types of operations (and their combinations): (1) the geometric symmetry operations (rotations, reflections, inversions) of rigid molecules, and (2) *isodynamic operations*, which take a nonrigid molecule into an energetically equivalent form by a physically reasonable process such as rotation about a single bond (as in ethane) or a molecular inversion (as in ammonia).[24]

See also

- Parity (physics) § Molecules
- Irreducible representation § Applications in theoretical physics and chemistry
- Woodward-Hoffmann rules § Correlation diagrams
- Hapticity § Hapticity and fluxionality
- Character table
- Crystallographic point group
- Point groups in three dimensions
- Symmetry of diatomic molecules
- Symmetry in quantum mechanics

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External links

- Point group symmetry (https://www.staff.ncl.ac.uk/j.p.goss/symmetry/) @ Newcastle University
- Molecular symmetry (http://www.ch.ic.ac.uk/local/symmetry/) @ Imperial College London
- Molecular Symmetry Online (https://telem.openu.ac.il/symmetry) @ The Open University of Israel
- Molecular Point Group Symmetry Tables (http://www.webqc.org/symmetry.php)
- Symmetry @ Otterbein (http://symmetry.otterbein.edu/)
- An internet lecture course on molecular symmetry @ Bergische Universitaet (http://www.ptc.uni-wuppertal.de/FMS_Overview.html)
- Character tables for point groups for chemistry Link (http://gernot-katzers-spice-pages.com/character_tables/index.html/)

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