Character tables for chemically important point groups

URL: http://www.mpip-mainz.mpg.de/~gelessus/group.html

by

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Introduction

For symmetrical molecules the application of group theory has proven to be very helpful. Examples where group theory can be applied successfully are molecular orbital theory, molecular spectroscopy, multipole expansions and ligand field theory. In general, group theoretical results can be used as classification scheme and/or to simplify numerical calculations. There are many books available which give an introduction to group theory and its applications to chemistry.

This WWW project gives a collection of character tables for chemically important point groups. Furthermore reducible representations can be reduced to irreducible representations. In case of molecular 3N representations and molecular vibrational representations the symmetry properties of the force constants up to the quartic force field are determined. The molecular point group and the corresponding 3N representation can be determined from cartesian or internal (Z-matrix) coordinates.

Currently the collection comprises 58 point groups (Fig. 1). All character tables were taken from the books of Salthouse/Ware, Cotton and Altmann/Herzig. Two examples are presented to show how to use the WWW pages.

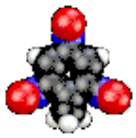
Altmann S. L.; Herzig P. Point-Group Theory Tables; Clarendon: Oxford, 1994

Cotton F. A. Chemical Applications of Group Theory: 3rd ed; Wiley: New York, 1990.

Salthouse J. A.; Ware M. J. Point Group Character Tables and Related Data; Cambridge University Press, 1972

Character tables for chemically important point groups

Nonaxial groups	C_1	C_s	C_i	-	-	-	-
C_n groups	C_2	C_3	C_4	C_5	C_6	C_7	C_8
D_n groups	D_2	D_3	D_4	D_5	D_6	D_7	D_8
C_{nv} groups	C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}
C_{nh} groups	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	-	-
D_{nh} groups	D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}
D_{nd} groups	D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}
S_n groups	S_2	S_4	S_6	S_8	S_{10}	S_{12}	-
Cubic groups	T	T_h	T_d	O	O_h	I	I_h
Linear groups	$C_{\infty v}$	$D_{\infty h}$	-	-	-	-	-



Help

Literature

Predefined reducible representations

Determine point group from molecular structure

Mirror Sites

Fig. 1

Last update September, 22nd 2000 by A. Gelessus

Example 1: BF_3 (D_{3h})

The equilibrium structure of BF_3 represents an example for a molecule with D_{3h} symmetry. If you select the point group D_{3h} from the point group table (Fig. 1) you get the following information (Fig. 2):

- Character table for D_{3h}.
- Additional information (number of symmetry elements, ...) for D_{3h}.
- Dialog box for the application of the reduction formula.
- Symmetry properties of the multipoles up to the 512-pole.

If you submit the Γ_{3N}-representation for BF_3 $(12, 0, -2, 4, -2, 2)$ in the dialog box for the reduction formula you get the following result (Fig. 3):

- The reduction of the Γ_{3N}-representation to irreducible representations:

$$\Gamma_{3N} = 1A_1^{'} + 1A_2^{'} + 3E^{'} + 2A_2^{''} + E^{''}$$

- The reduction of the Γ_{vib}-representation to irreducible representations, i.e. the vibrational modes of BF_3.

$$\Gamma_{vib} = 1A_1^{'} + 2E^{'} + 1A_2^{''}$$

- A table with information about allowed and forbidden transitions in IR and Raman spectra.
- The molecular potential energy surface V can be expressed in terms of normal ccordinates q_r.

$$V = \frac{1}{2}\sum_r \omega_r q_r^2 + \frac{1}{6}\sum_{rst} \phi_{rst} q_r q_s q_t + \frac{1}{24}\sum_{rstu} \phi_{rstu} q_r q_s q_t q_u + \ldots \qquad (1)$$

$$V = \frac{1}{2}\sum_r \omega_r q_r^2 + \sum_{r\le s\le t} k_{rst} q_r q_s q_t + \sum_{r\le s\le t\le u} k_{rstu} q_r q_s q_t q_u + \ldots \qquad (2)$$

  The number of force constants ϕ and k up to the quartic force field are given in columns 1 and 2 of the fifth table ('Number of force field parameters'). Only totally symmetrical force constants can be non-zero. The number of nonvanishing force constants k is given in the third column. (For optimized structures all first derivatives are zero. Since the normal coordinates are determined by diagonalization of the force constant matrix the coupling constants ϕ_{ij} and k_{ij} $(i \neq j)$ are all zero. This simplifies the expression for V to the form given in equations (1) and (2)).

- The sixth table ('Symmetry properties of force field parameters') lists the symmetry properties of all force constants. Only the totally symmetrical force constants are non-zero.
- Finally the number of independent internal coordinates for the molecule is determined.

Character table for point group D_{3h}

(x axis coincident with C'_2 axis)

D_{3h}	E	$2C_3$ (z)	$3C'_2$	σ_h (xy)	$2S_3$	$3\sigma_v$	linear functions, rotations	quadratic functions	cubic functions
A'_1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	$x(x^2-3y^2)$
A'_2	+1	+1	-1	+1	+1	-1	R_z	-	$y(3x^2-y^2)$
E'	+2	-1	0	+2	-1	0	(x, y)	(x^2-y^2, xy)	(xz^2, yz^2) $[x(x^2+y^2), y(x^2+y^2)]$
A''_1	+1	+1	+1	-1	-1	-1	-	-	-
A''_2	+1	+1	-1	-1	-1	+1	z	-	z^3, $z(x^2+y^2)$
E''	+2	-1	0	-2	+1	0	(R_x, R_y)	(xz, yz)	$[xyz, z(x^2-y^2)]$

Additional information

Number of symmetry elements	h = 12
Number of irreducible representations	n = 6
Abelian group	no
Subgroups	**C_s , C_2 , C_3 , D_3 , C_{2v} , C_{3v} , C_{3h}**
Optical Isomerism (Chirality)	no

Reduction formula for point group D_{3h}

Type of representation

$\Gamma_{general}$ Γ_{3N} Γ_{vib}

E	**$2C_3$ (z)**	**$3C'_2$**	**σ_h (xy)**	**$2S_3$**	**$3\sigma_v$**
0	0	0	0	0	0

Submit
Reset

Multipoles

dipole (p)	$E'+A''_2$
quadrupole (d)	$A'_1+E'+E''$
octopole (f)	$A'_1+A'_2+E'+A''_2+E''$
hexadecapole (g)	$A'_1+2E'+A''_1+A''_2+E''$
32-pole (h)	$A'_1+A'_2+2E'+A''_2+2E''$
64-pole (i)	$2A'_1+A'_2+2E'+A''_1+A''_2+2E''$
128-pole (j)	$A'_1+A'_2+3E'+A''_1+2A''_2+2E''$
256-pole(k)	$2A'_1+A'_2+3E'+A''_1+A''_2+3E''$
512-pole (l)	$2A'_1+2A'_2+3E'+A''_1+2A''_2+3E''$

First nonvanishing multipole: quadrupole

Literature

- *A. Gelessus, W. Thiel and W. Weber, J. Chem. Educ.* ***72****, 505 (1995)*
  Multipoles and Symmetry

Reduction formula for point group D_{3h}

Your representation

E	$2C_3$ (z)	$3C'_2$	σ_h (xy)	$2S_3$	$3\sigma_v$
12	0	-2	4	-2	2

can be reduced to

A'_1	A'_2	E'	A''_1	A''_2	E''
1	1	3	0	2	1

Substraction of translational and rotational contributions results in

A'_1	A'_2	E'	A''_1	A''_2	E''
1	0	2	0	1	0

Force field analysis

Infrared and Raman activities (harmonic approximation)

Method	A'_1	A'_2	E'	A''_1	A''_2	E''
Infrared	-	-	+	-	+	-
Raman	+	-	+	-	-	+

Number of force field parameters

Force field	No. 1	No. 2	No. 3
linear	6	6	1
quadratic	36	21	5
cubic	216	56	9
quartic	1296	126	19

No. 1 : Total number of force constants Φ.
No. 2 : Total number of force constants k.
No. 3 : Total number of nonvanishing force constants k.

Symmetry properties of force field parameters

Force field	A'_1	A'_2	E'	A''_1	A''_2	E''
linear	1	0	2	0	1	0
quadratic	5	1	5	0	1	2
cubic	9	5	13	1	5	5
quartic	19	9	29	5	9	13

Number of independant internal coordinates	1

Literature

- *J.K.G. Watson, J. Mol. Spec.* ***41*** *229 (1972)*
The Numbers of Structural Parameters and Potential Constants of Molecules

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Example 2: C_2H_4 (D_{2h})

In this example the point group and the Γ_{3N}-representation are determined from the molecular coordinates. Fig. 4 shows the input for ethen in internal coordinates (Z-matrix). Upon submitting the point group and Γ_{3N}-representation for ethen for ethen is determined. The subgroups and Γ_{3N}-representations for the subgroups are also included (Fig. 5). This information can be further processed to get the force analysis for ethen (Fig. 6).

Determine point group from internal coordinates

Bond lengths are given in units of Angstrom Angles are given in units of Degree

Reference Number I	Atom Type	Bond Length NA I	Bond Angle NB NA I	Twist Angle NC NB NA I	NA	NB	NC
1	C	-	-	-	-	-	-
2	C	1.45	-	-	1	-	-
3	H	1.1	110.0	-	1	2	-
4	H	1.1	110.0	180.0	1	2	3
5	H	1.1	110.0	180.0	2	1	3
6	H	1.1	110.0	180.0	2	1	4
7	None	0.0	0.0	0.0	1	1	1
8	None	0.0	0.0	0.0	1	1	1
9	None	0.0	0.0	0.0	1	1	1
10	None	0.0	0.0	0.0	1	1	1
11	None	0.0	0.0	0.0	1	1	1
12	None	0.0	0.0	0.0	1	1	1
13	None	0.0	0.0	0.0	1	1	1
14	None	0.0	0.0	0.0	1	1	1
15	None	0.0	0.0	0.0	1	1	1
16	None	0.0	0.0	0.0	1	1	1
17	None	0.0	0.0	0.0	1	1	1
18	None	0.0	0.0	0.0	1	1	1
19	None	0.0	0.0	0.0	1	1	1
20	None	0.0	0.0	0.0	1	1	1
21	None	0.0	0.0	0.0	1	1	1
22	None	0.0	0.0	0.0	1	1	1
23	None	0.0	0.0	0.0	1	1	1
24	None	0.0	0.0	0.0	1	1	1
25	None	0.0	0.0	0.0	1	1	1
26	None	0.0	0.0	0.0	1	1	1
27	None	0.0	0.0	0.0	1	1	1
28	None	0.0	0.0	0.0	1	1	1
29	None	0.0	0.0	0.0	1	1	1
30	None	0.0	0.0	0.0	1	1	1

Submit Reset

Fig. 4

Determine point group

Number of atoms	6
Sum formula	$C_2 H_4$
Molecular weight	28.03

Z-matrix									
Atom Number	Reference Number I	Atomic Symbol	Atomic Number	Bond Length (Angstrom) NA I	Bond Angle (Degree) NB NA I	Twist Angle (Degree) NC NB NA I	NA	NB	NC
1	1	C	6	0.000000	0.000000	0.000000	0	0	0
2	2	C	6	1.450000	0.000000	0.000000	1	0	0
3	3	H	1	1.100000	110.000000	0.000000	1	2	0
4	4	H	1	1.100000	110.000000	180.000000	1	2	3
5	5	H	1	1.100000	110.000000	180.000000	2	1	3
6	6	H	1	1.100000	110.000000	180.000000	2	1	4

Cartesian coordinates					
Atom Number	Atomic Symbol	Atomic Number	x-Coordinate (Angstrom)	y-Coordinate (Angstrom)	z-Coordinate (Angstrom)
1	C	6	0.000000	0.000000	0.000000
2	C	6	1.450000	0.000000	0.000000
3	H	1	-0.376222	1.033662	0.000000
4	H	1	-0.376222	-1.033662	0.000000
5	H	1	1.826222	-1.033662	0.000000
6	H	1	1.826222	1.033662	0.000000

Rotational Analysis	
Rotational Constant A (GHz)	117.3346
Rotational Constant B (GHz)	28.8729
Rotational Constant C (GHz)	23.1711
Ray's asymmetry parameter	-0.8789
Classification : Asymmetric top	

Symmetry adapted cartesian coordinates					
Atom Number	Atomic Symbol	Atomic Number	x-Coordinate (Angstrom)	y-Coordinate (Angstrom)	z-Coordinate (Angstrom)
1	C	6	-0.725000	0.000000	0.000000
2	C	6	0.725000	0.000000	0.000000
3	H	1	-1.101222	-1.033662	0.000000
4	H	1	-1.101222	1.033662	0.000000
5	H	1	1.101222	1.033662	0.000000
6	H	1	1.101222	-1.033662	0.000000

Determined point group	**D_{2h}**
Subgroups	**C_s , C_i , C_2 , C_{2v} , C_{2h}**

Γ_{3N} representation									
group	E	C_2 (z)	C_2 (y)	C_2 (x)	i	σ (xy)	σ (xz)	σ (yz)	-
D_{2h}	18	0	0	-2	0	6	2	0	Submit
C_s	18	-	-	-	-	6	-	-	Submit
C_s	18	-	-	-	-	-	2	-	Submit
C_s	18	-	-	-	-	-	-	0	Submit
C_i	18	-	-	-	0	-	-	-	Submit
C_2	18	0	-	-	-	-	-	-	Submit
C_2	18	-	0	-	-	-	-	-	Submit
C_2	18	-	-	-2	-	-	-	-	Submit
C_{2v}	18	0	-	-	-	-	2	0	Submit
C_{2v}	18	-	0	-	-	6	-	0	Submit
C_{2v}	18	-	-	-2	-	6	2	-	Submit
C_{2h}	18	0	-	-	0	6	-	-	Submit
C_{2h}	18	-	0	-	0	-	2	-	Submit
C_{2h}	18	-	-	-2	0	-	-	0	Submit

Fig. 5

Reduction formula for point group D_{2h}

Your representation

E	C_2 (z)	C_2 (y)	C_2 (x)	i	σ (xy)	σ (xz)	σ (yz)
18	0	0	-2	0	6	2	0

can be reduced to

A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
3	3	2	1	1	2	3	3

Substraction of translational and rotational contributions results in

A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
3	2	1	0	1	1	2	2

Force field analysis

Infrared and Raman activities (harmonic approximation)

Method	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
Infrared	-	-	-	-	-	+	+	+
Raman	+	+	+	+	-	-	-	-

Number of force field parameters

Force field	No. 1	No. 2	No. 3
linear	12	12	3
quadratic	144	78	18
cubic	1728	364	60
quartic	20736	1365	216

No. 1 : Total number of force constants ϕ.
No. 2 : Total number of force constants k.
No. 3 : Total number of nonvanishing force constants k.

Symmetry properties of force field parameters

Force field	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
linear	3	2	1	0	1	1	2	2
quadratic	18	11	7	6	7	7	11	11
cubic	60	53	38	31	38	38	53	53
quartic	216	188	148	141	148	148	188	188

Number of independant internal coordinates	3

Literature

- *J.K.G. Watson, J. Mol. Spec.* ***41*** *229 (1972)*
The Numbers of Structural Parameters and Potential Constants of Molecules

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Citations

Examples of web pages having links to 'Character tables for chemically important point groups'

- Open Directory Project
  http://www.dmoz.org/Science/Math/Algebra/Group_Theory
- The Chemistry Information Service
  www.chemie.de
- Chemdex
  http://www.shef.ac.uk/chemistry/chemdex/chemdex/spectroscopy.html
- Institute of Theoretical Chemistry, University of Nijmegen
  http://www.theochem.kun.nl/local.html
- Institute of Organic Chemistry, University of Zurich
  http://www.unizh.ch/oci/diversa/BookMarks/BookMarks.shtml
- College of Arts and Sciences, Arkansas State University
  http://www.cas.astate.edu/draganjac
- University of Exeter
  http://newton.ex.ac.uk/people/goss/symmetry/links.html
- Central Connecticut State University
  http://cchem2.ccsu.edu/grouptheory/group.html
- Max Planck Institute for Coal Research
  http://www.mpi-muelheim.mpg.de/kofo/institut/arbeitsbereiche/thiel/thiel_themen.html