Vibration Spectroscopy

Tables for Factor Group and Point Group Analysis

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Comments

Title line

Contains the point group at the left and right sides and the crystallographic spacegroup in the center of the page.

Character tables

The vibration types or species are named according to the symmetry operations they represent as follows:

A ..... symmetric with respect to the principal axis of symmetry
B..... antisymmetric with respect to the principal axis of symmetry
E..... doubly degenerate vibrations, the irreducible representation is two-dimensional, i.e., a 2 × 2 matrix
F ..... triply degenerate vibrations, i.e., a three-dimensional representation
g and *u* (subscripts) .... symmetric and antisymmetric with respect to a center of symmetry (from german *gerade* and *ungerade*)
1 and *2* (subscripts) .... symmetric and antisymmetric with respect to a rotation axis (C_p) or a rotation-reflection axis (S_p) other than the principal axis or, in those point groups with only one symmetry axis, with respect to a plane of symmetry
‘ and “ (superscript) .... symmetric or antisymmetric with respect to a plane of symmetry
Σ^+ ..... symmetric with respect to a plane of symmetry through the molecular axis (for linear molecules)
Σ^- ..... antisymmetric with respect to a plane of symmetry through the molecular axis (for linear molecules)
Π, Δ, Φ..... degenerate vibrations (linear molecules) with a degree of degeneracy increasing in this order

Unnamed rows belong to the previously named vibration (double degenerate vibrations represented by to rows).
The electric moment belongs to the same species as the translations.
Infrared active vibrations must involve a change in the dipole moment.

Selection rules

Selection rules are represented in matrix format where a mark in a matrix element indicate a forbidden vibration as follows:

x.....this combination band represents a forbidden vibration
n .....this symmetry species raised to the n'th power (*n* = any integer number) represents a forbidden overtone
o .....this symmetry species raised to the o'th power (*o* = odd integer numbers) represents a forbidden overtone
e.....this symmetry species raised to the e'th power (*e* = even integer numbers) represents a forbidden overtone
1 .....this symmetry species represents a forbidden vibration

Wyckoff sites

A repetition of the appropriate row of the Wyckoff site table on page 3.

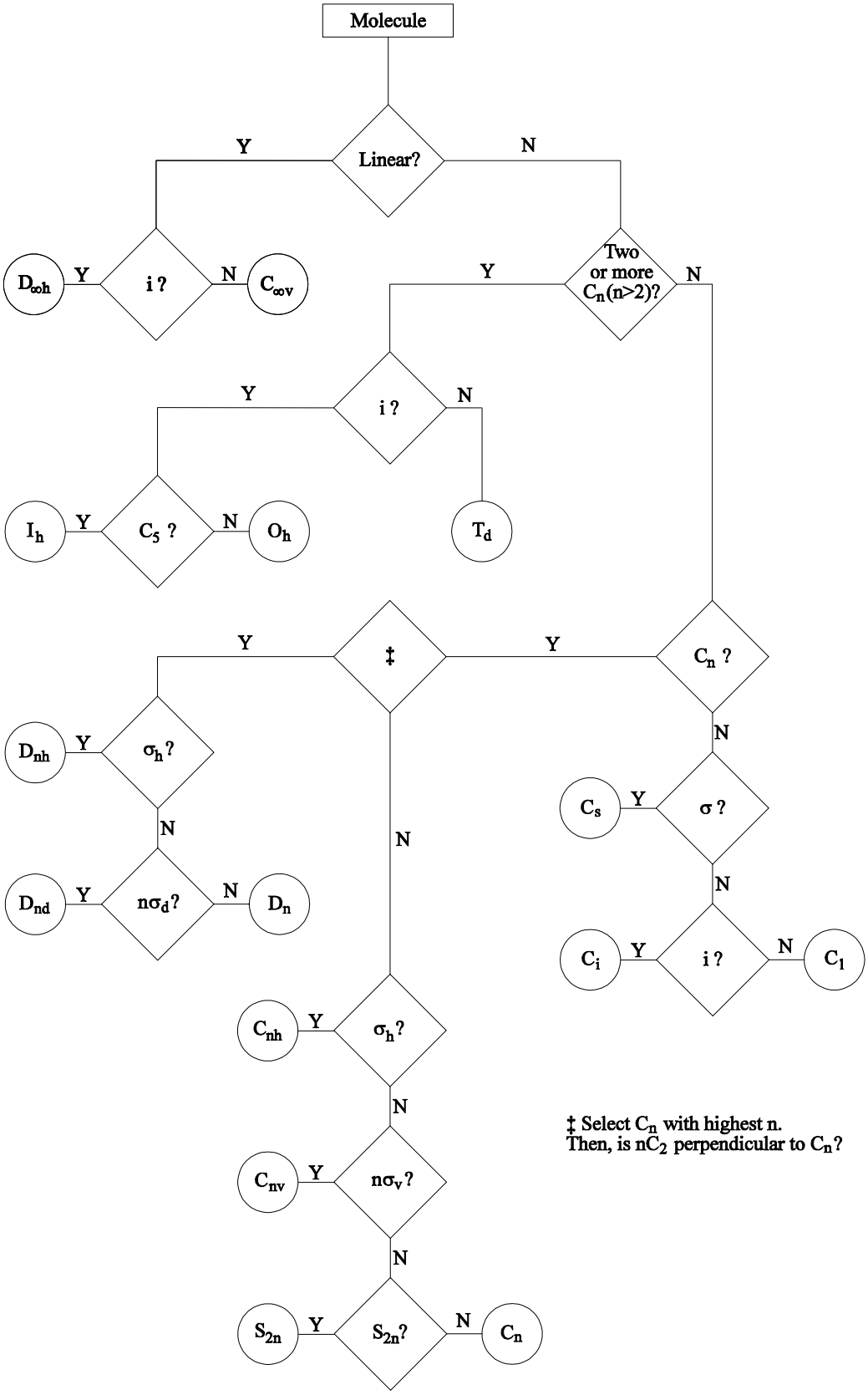
Adams - Newton table 1 & 3

The tables were originally published in 1970 by Prof. D.M. Adams and D.C. Newton, Department of Chemistry, University of Leicester, LE1 7RH, England.

Raman depolarised bands

The depolarisation ratio is defined as $\rho = I_\perp / I_{||}$ with $0 \le \rho \le 0.75$. Polarised Raman bands ($\rho \approx 0$) is caused by totally symmetric vibrations.

Determination of Point Group



Point group	Space group	Allowed sites and their Wyckoff notation							
$C_{\infty v}$	A10								
C_1	1	C_1 - A							
C_2	3	C_2 - A	C_1 - E						
C_{2h}	10	C_{2h} - A	C_2 - I	C_s - M	C_1 - O				
C_{2v}	25	C_{2v} - A	C_s(zx) - E	C_s(yz) - G	C_1 - I				
C_3	143	C_3 - A	C_1 - D						
C_{3h}	174	C_{3h} - A	C_3 - G	C_s - J	C_1 - L				
C_{3v}	156	C_{3v} - A	C_s - D	C_1 - E					
C_4	75	C_4 - A	C_1 - D						
C_{4h}	83	C_{4h} - A	C_4 - G	C_s - J	C_1 - L				
C_{4v}	99	C_{4v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - G				
C_5	A2								
C_{5h}	A4								
C_{5v}	A3								
C_6	168	C_6 - A	C_1 - D						
C_{6h}	175	C_{6h} - A	C_6 - E	C_s - J	C_1 - L				
C_{6v}	183	C_{6v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - F				
C_i	2	C_i - A	C_1 - I						
C_s	6	C_s - A	C_1 - C						
$D_{\infty h}$	A11								
D_2	16	D_2 - A	C_2(x) - I	C_2(y) - M	C_2(z) - Q	C_1 - U			
D_{2d}	111	D_{2d} - A	C_{2v} - G	$C_2(C_2')$ - I	C_s - N	C_1 - O			
D_{2h}	47	D_{2h} - A	C_{2v}(x) - I	C_{2v}(y) - M	C_{2v}(z) - Q	C_s(yz) - U	C_s(zx) - W	C_s(xy) - Y	C_1 - ∝
D_3	149	D_3 - A	C_3 - G	C_2 - J	C_1 - L				
D_{3d}	162	D_{3d} - A	C_{3v} - E	C_2 - I	C_s - K	C_1 - L			
D_{3h}	187	D_{3h} - A	C_{3v} - G	C_{2v} - J	$C_s(\sigma_h)$ - L	$C_s(\sigma_v)$ - N	C_1 - O		
D_4	89	D_4 - A	C_4 - G	$C_2(C_2'')$ - J	$C_2(C_2')$ - L	C_1 - P			
D_{4d}	A1								
D_{4h}	123	D_{4h} - A	C_{4v} - G	$C_{2v}(C_2'')$ - J	$C_{2v}(C_2')$ - L	$C_s(\sigma_h)$ - P	$C_s(\sigma_d)$ - R	$C_s(\sigma_v)$ - S	C_1 - U
D_5	A5								
D_{5d}	A6								
D_{5h}	A7								
D_6	177	D_6 - A	C_6 - E	$C_2(C_2')$ - J	$C_2(C_2'')$ - L	C_1 - N			
D_{6d}	A8								
D_{6h}	191	D_{6h} - A	C_{6v} - E	$C_{2v}(C_2')$ - J	$C_{2v}(C_2'')$ - L	$C_s(\sigma_v)$ - N	$C_s(\sigma_d)$ - O	$C_s(\sigma_h)$ - P	C_1 - R
O	207	O - A	C_4 - E	C_3 - G	$C_2(C_2')$ - I	C_1 - K			
O_h	221	O_h - A	C_{4v} - E	C_{3v} - G	C_{2v} - I	$C_s(\sigma_h)$ - K	$C_s(\sigma_d)$ - M	C_1 - N	
S_4	81	S_4 - A	C_1 - H						
S_6	147	S_6 - A	C_1 - G						
S_8	A9								
T	195	T - A	C_3 - E	C_2 - F	C_1 -J				
T_d	215	T_d - A	C_{3v} - E	C_{2v} - F	C_s - I	C_1 - J			
T_h	200	T_h - A	C_3 - I	C_{2v} - E	C_s - J	C_1 -L			

Symmetry elements: I

C_1	I
A	1

Selection rules, forbidden vibrations

Infrared:

	A
A	

(None)

Raman:

	A
A	

(None)

C_1	1	C_1 - A							

Wyckoff	C_1 A	Rotatory A
1A	3	3

Wyckoff	Vector A
1A	1

Symmetry elements: i

C_i	I	i		
A_g	1	1	R_x, R_y, R_z	x^2, y^2, z^2, xy, xz, yz
A_u	1	-1	T_x, T_y, T_z	

Selection rules, forbidden vibrations

Infrared:

	A_g	A_u
A_g		
A_u		

(Missing information)

Raman:

	A_g	A_u
A_g		
A_u		

(Missing information)

C_i	2	C_i - A	C_1 - I						

	C_i		Rotatory	
Wyckoff	A_g	A_u	A_g	A_u
1 A-H	0	3	3	0
2 I	3	3	3	3

	Vector	
Wyckoff	A_g	A_u
1 A-H	1	0
2 I	1	1

Symmetry elements: C_2

C_2	I	$C_2(z)$		
A	1	1	T_z, R_z	x^2, y^2, z^2, xy
B	1	-1	T_x, T_y, R_x, R_y	yz, xz

Selection rules, forbidden vibrations

Infrared:

	A	B
A		
B		

(None)

Raman:

	A	B
A		
B		

(None)

C_2	3	C_2 - A	C_1 - E						

	C_2		Rotatory	
Wyckoff	A	B	A	B
1 A-D	1	2	1	2
2 E	3	3	3	3

	Vector	
Wyckoff	A	B
1 A-D	1	0
2 E	1	1

Symmetry elements: σ

C_s	I	σ(xy)		
A'	1	1	T_x, T_y, R_z	x^2, y^2, z^2, xy
A"	1	-1	T_z, R_x, R_y	yz, xz

Selection rules, forbidden vibrations

Infrared:

	A'	A"
A'		
A"		

(None)

Raman:

	A'	A"
A'		
A"		

(None)

C_s	6	C_s - A	C_1 - C						

	C_s		Rotatory	
Wyckoff	A'	A"	A'	A"
1 A-B	2	1	1	2
2 C	3	3	3	3

	Vector	
Wyckoff	A'	A"
1 A-B	1	0
2 C	1	1

Symmetry elements: C_2, σ_h, S_2, i

C_{2h}	I	$C_2(z)$	$\sigma_h(xy)$	i		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
A_u	1	1	-1	-1	T_z	
B_g	1	-1	-1	1	R_x, R_y	yz, xz
B_u	1	-1	1	-1	T_x, T_y	

Selection rules, forbidden vibrations

Infrared:

	A_g	A_u	B_g	B_u
A_g	n		x	
A_u		e		x
B_g	x		n	
B_u		x		e

Raman:

	A_g	A_u	B_g	B_u
A_g		x		x
A_u	x	o	x	
B_g		x		x
B_u	x		x	o

C_{2h}	10	C_{2h} - A	C_2 - I	C_s - M	C_1 - O				

	C_{2h}				Rotatory			
Wyckoff	A_g	B_g	A_u	B_u	A_g	B_g	A_u	B_u
1 A-H	0	0	1	2	1	2	0	0
2 I-L	1	2	1	2	1	2	1	2
2 M-N	2	1	1	2	1	2	2	1
4 O	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A_g	B_g	A_u	B_u
1 A-H	1	0	0	0
2 I-L	1	0	1	0
2 M-N	1	0	0	1
4 O	1	1	1	1

Symmetry elements: $3C_2$

D_2	I	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	-1	-1	T_z, R_z	xy
B_2	1	-1	1	-1	T_y, R_y	xz
B_3	1	-1	-1	1	T_x, R_x	yz

Selection rules, forbidden vibrations

Infrared:

	A	B_1	B_2	B_3
A				
B_1				
B_2				
B_3				

(Missing information)

Raman:

	A	B_1	B_2	B_3
A				
B_1				
B_2				
B_3				

(Missing information)

D_2	16	D_2 - A	$C_2(x)$ - I	$C_2(y)$ - M	$C_2(z)$ - Q	C_1 - U			

	D_2				Rotatory			
Wyckoff	A	B_1	B_2	B_3	A	B_1	B_2	B_3
1 A-H	0	1	1	1	0	1	1	1
2 I-L	1	2	2	1	1	2	2	1
2 M-P	1	2	1	2	1	2	1	2
2 Q-T	1	1	2	2	1	1	2	2
4 U	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A	B_1	B_2	B_3
1 A-H	1	0	0	0
2 I-L	1	0	0	1
2 M-P	1	0	1	0
2 Q-T	1	1	0	0
4 U	1	1	1	1

Symmetry elements: C_2, $2\sigma_v$

C_{2v}	I	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	T_z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	T_x, R_y	xz
B_2	1	-1	-1	1	T_y, R_x	yz

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2
A_1		x		
A_2	x	o		
B_1				x
B_2			x	

Raman:

	A_1	A_2	B_1	B_2
A_1				
A_2				
B_1				
B_2				

(None)

C_{2v}	25	C_{2v} - A	$C_s(zx)$ - E	$C_s(yz)$ - G	C_1 - I				

	C_{2v}				Rotatory			
Wyckoff	A_1	A_2	B_1	B_2	A_1	A_2	B_1	B_2
1 A-D	1	0	1	1	0	1	1	1
2 E-F	2	1	2	1	1	2	1	2
2 G-H	2	1	1	2	1	2	2	1
4 I	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A_1	A_2	B_1	B_2
1 A-D	1	0	0	0
2 E-F	1	0	1	0
2 G-H	1	0	0	1
4 I	1	1	1	1

Symmetry elements: i, $3C_2$, 3σ

$D_{2h} = V_h$	I	σ(xy)	σ(xz)	σ(yz)	i	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
A_u	1	-1	-1	-1	-1	1	1	1		
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{1u}	1	-1	1	1	-1	1	-1	-1	T_z	
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{2u}	1	1	-1	1	-1	-1	1	-1	T_y	
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
B_{3u}	1	1	1	-1	-1	-1	-1	1	T_x	

Selection rules, forbidden vibrations

Infrared:

	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
A_g	n	x	x	x	x			
B_{1g}	x	n	x	x	x	x	x	
B_{2g}	x	x	n	x				
B_{3g}	x	x	x	n				
A_u	x	x			n	x	x	x
B_{1u}		x			x	e	x	x
B_{2u}		x			x	x	e	x
B_{3u}					x	x	x	e

Raman:

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

Cont.

D_{2h}	47	D_{2h} - A	$C_{2v}(x)$ - I	$C_{2v}(y)$ - M	$C_{2v}(z)$ - Q	$C_s(yz)$ - U	$C_s(zx)$ - W	$C_s(xy)$ - Y	C_1 - ∝

	D_{2h}								Rotatory							
Wyckhoff	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
1 A-H	0	0	0	0	0	1	1	1	0	1	1	1	0	0	0	0
2 I-L	1	1	1	0	0	1	1	1	0	1	1	1	1	1	1	0
2 M-P	1	1	0	1	0	1	1	1	0	1	1	1	1	1	0	1
2 Q-T	1	0	1	1	0	1	1	1	0	1	1	1	1	0	1	1
4 U-V	2	1	1	2	1	2	2	1	1	2	2	1	2	1	1	2
4 W-X	2	1	2	1	1	2	1	2	1	2	1	2	2	1	2	1
4 Y-Z	2	2	1	1	1	1	2	2	1	1	2	2	2	2	1	1
8 α	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3

	Vector							
Wyckoff	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
1 A-H	1	0	0	0	0	0	0	0
2 I-L	1	0	0	0	0	0	0	1
2 M-P	1	0	0	0	0	0	1	0
2 Q-T	1	0	0	0	0	1	0	0
4 U-V	1	0	0	1	0	1	1	0
4 W-X	1	0	1	0	0	1	0	1
4 Y-Z	1	1	0	0	0	0	1	1
8 α	1	1	1	1	1	1	1	1

Symmetry elements: C_4

C_4	I	C_4^1	C_2	C_4^3		
A	1	1	1	1	T_z, R_z	z^2, $x^2 + y^2$
B	1	-1	1	-1		$x^2 - y^2$, xy
E	1	i	-1	-i	(T_x, T_y) (R_x, R_y)	(xz, yz)
	1	-i	-1	i		

$i = -1^{½}$

Selection rules, forbidden vibrations

Infrared:

	A	B	E
A			
B			
E			

(Missing information)

Raman:

	A	B	E
A			
B			
E			

(Missing information)

C_4	75	C_4 - A	C_1 - D						

	C_4			Rotatory		
Wyckoff	A	B	E	A	B	E
1 A-B	1	0	1	1	0	1
2 C	1	1	2	1	1	2
4 D	3	3	3	3	3	3

	Vector		
Wyckoff	A	B	E
1 A-B	1	0	0
2 C	1	1	0
4 D	1	1	1

Symmetry elements: C_2, S_4

S_4	I	S_4^1	C_2	S_4^3		
A	1	1	1	1	R_z	z^2, $x^2 + y^2$
B	1	-1	1	-1	T_z	$x^2 - y^2$, xy
E	1	i	-1	-i	(T_x, T_y) (R_x, R_y)	(xz, yz)
	1	-i	-1	i		

$i = -1^{½}$

Selection rules, forbidden vibrations

Infrared:

	A	B	E
A			
B			
E			

(Missing information)

Raman:

	A	B	E
A			
B			
E			

(Missing information)

S_4	81	S_4 - A	C_1 - H						

	S_4			Rotatory		
Wyckoff	A	B	E	A	B	E
1 A-D	0	1	1	1	0	1
2 E-G	1	1	2	1	1	2
4 H	3	3	3	3	3	3

	Vector		
Wyckoff	A	B	E
1 A-D	1	0	0
2 E-G	1	1	0
4 H	1	1	1

Symmetry elements: i, C_4, σ_h

C_{4h}	I	C_4^1	C_2	C_4^3	i	S_4^3	σ_h	S_4^1		
A_g	1	1	1	1	1	1	1	1	R_z	z^2, $x^2 + y^2$
B_g	1	-1	1	-1	1	-1	1	-1		$x^2 - y^2$, xy
E_g	1	i	-1	-i	1	I	-1	-i	(R_x, R_y)	(xz, yz)
	1	-i	-1	i	1	-i	-1	i		
A_u	1	1	1	1	-1	-1	-1	-1	T_z	
B_u	1	-1	1	-1	-1	1	-1	1		
E_u	1	i	-1	-i	-1	-i	1	i	(T_x, T_y)	
	1	-i	-1	i	-1	i	1	-i		

$i = -1^{½}$

Selection rules, forbidden vibrations

Infrared:

	A_g	B_g	E_g	A_u	B_u	E_u
A_g						
B_g						
E_g						
A_u						
B_u						
E_u						

(Missing information)

Raman:

	A_g	B_g	E_g	A_u	B_u	E_u
A_g						
B_g						
E_g						
A_u						
B_u						
E_u						

(Missing information)

C_{4h}	83	C_{4h} - A	C_4 - G	C_s - J	C_1 - L				

	C_{4h}						Rotatory					
Wyckhoff	A_g	B_g	E_g	A_u	B_u	E_u	A_g	B_g	E_g	A_u	B_u	E_u
1 A-D	0	0	0	1	0	1	1	0	1	0	0	0
2 E-F	0	0	0	1	1	2	1	1	2	0	0	0
2 G-H	1	0	1	1	0	1	1	0	1	1	0	1
4 I	1	1	2	1	1	2	1	1	2	1	1	2
4 J-K	2	2	1	1	1	2	1	1	2	2	2	1
8 L	3	3	3	3	3	3	3	3	3	3	3	3

Cont.

	Vector					
Wyckoff	A_g	B_g	E_g	A_u	B_u	E_u
1 A-D	1	0	0	0	0	0
2 E-F	1	1	0	0	0	0
2 G-H	1	0	0	1	0	0
4 I	1	1	0	1	1	0
4 J-K	1	1	0	0	0	1
8 L	1	1	1	1	1	1

Symmetry elements: C_4, C_2

D_4	I	$2C_4$	C_2	$2C_2'$	$2C_2''$		
A_1	1	1	1	1	1		z^2, x^2+y^2
A_2	1	1	1	-1	-1	T_z, 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	(T_x, T_y) (R_x, R_y)	(xz, yz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E
A_1					
A_2					
B_1					
B_2					
E					

(Missing information)

Raman:

	A_1	A_2	B_1	B_2	E
A_1					
A_2					
B_1					
B_2					
E					

(Missing information)

D_4	89	D_4 - A	C_4 - G	$C_2(C_2'')$ - J	$C_2(C_2')$ - L	C_1 - P			

	D_4					Rotatory				
Wyckoff	A_1	A_2	B_1	B_2	E	A_1	A_2	B_1	B_2	E
1 A-D	0	1	0	0	1	0	1	0	0	1
2 E-F	0	1	0	1	2	0	1	0	1	2
2 G-H	1	1	0	0	2	1	1	0	0	2
4 I	1	1	1	1	4	1	1	1	1	4
4 J-K	1	2	2	1	3	1	2	2	1	3
4 L-O	1	2	1	2	3	1	2	1	2	3
8 P	3	3	3	3	6	3	3	3	3	6

Cont.

	Vector				
Wyckoff	A_1	A_2	B_1	B_2	E
1 A-D	1	0	0	0	0
2 E-F	1	0	1	0	0
2 G-H	1	1	0	0	0
4 I	1	1	1	1	0
4 J-K	1	0	0	1	1
4 L-O	1	0	1	0	1
8 P	1	1	1	1	2

Symmetry elements: C_4, $4\sigma_v$

C_{4v}	I	$2C_4(z)$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	T_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	(T_x, T_y) (R_x, R_y)	(yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E
A_1		x	x	x	
A_2	x	o	x	x	
B_1	x	x	o	x	
B_2	x	x	x	o	
E					

Raman:

	A_1	A_2	B_1	B_2	E
A_1		x			
A_2	x	o			
B_1				x	
B_2			x		
E					

C_{4v}	99	C_{4v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - G				

	C_{4v}					Rotatory				
Wyckoff	A_1	A_2	B_1	B_2	E	A_1	A_2	B_1	B_2	E
1 A-B	1	0	0	0	1	0	1	0	0	1
2 C	1	0	1	0	2	0	1	0	1	2
4 D	2	1	1	2	3	1	2	2	1	3
4 E-F	2	1	2	1	3	1	2	1	2	3
8 G	3	3	3	3	6	3	3	3	3	6

	Vector				
Wyckoff	A_1	A_2	B_1	B_2	E
1 A-B	1	0	0	0	0
2 C	1	0	1	0	0
4 D	1	0	0	1	1
4 E-F	1	0	1	0	1
8 G	1	1	1	1	2

Symmetry elements: $3D_2$, S_4, $2\sigma_d$

D_{2d}	I	$2S_4(z)$	S_4^2	$2C_2$	$2\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
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	T_z	xy
E	2	0	-2	0	0	(T_x, T_y) (R_x, R_y)	(yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E
A_1	n	x	x		
A_2	x	n		x	
B_1	x		n	x	
B_2		x	x	e	
E					

Raman:

	A_1	A_2	B_1	B_2	E
A_1		x			
A_2	x	o			
B_1				x	
B_2			x		
E					

D_{2d}	111	D_{2d} - A	C_{2v} - G	$C_2(C_2')$ - I	C_s - N	C_1 - O			

	D_{2d}					Rotatory				
Wyckoff	A_1	A_2	B_1	B_2	E	A_1	A_2	B_1	B_2	E
1 A-D	0	0	0	1	1	0	1	0	0	1
2 E-F	0	1	0	1	2	0	1	0	1	2
2 G-H	1	0	0	1	2	0	1	1	0	2
4 I-L	1	2	1	2	3	1	2	1	2	3
4 M	1	1	1	1	4	1	1	1	1	4
4 N	2	1	1	2	3	1	2	2	1	3
8 O	3	3	3	3	6	3	3	3	3	6

Cont.

	Vector				
Wyckoff	A_1	A_2	B_1	B_2	E
1 A-D	1	0	0	0	0
2 E-F	1	0	1	0	0
2 G-H	1	0	0	1	0
4 I-L	1	0	1	0	1
4 M	1	1	1	1	0
4 N	1	0	0	1	1
8 O	1	1	1	1	2

Symmetry elements: i, $4C_2$, C_4, S_4, $4\sigma_v$, σ_h

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

Selection rules, forbidden vibrations

Infrared:

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
A_{1g}	n	x	x	x	x	x		x	x	
A_{2g}	x	n	x	x	x		x	x	x	
B_{1g}	x	x	n	x	x	x	x	x		
B_{2g}	x	x	x	n	x	x	x		x	
E_g	x	x	x	x	n					
A_{1u}	x		x	x		n	x	x	x	x
A_{2u}		x	x	x		x	e	x	x	x
B_{1u}	x	x	x			x	x	n	x	x
B_{2u}	x	x		x		x	x	x	n	x
E_u						x	x	x	x	e

Raman:

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
A_{1g}		x				x	x	x	x	x
A_{2g}	x	o				x	x	x	x	x
B_{1g}				x		x	x	x	x	x
B_{2g}			x			x	x	x	x	x
E_g						x	x	x	x	x
A_{1u}	x	x	x	x	x	o				
A_{2u}	x	x	x	x	x		o			
B_{1u}	x	x	x	x	x			o		
B_{2u}	x	x	x	x	x				o	
E_u	x	x	x	x	x					o

Cont.

D_{4h}	123	D_{4h} - A	C_{4v} - G	$C_{2v}(C_2'')$ - J	$C_{2v}(C_2')$ - L	$C_s(\sigma_h)$ - P	$C_s(\sigma_d)$ - R	$C_s(\sigma_v)$ - S	C_1 - U

	D_{4h}										Rotatory									
Wyckoff	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
1 A-D	0	0	0	0	0	0	1	0	0	1	0	1	0	0	1	0	0	0	0	0
2 E-F	0	0	0	0	0	0	1	0	1	2	0	1	0	1	2	0	0	0	0	0
2 G-H	1	0	0	0	1	0	1	0	0	1	0	1	0	0	1	1	0	0	0	1
4 I	1	0	1	0	2	0	1	0	1	2	0	1	0	1	2	1	0	1	0	2
4 J-K	1	1	1	1	1	0	1	1	0	2	0	1	1	0	2	1	1	1	1	1
4 L-O	1	1	1	1	1	0	1	0	1	2	0	1	0	1	2	1	1	1	1	1
8 P-Q	2	2	2	2	2	1	1	1	1	4	1	1	1	1	4	2	2	2	2	2
8 R	2	1	1	2	3	1	2	2	1	3	1	2	2	1	3	2	1	1	2	3
8 S-T	2	1	2	1	3	1	2	1	2	3	1	2	1	2	3	2	1	2	1	3
16 U	3	3	3	3	6	3	3	3	3	6	3	3	3	3	6	3	3	3	3	6

	Vector									
Wyckoff	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
1 A-D	1	0	0	0	0	0	0	0	0	0
2 E-F	1	0	1	0	0	0	0	0	0	0
2 G-H	1	0	0	0	0	0	1	0	0	0
4 I	1	0	1	0	0	0	1	0	1	0
4 J-K	1	0	0	1	0	0	0	0	0	1
4 L-O	1	0	1	0	0	0	0	0	0	1
8 P-Q	1	1	1	1	0	0	0	0	0	2
8 R	1	0	0	1	1	0	1	1	0	1
8 S-T	1	0	1	0	1	0	1	0	1	1
16 U	1	1	1	1	2	1	1	1	1	2

Symmetry elements: C_3

C_3	I	C_3^1	C_3^2		
A	1	1	1	T_z, R_z	$x^2 + y^2$, z^2
E	1	ε	ε^*	(T_x, T_y) (R_x, R_y)	($x^2 - y^2$, xy, yz, xz)
	1	ε^*	ε		

$\varepsilon = \exp(2\pi i/3) = 1^{1/3}$ $\varepsilon^* = \exp(-2\pi i/3) = \exp(4\pi i/3) = 1^{2/3}$

Selection rules, forbidden vibrations

Infrared:

	A	E
A		
E		

(Missing information)

Raman:

	A	E
A		
E		

(Missing information)

C_3	143	C_3 - A	C_1 - D						

	C_3		Rotatory	
Wyckoff	A	E	A	E
1 A-C	1	1	1	1
3 D	3	3	3	3

	Vector	
Wyckoff	A	E
1 A-C	1	0
3 D	1	1

Symmetry elements: i, C_3, S_6

S_6	I	C_3^1	C_3^2	i	S_6^5	S_6^1		
A_g	1	1	1	1	1	1	R_z	z^2, $x^2 + y^2$
E_g	1	ε	ε^*	1	ε	ε^*	(R_x, R_y)	($x^2 - y^2$, xy, xz, yz)
	1	ε^*	ε	1	ε^*	ε		
A_u	1	1	1	-1	-1	-1	T_z	
E_u	1	ε	ε^*	-1	-ε	$-\varepsilon^*$	(T_x, T_y)	
	1	ε^*	ε	-1	$-\varepsilon^*$	-ε		

$\varepsilon = \exp(2\pi i/3) = 1^{1/3}$ $\varepsilon^* = \exp(-2\pi i/3) = \exp(4\pi i/3) = 1^{2/3}$

Selection rules, forbidden vibrations

Infrared:

	A_g	E_g	A_u	E_u
A_g				
E_g				
A_u				
E_u				

(Missing information)

Raman:

	A_g	E_g	A_u	E_u
A_g				
E_g				
A_u				
E_u				

(Missing information)

S_6	147	S_6 - A	C_1 - G						

	S_6				Rotatory			
Wyckoff	A_g	E_g	A_u	E_u	A_g	E_g	A_u	E_u
1 A-B	0	0	1	1	1	1	0	0
2 C-D	1	1	1	1	1	1	1	1
3 E-F	0	0	3	3	3	3	0	0
6 G	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A_g	E_g	A_u	E_u
1 A-B	1	0	0	0
2 C-D	1	0	1	0
3 E-F	1	1	0	0
6 G	1	1	1	1

Symmetry elements: $3C_2$, C_3

D_3	I	$2C_3$	$3C_2$		
A_1	1	1	1		z^2, $x^2 + y^2$
A_2	1	1	-1	T_z, R_z	
E	2	-1	0	(T_x, T_y) (R_x, R_y)	($x^2 - y^2$, xy, xz, yz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E
A_1			
A_2			
E			

(Missing information)

Raman:

	A_1	A_2	E
A_1			
A_2			
E			

(Missing information)

D_3	149	D_3 - A	C_3 - G	C_2 - J	C_1 - L				

	D_3			Rotatory		
Wyckoff	A_1	A_2	E	A_1	A_2	E
1 A-F	0	1	1	0	1	1
2 G-I	1	1	2	1	1	2
3 J-K	1	2	3	1	2	3
6 L	3	3	6	3	3	6

	Vector		
Wyckoff	A_1	A_2	E
1 A-F	1	0	0
2 G-I	1	1	0
3 J-K	1	0	1
6 L	1	1	2

Symmetry elements: C_3, $3\sigma_v$

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

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E
A_1		x	
A_2	x	o	
E			

Raman:

	A_1	A_2	E
A_1		x	
A_2	x	o	
E			

C_{3v}	156	C_{3v} - A	C_s - D	C_1 - E					

	C_{3v}			Rotatory		
Wyckoff	A_1	A_2	E	A_1	A_2	E
1 A-C	1	0	1	0	1	1
3 D	2	1	3	1	2	3
6 E	3	3	6	3	3	6

	Vector		
Wyckoff	A_1	A_2	E
1 A-C	1	0	0
3 D	1	0	1
6 E	1	1	2

Symmetry elements: i, $3C_2$, C_3, S_6, $3\sigma_d$

$D_{3d} \equiv S_{6v}$	I	$2S_6(z)$	$2S_6^2$	S_6^3	$3C_2$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		$x^2 + y^2$, z^2
A_{1u}	1	-1	1	-1	1	-1		
A_{2g}	1	1	1	1	-1	-1	R_z	
A_{2u}	1	-1	1	-1	-1	1	T_z	
E_g	2	-1	-1	2	0	0	(R_x, R_y)	($x^2 - y^2$, xy)
E_u	2	1	-1	-2	0	0	(T_x, T_y)	(yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_1	A_2	A_2	E_g	E_u
A_1	n	x	x		x	
A_1	x	n		x		x
A_2	x		n	x	x	
A_2		x	x	e		x
E_g	x		x		n	
E_u		x		x		e

Raman:

	A_1	A_1	A_2	A_2	E_g	E_u
A_1		x	x	x		x
A_1	x	o	x	x	x	
A_2	x	x	o	x		x
A_2	x	x	x	o	x	
E_g		x		x		x
E_u	x		x		x	o

D_{3d}	162	D_{3d} - A	C_{3v} - E	C_2 - I	C_s - K	C_1 - L			

	D_{3d}						Rotatory					
Wyckoff	A_{1g}	A_{2g}	E_g	A_{1u}	A_{2u}	E_u	A_{1g}	A_{2g}	E_g	A_{1u}	A_{2u}	E_u
1 A-B	0	0	0	0	1	1	0	1	1	0	0	0
2 C-D	0	1	1	0	1	1	0	1	1	0	1	1
2 E	1	0	1	0	1	1	0	1	1	1	0	1
3 F-G	0	0	0	1	2	3	1	2	3	0	0	0
4 H	1	1	2	1	1	2	1	1	2	1	1	2
6 I-J	1	2	3	1	2	3	1	2	3	1	2	3
6 K	2	1	3	1	2	3	1	2	3	2	1	3
12 L	3	3	6	3	3	6	3	3	6	3	3	6

Cont.

	Vector					
Wyckoff	A_{1g}	A_{2g}	E_g	A_{1u}	A_{2u}	E_u
1 A-B	1	0	0	0	0	0
2 C-D	1	0	0	1	0	0
2 E	1	0	0	0	1	0
3 F-G	1	0	1	0	0	0
4 H	1	1	0	1	1	0
6 I-J	1	0	1	1	0	1
6 K	1	0	1	0	1	1
12 L	1	1	2	1	1	2

Symmetry elements: C_6

C_6	I	C_6^1	C_3^1	C_2	C_3^2	C_6^5		
A	1	1	1	1	1	1	T_z, R_z	z^2, $x^2 + y^2$
B	1	-1	1	-1	1	-1		
E_1	1	ε	$-\varepsilon^*$	-1	-ε	ε^*	(T_x, T_y) (R_x, $R_{y)}$	(xz, yz)
	1	ε^*	-ε	-1	$-\varepsilon^*$	ε		
E_2	1	$-\varepsilon^*$	-ε	1	$-\varepsilon^*$	-ε		(x^2 - y^2, xy)
	1	-ε	$-\varepsilon^*$	1	-ε	-ε		

$\varepsilon = \exp(2\pi i/6)$ $\varepsilon^* = \exp(-2\pi i/6)$

Selection rules, forbidden vibrations

Infrared:

	A	B	E_1	E_2
A				
B				
E_1				
E_2				

(Missing information)

Raman:

	A	B	E_1	E_2
A				
B				
E_1				
E_2				

(Missing information)

C_6	168	C_6 - A	C_1 - D						

	C_6				Rotatory			
Wyckoff	A	B	E_1	E_2	A	B	E_1	E_2
1 A	1	0	1	0	1	0	1	0
2 B	1	1	1	1	1	1	1	1
3 C	1	2	2	1	1	2	2	1
6 D	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A	B	E_1	E_2
1 A	1	0	0	0
2 B	1	1	0	0
3 C	1	0	0	1
6 D	1	1	1	1

Symmetry elements: C_3, σ_h

C_{3h}	I	C_3	σ_h	S_3		
A'	1	1	1	1	R_z	$x^2 + y^2, z^2$
A"	1	1	-1	-1	T_z	
E'	2	-1	2	-1	(T_x, T_y)	$(x^2 - y^2, xy)$
E"	2	-1	-2	1	(R_x, R_y)	(yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A'	A"	E'	E"
A'	n			x
A"		e	x	
E'		x		
E"	x			n

Raman:

	A'	A"	E'	E"
A'		x		
A"	x	o		
E'				
E"				

C_{3h}	174	C_{3h} - A	C_3 - G	C_s - J	C_1 - L				

	C_{3h}				Rotatory			
Wyckoff	A'	E'	A"	E"	A'	E'	A"	E"
1 A-F	0	1	1	0	1	0	0	1
2 G-I	1	1	1	1	1	1	1	1
3 J-K	2	2	1	1	1	1	2	2
6 L	3	3	3	3	3	3	3	3

	Vector			
Wyckoff	A'	E'	A"	E"
1 A-F	1	0	0	0
2 G-I	1	0	1	0
3 J-K	1	1	0	0
6 L	1	1	1	1

Symmetry elements: i, C_6, σ_h

C_{6h}	I	C_6^1	C_3^1	C_2	C_3^2	C_6^5	i	S_3^5	S_6^5	σ_h	S_6^1	S_3^1		
A_g	1	1	1	1	1	1	1	1	1	1	1	1	R_z	z^2, $x^2 + y^2$
B_g	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		
E_{1g}	1	ε	$-\varepsilon^*$	-1	-ε	ε^*	1	ε	$-\varepsilon^*$	-1	-ε	ε^*	(R_x, R_y)	(xz, yz)
	1	ε^*	-ε	-1	$-\varepsilon^*$	ε	1	ε^*	-ε	-1	$-\varepsilon^*$	ε		
E_{2g}	1	$-\varepsilon^*$	-ε	1	$-\varepsilon^*$	-ε	1	$-\varepsilon^*$	-ε	1	$-\varepsilon^*$	-ε		($x^2 - y^2$, xy)
	1	-ε	$-\varepsilon^*$	1	-ε	$-\varepsilon^*$	1	-ε	$-\varepsilon^*$	1	-ε	$-\varepsilon^*$		
A_u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	T_z	
B_u	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		
E_{1u}	1	ε	$-\varepsilon^*$	-1	-ε	ε^*	-1	-ε	ε^*	1	ε	$-\varepsilon^*$	(T_x, T_y)	
	1	ε^*	-ε	-1	$-\varepsilon^*$	ε	-1	$-\varepsilon^*$	ε	1	ε^*	-ε		
E_{2u}	1	$-\varepsilon^*$	-ε	1	$-\varepsilon^*$	-ε	-1	ε^*	ε	-1	ε^*	ε		
	1	-ε	$-\varepsilon^*$	1	-ε	$-\varepsilon^*$	-1	ε	ε^*	-1	ε	ε^*		

$\varepsilon = \exp(2\pi i/6)$ $\varepsilon^* = \exp(-2\pi i/6)$

Selection rules, forbidden vibrations

Infrared:

	A_g	B_g	E_{1g}	E_{2g}	A_u	B_u	E_{1u}	E_{2u}
A_g								
B_g								
E_{1g}								
E_{2g}								
A_u								
B_u								
E_{1u}								
E_{2u}								

(Missing information)

Raman:

	A_g	B_g	E_{1g}	E_{2g}	A_u	B_u	E_{1u}	E_{2u}
A_g								
B_g								
E_{1g}								
E_{2g}								
A_u								
B_u								
E_{1u}								
E_{2u}								

(Missing information)

Cont.

C_{6h}	175	C_{6h} - A	C_6 - E	C_s - J	C_1 - L				

	C_{6h}								Rotatory							
Wyckoff	A_g	B_g	E_{1g}	E_{2g}	A_u	B_u	E_{1u}	E_{2u}	A_g	B_g	E_{1g}	E_{2g}	A_u	B_u	E_{1u}	E_{2u}
1 A-B	0	0	0	0	1	0	1	0	1	0	1	0	0	0	0	0
2 C-D	0	1	0	1	1	0	1	0	1	0	1	0	0	1	0	1
2 E	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
3 F-G	0	0	0	0	1	2	2	1	1	2	2	1	0	0	0	0
4 H	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6 I	1	2	2	1	1	2	2	1	1	2	2	1	1	2	2	1
6 J-K	2	1	1	2	1	2	2	1	1	2	2	1	2	1	1	2
12 L	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3

	Vector							
Wyckoff	A_g	B_g	E_{1g}	E_{2g}	A_u	B_u	E_{1u}	E_{2u}
1 A-B	1	0	0	0	0	0	0	0
2 C-D	1	0	0	0	0	1	0	0
2 E	1	0	0	0	1	0	0	0
3 F-G	1	0	0	1	0	0	0	0
4 H	1	1	0	0	1	1	0	0
6 I	1	0	0	1	1	0	0	1
6 J-K	1	0	0	1	0	1	1	0
12 L	1	1	1	1	1	1	1	1

Symmetry elements: $6C_2$, C_6

D_6	I	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$		
A_1	1	1	1	1	1	1		z^2, $x^2 + y^2$
A_2	1	1	1	1	-1	-1	T_z, R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	(T_x, T_y) (R_x, R_y)	(xz, yz)
E_2	2	-1	-1	2	0	0		($x^2 - y^2$, xy)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E_1	E_2
A_1						
A_2						
B_1						
B_2						
E_1						
E_2						

(Missing information)

Raman:

	A_1	A_2	B_1	B_2	E_1	E_2
A_1						
A_2						
B_1						
B_2						
E_1						
E_2						

(Missing information)

D_6	177	D_6 - A	C_6 - E	$C_2(C_2')$ - J	$C_2(C_2'')$ - L	C_1 - N			

	D_6						Rotatory					
Wyckoff	A_1	A_2	B_1	B_2	E_1	E_2	A_1	A_2	B_1	B_2	E_1	E_2
1 A-B	0	1	0	0	1	0	0	1	0	0	1	0
2 C-D	0	1	1	0	1	1	0	1	1	0	1	1
2 E	1	1	0	0	2	0	1	1	0	0	2	0
3 F-G	0	1	1	1	2	1	0	1	1	1	2	1
4 H	1	1	1	1	2	2	1	1	1	1	2	2
6 I	1	1	2	2	4	2	1	1	2	2	4	2
6 J-K	1	2	1	2	3	3	1	2	1	2	3	3
6 L-M	1	2	2	1	3	3	1	2	2	1	3	3
12 N	3	3	3	3	6	6	3	3	3	3	6	6

Cont.

	Vector					
Wyckoff	A_1	A_2	B_1	B_2	E_1	E_2
1 A-B	1	0	0	0	0	0
2 C-D	1	0	0	1	0	0
2 E	1	1	0	0	0	0
3 F-G	1	0	0	0	0	1
4 H	1	1	1	1	0	0
6 I	1	1	0	0	0	2
6 J-K	1	0	1	0	1	1
6 L-M	1	0	0	1	1	1
12 N	1	1	1	1	2	2

Symmetry elements:

D_{6v}	I	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	T_z	z^2, $x^2 + y^2$
A_2	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	(T_x, T_y) (R_x, R_y)	(xz, yz)
E_2	2	-1	-1	2	0	0		(x^2 - y^2, xy)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E_1	E_2
A_1						
A_2						
B_1						
B_2						
E_1						
E_2						

(Missing information)

Raman:

	A_1	A_2	B_1	B_2	E_1	E_2
A_1						
A_2						
B_1						
B_2						
E_1						
E_2						

(Missing information)

C_{6v}	183	C_{6v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - F				

	D_{6v}						Rotatory					
Wyckoff	A_1	A_2	B_1	B_2	E_1	E_2	A_1	A_2	B_1	B_2	E_1	E_2
1 A	1	0	0	0	1	0	0	1	0	0	1	0
2 B	1	0	1	0	1	1	0	1	0	1	1	1
3 C	1	0	1	1	2	1	0	1	1	1	2	1
6 D	2	1	1	2	3	3	1	2	2	1	3	3
6 E	2	1	2	1	3	3	1	2	1	2	3	3
12 F	3	3	3	3	6	6	3	3	3	3	6	6

Cont.

	Vector					
Wyckoff	A_1	A_2	B_1	B_2	E_1	E_2
1 A	1	0	0	0	0	0
2 B	1	0	1	0	0	0
3 C	1	0	0	0	0	1
6 D	1	0	0	1	1	1
6 E	1	0	1	0	1	1
12 F	1	1	1	1	2	2

Symmetry elements: $3C_2$, C_3, $3\sigma_v$, σ_h

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

Selection rules, forbidden vibrations

Infrared:

	A_1'	A_1	A_2'	A_2	E'	E''
A_1'	n	x	x			x
A_1	x	n		x	x	
A_2'	x		n	x		x
A_2		x	x	e	x	
E'		x		x		
E''	x		x			n

Raman:

	A_1'	A_1	A_2'	A_2	E'	E''
A_1'		x	x	x		
A_1	x	o	x	x		
A_2'	x	x	o	x		
A_2	x	x	x	o		
E'						
E''						

D_{3h}	187	D_{3h} - A	C_{3v} - G	C_{2v} - J	$C_s(\sigma_h)$ - L	$C_s(\sigma_v)$ - N	C_1 - O		

	D_{3h}						Rotatory					
Wyckoff	A_1'	A_2'	E'	A_1''	A_2''	E''	A_1'	A_2'	E'	A_1''	A_2''	E''
1 A-F	0	0	1	0	1	0	0	1	0	0	0	1
2 G-I	1	0	1	0	1	1	0	1	1	1	0	1
3 J-K	1	1	2	0	1	1	0	1	1	1	1	2
6 L-M	2	2	4	1	1	2	1	1	2	2	2	4
6 N	2	1	3	1	2	3	1	2	3	2	1	3
12 O	3	3	6	3	3	6	3	3	6	3	3	6

Cont.

	Vector					
Wyckoff	A_1'	A_2'	E'	A_1''	A_2''	E''
1 A-F	1	0	0	0	0	0
2 G-I	1	0	0	0	1	0
3 J-K	1	0	1	0	0	0
6 L-M	1	1	2	0	0	0
6 N	1	0	1	0	1	1
12 O	1	1	2	1	1	2

Symmetry elements: i, $6C_2$, C_6, S_6, $6\sigma_v$, σ_h

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

Selection rules, forbidden vibrations

Infrared:

	A_{1g}	A_{1u}	A_{2g}	A_{2u}	B_{1g}	B_{1u}	B_{2g}	B_{2u}	E_{1g}	E_{1u}	E_{2g}	E_{2u}
A_{1g}	n		x		x	x	x	x	x	x	x	x
A_{1u}		n		x	x	x	x	x	x	x	x	x
A_{2g}	x		n	x	x	x	x	x	x	x	x	x
A_{2u}		x	x	e	x	x	x	x		x	x	x
B_{1g}	x	x	x	x	n	x			x	x	x	
B_{1u}	x	x	x	x	x	n	x	x	x	x		x
B_{2g}	x	x	x	x		x	n	x	x	x		
B_{2u}	x	x	x	x		x	x	n	x	x		
E_{1g}	x	x	x		x	x	x	x	n		x	
E_{1u}	x	x	x	x	x	x	x	x		e		x
E_{2g}	x	x	x	x	x				x		n	
E_{2u}	x	x	x	x		x				x		e

Raman:

	A_{1g}	A_{1u}	A_{2g}	A_{2u}	B_{1g}	B_{1u}	B_{2g}	B_{2u}	E_{1g}	E_{1u}	E_{2g}	E_{2u}
A_{1g}		x	x	x	x	x	x	x		x		x
A_{1u}	x	o	x	x	x	x	x	x	x		x	
A_{2g}	x	x	o	x	x	x	x	x		x		x
A_{2u}	x	x	x	o	x	x	x	x	x		x	
B_{1g}	x	x	x	x	o	x	x	x		x		x
B_{1u}	x	x	x	x	x	o	x	x	x		x	
B_{2g}	x	x	x	x	x	x	o	x		x		x
B_{2u}	x	x	x	x	x	x	x	o	x		x	
E_{1g}		x		x		x		x		x		
E_{1u}	x		x		x		x		x	o	x	x
E_{2g}		x		x		x		x		x		x
E_{2u}	x		x		x		x			x	x	o

Cont.

D_{6h}	191	D_{6h} - A	C_{6v} - E	$C_{2v}(C_2')$ - J	$C_{2v}(C_2'')$ - L	$C_s(\sigma_v)$ - N	$C_s(\sigma_d)$ - O	$C_s(\sigma_h)$ - P	C_1 - R

	D_{6h}												Rotatory											
Wyckoff	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
1 A-B	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	1	0	0	0	0	0	0	0
2 C-D	0	0	1	0	0	1	0	1	0	0	1	0	0	1	0	0	1	0	0	0	1	0	0	1
2 E	1	0	0	0	1	0	0	1	0	0	1	0	0	1	0	0	1	0	1	0	0	0	1	0
3 F-G	0	0	0	0	0	0	0	1	1	1	2	1	0	1	1	1	2	1	0	0	0	0	0	0
4 H	1	0	1	0	1	1	0	1	0	1	1	1	0	1	0	1	1	1	1	0	1	0	1	1
6 I	1	0	1	1	2	1	0	1	1	1	2	1	0	1	1	1	2	1	1	0	1	1	2	1
6 J-K	1	1	0	1	1	2	0	1	1	1	2	1	0	1	1	1	2	1	1	1	0	1	1	2
6 L-M	1	1	1	0	1	2	0	1	1	1	2	1	0	1	1	1	2	1	1	1	1	0	1	2
12 N	2	1	1	2	3	3	1	2	2	1	3	3	1	2	2	1	3	3	2	1	1	2	3	3
12 O	2	1	2	1	3	3	1	2	1	2	3	3	1	2	1	2	3	3	2	1	2	1	3	3
12 P-Q	2	2	1	1	2	4	1	1	2	2	4	2	1	1	2	2	4	2	2	2	1	1	2	4
24 R	3	3	3	3	6	6	3	3	3	3	6	6	3	3	3	3	6	6	3	3	3	3	6	6

	Vector											
Wyckoff	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
1 A-B	1	0	0	0	0	0	0	0	0	0	0	0
2 C-D	1	0	0	0	0	0	0	0	0	1	0	0
2 E	1	0	0	0	0	0	0	1	0	0	0	0
3 F-G	1	0	0	0	0	1	0	0	0	0	0	0
4 H	1	0	1	0	0	0	0	1	0	1	0	0
6 I	1	0	0	0	0	1	0	1	0	0	0	1
6 J-K	1	0	0	0	0	1	0	0	1	0	1	0
6 L-M	1	0	0	0	0	1	0	0	0	1	1	0
12 N	1	0	0	1	1	1	0	1	1	0	1	1
12 O	1	0	1	0	1	1	0	1	0	1	1	1
12 P-Q	1	1	0	0	0	2	0	0	1	1	2	0
24 R	1	1	1	1	2	2	1	1	1	1	2	2

Symmetry elements: $3C_2$, $4C_3$

T	I	$4C_3$	$4C_3^2$	$3C_2$		
A	1	1	1	1		$x^2 + y^2 + z^2$
E	1	ε	ε^*	1		$x^2 + y^2 - 2z^2$, $x^2 - y^2$
	1	ε^*	ε	1		
F	3	0	0	-1	(T_x, T_y, T_z) (R_x, R_y, R_z)	(xy, yz, xz)

$\varepsilon = \exp(2\pi i/3)$ $\varepsilon^* = \exp(-2\pi i/3)$

Selection rules, forbidden vibrations

Infrared:

	A	E	F
A			
E			
F			

(Missing information)

Raman:

	A	E	F
A			
E			
F			

(Missing information)

T	195	T - A	C_3 - E	C_2 - F	C_1 -J				

	T			Rotatory		
Wyckoff	A	E	F	A	E	F
1 A-B	0	0	1	0	0	1
3 C-D	0	0	3	0	0	3
4 E	1	1	3	1	1	3
6 F-I	1	1	5	1	1	5
12 J	3	3	9	3	3	9

	Vector		
Wyckoff	A	E	F
1 A-B	1	0	0
3 C-D	1	1	0
4 E	1	0	1
6 F-I	1	1	1
12 J	1	1	3

Symmetry elements: i, $3C_2$, $4C_3$, $4S_4$, $3\sigma_d$

T	I	$4C_3$	$4C_3^2$	$3C_2$	I	$4S_6$	$4S_6^5$	$3\sigma_h$		
A_g	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_u	1	1	1	1	-1	-1	-1	-1		
E_g	1	ε	ε*	1	1	ε	ε*	1		$(x^2 + y^2 - 2z^2, x^2 - y^2)$
	1	ε*	ε	1	1	ε*	ε	1		
E_u	1	ε	ε*	1	-1	−ε	−ε*	-1		
	1	ε*	ε	1	-1	−ε*	−ε	-1		
F_g	3	0	0	-1	1	0	0	-1	(R_x, R_y, R_z)	(xy, yz, xz)
F_u	3	0	0	-1	-1	0	0	1	(T_x, T_y, T_z)	

$\varepsilon = \exp(2\pi i/3)$ $\varepsilon = \exp(-2\pi i/3)$

Selection rules, forbidden vibrations

Infrared:

	A_g	A_u	E_g	E_u	F_g	F_u
A_g						
A_u						
E_g						
E_u						
F_g						
F_u						

(Missing information)

Raman:

	A_g	A_u	E_g	E_u	F_g	F_u
A_g						
A_u						
E_g						
E_u						
F_g						
F_u						

(Missing information)

T_h	200	T_h - A	C_3 - I	C_{2v} - E	C_s - J	C_1 -L			

	T_h						Rotatory					
Wyckoff	A_g	E_g	F_g	A_u	E_u	F_u	A_g	E_g	F_g	A_u	E_u	F_u
1 A-B	0	0	0	0	0	1	0	0	1	0	0	0
3 C-D	0	0	0	0	0	3	0	0	3	0	0	0
6 E-H	1	1	2	0	0	3	0	0	3	1	1	2
8 I	1	1	3	1	1	3	1	1	3	1	1	3
12 J-K	2	2	4	1	1	5	1	1	5	2	2	4
24 L	3	3	9	3	3	9	3	3	9	3	3	9

Cont.

	Vector					
Wyckoff	A_g	E_g	F_g	A_u	E_u	F_u
1 A-B	1	0	0	0	0	0
3 C-D	1	1	0	0	0	0
6 E-H	1	1	0	0	0	1
8 I	1	0	1	1	0	1
12 J-K	1	1	1	0	0	2
24 L	1	1	3	1	1	3

Symmetry elements: $6C_2$, $4C_3$, $3C_4$

O	I	$8C_3$	$3C_2$	$6C_4$	$6C_2'$		
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		$(x^2 + y^2 - 2z^2, x^2 - y^2)$
F_1	3	0	-1	1	-1	(R_x, R_y, R_z)	(T_x, T_y, T_z)
F_2	3	0	-1	-1	1		(xy, yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E	F_1	F_2
A_1					
A_2					
E					
F_1					
F_2					

(Missing information)

Raman:

	A_1	A_2	E	F_1	F_2
A_1					
A_2					
E					
F_1					
F_2					

(Missing information)

O	207	O - A	C_4 - E	C_3 - G	$C_2(C_2')$ - I	C_1 - K			

	O					Rotatory				
Wyckoff	A_1	A_2	E	F_1	F_2	A_1	A_2	E	F_1	F_2
1 A-B	0	0	0	1	0	0	0	0	1	0
3 C-D	0	0	0	2	1	0	0	0	2	1
6 E-F	1	0	1	3	2	1	0	1	3	2
8 G	1	1	2	3	3	1	1	2	3	3
12 H	1	1	2	5	5	1	1	2	5	5
12 I-J	1	2	3	5	4	1	2	3	5	4
24 K	3	3	6	9	9	3	3	6	9	9

Cont.

	Vector				
Wyckoff	A_1	A_2	E	F_1	F_2
1 A-B	1	0	0	0	0
3 C-D	1	0	1	0	0
6 E-F	1	0	1	1	0
8 G	1	1	0	1	1
12 H	1	1	2	1	1
12 I-J	1	0	1	1	2
24 K	1	1	2	3	3

Symmetry elements: $3C_2$, $4C_3$, $3S_4$

T_d	I	$8C_3$	$6\sigma_d$	$6S_4$	$3S_4^2$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	-1	-1	1		
E	2	-1	0	0	2		$(x^2 + y^2 - 2z^2, x^2 - y^2)$
F_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
F_2	3	0	1	-1	-1	(T_x, T_y, T_z)	(xy, yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E	F_1	F_2
A_1	n	x	x	x	
A_2	x	n	x		x
E	x	x	n		
F_1	x			n	
F_2		x			

Raman:

	A_1	A_2	E	F_1	F_2
A_1		x		x	
A_2	x	o			x
E					
F_1	x			n	
F_2		x			

T_d	215	T_d - A	C_{3v} - E	C_{2v} - F	C_s - I	C_1 - J			

	T_d					Rotatory				
Wyckoff	A_1	A_2	E	F_1	F_2	A_1	A_2	E	F_1	F_2
1 A-B	0	0	0	0	1	0	0	0	1	0
3 C-D	0	0	0	1	2	0	0	0	2	1
4 E	1	0	1	1	2	0	1	1	2	1
6 F-G	1	0	1	2	3	0	1	1	3	2
12 H	1	1	2	5	5	1	1	2	5	5
12 I	2	1	3	4	5	1	2	3	5	4
24 J	3	3	6	9	9	3	3	6	9	9

Cont.

	Vector				
Wyckoff	A_1	A_2	E	F_1	F_2
1 A-B	1	0	0	0	0
3 C-D	1	0	1	0	0
4 E	1	0	0	0	1
6 F-G	1	0	1	0	1
12 H	1	1	2	1	1
12 I	1	0	1	1	2
24 J	1	1	2	3	3

Symmetry elements: i, $6C_2$, $4C_3$, $3C_4$, $3S_4$, $4S_6$, $9\sigma_d$

O_h	I	$8C_3$	$6C_2$	$6C_4$	$3C_4^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(x^2 + y^2 - 2z^2, x^2 - y^2)$
E_u	2	-1	0	0	2	-2	0	1	-2	0		
F_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
F_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(T_x, T_y, T_z)	
F_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xy, yz, xz)
F_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

Selection rules, forbidden vibrations

Infrared:

	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_g	E_u	F_{1g}	F_{1u}	F_{2g}	F_{2u}
A_{1g}	n	x	x	x	x	x	x		x	x
A_{1u}	x	n	x	x	x	x		x	x	x
A_{2g}	x	x	n	x	x	x	x	x	x	
A_{2u}	x	x	x	n	x	x	x	x		x
E_g	x	x	x	x	n	x	x		x	
E_u	x	x	x	x	x	n		x		x
F_{1g}	x		x	x	x		n		x	
F_{1u}		x	x	x		x		n>1		x
F_{2g}	x	x	x		x		x		n	
F_{2u}	x	x		x		x		x		n

Raman:

	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_g	E_u	F_{1g}	F_{1u}	F_{2g}	F_{2u}
A_{1g}		x	x	x		x	x	x		x
A_{1u}	x	o	x	x	x		x	x	x	
A_{2g}	x	x	o	x		x		x	x	x
A_{2u}	x	x	x	o	x		x		x	x
E_g		x		x		x		x		x
E_u	x		x		x	n	x		x	
F_{1g}	x	x		x		x	1	x		x
F_{1u}	x	x	x		x		x	n	x	
F_{2g}		x	x	x		x		x		x
F_{2u}	x		x	x	x		x		x	n

Cont.

O_h	221	O_h - A	C_{4v} - E	C_{3v} - G	C_{2v} - I	$C_s(\sigma_h)$ - K	$C_s(\sigma_d)$ - M	C_1 - N	

	O_h									Rotatory									
Wyckoff	A_{1g}	A_{2g}	E_g	F_{1g}	F_{2g}	A_{1u}	A_{2u}	E_u	F_{1u}	F_{2u}	A_{1g}	A_{2g}	E_g	F_{1g}	F_{2g}	A_{1u}	A_{2u}	E_u	F_{1u}	F_{2u}
1 A-B	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0
3 C-D	0	0	0	0	0	0	0	0	2	1	0	0	0	2	1	0	0	0	0	0
6 E-F	1	0	1	1	1	0	0	0	2	1	0	0	0	2	1	1	0	1	1	1
8 G	1	0	1	1	2	0	1	1	2	1	0	1	1	2	1	1	0	1	1	2
12 H	1	1	2	2	2	0	0	0	3	3	0	0	0	3	3	1	1	2	2	2
12 I-J	1	1	2	2	2	0	1	1	3	2	0	1	1	3	2	1	1	2	2	2
24 K-L	2	2	4	4	4	1	1	2	5	5	1	1	2	5	5	2	2	4	4	4
24 M	2	1	3	4	5	1	2	3	5	4	1	2	3	5	4	2	1	3	4	5
48 N	3	3	6	9	9	3	3	6	9	9	3	3	6	9	9	3	3	6	9	9

	Vector									
Wyckoff	A_{1g}	A_{2g}	E_g	F_{1g}	F_{2g}	A_{1u}	A_{2u}	E_u	F_{1u}	F_{2u}
1 A-B	1	0	0	0	0	0	0	0	0	0
3 C-D	1	0	1	0	0	0	0	0	0	0
6 E-F	1	0	1	0	0	0	0	0	1	0
8 G	1	0	0	0	1	0	1	0	1	0
12 H	1	1	2	0	0	0	0	0	1	1
12 I-J	1	0	2	0	1	0	0	0	1	1
24 K-L	1	1	2	1	1	0	0	0	2	2
24 M	1	0	1	1	2	0	1	1	2	1
48 N	1	1	2	3	3	1	1	2	3	3

Symmetry elements: $4C_2$, C_4, S_8, $4\sigma_d$

D_{4d}	I	$2S_8(z)$	$2S_8^2$	$2S_8^3$	S_8^4	$4C_2$	$4\sigma_d$		
A_1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	1	-1		
B_2	1	-1	1	-1	1	-1	1	T_z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	(T_x, T_y)	
E_2	2	0	-2	0	2	0	0		$(x^2 - y^2, xy)$
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0	(R_x, R_y)	(yz, xz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E_1	E_2	E_3
A_1	1+e	x	x			x	x
A_2	x	1+e		x		x	x
B_1	x		1+e	x	x	x	
B_2		x	x	e	x	x	
E_1			x	x	e		
E_2	x	x	x	x		1	
E_3	x	x					1+e

Raman:

	A_1	A_2	B_1	B_2	E_1	E_2	E_3
A_1			x	x	x		
A_2		o	x	x	x		
B_1	x	x	o	x			x
B_2	x	x	x	o			x
E_1	x	x			o		
E_2							
E_3			x	x			

Symmetry elements: C_5

C_5	I	C_5^1	C_5^2	C_5^3	C_5^4		
A	1	1	1	1	1	T_z, R_z	$x^2 + y^2$, z^2
E_1	1	ε	ε^2	ε^{2*}	ε^*	(T_x, T_y) (R_x, R_y)	(xz, yz)
	1	ε^*	ε^{2*}	ε^2	ε		
E_2	1	ε^2	ε^*	ε	ε^{2*}		($x^2 - y^2$, xy)
	1	ε^{2*}	ε	ε^*	ε^2		

$\varepsilon = \exp(2\pi i/5) = 1^{1/5}$ $\varepsilon^* = \exp(-2\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A	E_1	E_2
A			
E_1			
E_2			

(Missing information)

Raman:

	A	E_1	E_2
A			
E_1			
E_2			

(Missing information)

Symmetry elements:

C_{5v}	I	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	T_z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	R_z	
E_1	2	a	b	0	(T_x, T_y) (R_x, R_y)	(xz, yz)
E_2	2	b	a	0		$(x^2 - y^2, xy)$

$a = 2 \cos 2\pi/5 = \exp(2\pi i/5) + \exp(-2\pi i/5)$ $b = 2 \cos 4\pi/5 = \exp(4\pi i/5) + \exp(-4\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E_1	E_2
A_1				
A_2				
E_1				
E_2				

(Missing information)

Raman:

	A_1	A_2	E_1	E_2
A_1				
A_2				
E_1				
E_2				

(Missing information)

Symmetry elements:

C_{5v}	I	C_5^1	C_5^2	C_5^3	C_5^4	σ_h	S_5^1	S_5^7	S_5^3	S_5^9		
A'	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_1'	1	ε	ε^2	ε^{2*}	ε^*	1	ε	ε^2	ε^{2*}	ε^*	(T_x, T_y)	
	1	ε^*	ε^{2*}	ε^*	ε	1	ε^*	ε^{2*}	ε^2	ε		
E_2'	1	ε^2	ε^*	ε	ε^{2*}	1	ε^2	ε^*	ε	ε^{2*}		($x^2 - y^2$, xy)
	1	ε^{2*}	ε	ε^*	ε^2	1	ε^{2*}	ε	ε^*	ε^2		
A"	1	1	1	1	1	-1	-1	-1	-1	-1	T_z	
E_1'	1	ε	ε^2	ε^{2*}	ε^*	-1	$-\varepsilon$	$-\varepsilon^2$	$-\varepsilon^{2*}$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)
	1	ε^*	ε^{2*}	ε^2	ε	-1	$-\varepsilon^*$	$-\varepsilon^{2*}$	$-\varepsilon^2$	$-\varepsilon$		
E_2"	1	ε^2	ε^*	ε	ε^{2*}	-1	$-\varepsilon^2$	$-\varepsilon^*$	$-\varepsilon$	$-\varepsilon^{2*}$		
	1	ε^{2*}	ε	ε^*	ε^2	-1	$-\varepsilon^{2*}$	$-\varepsilon$	$-\varepsilon^*$	$-\varepsilon^2$		

$\varepsilon = \exp(2\pi i/5) = -1^{1/5}$ $\varepsilon^* = \exp(-2\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A'	E_1'	E_2'	A"	E_1"	E_2"
A'						
E_1'						
E_2'						
A"						
E_1"						
E_2"						

(Missing information)

Raman:

	A'	E_1'	E_2'	A"	E_1"	E_2"
A'						
E_1'						
E_2'						
A"						
E_1"						
E_2"						

(Missing information)

Symmetry elements:

D_5	I	$2C_5$	$2C_5^2$	$5C_2$		
A_1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	-1	T_z, R_z	
E_1	2	a	b	0	(T_x, T_y) (R_x, R_y)	(xz, yz)
E_2	2	b	a	0		$(x^2 - y^2, xy)$

$a = 2 \cos 2\pi/5 = \exp(2\pi i/5) + \exp(-2\pi i/5)$ $b = 2 \cos 4\pi/5 = \exp(4\pi i/5) + \exp(-4\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	E_1	E_2
A_1				
A_2				
E_1				
E_2				

(Missing information)

Raman:

	A_1	A_2	E_1	E_2
A_1				
A_2				
E_1				
E_2				

(Missing information)

Symmetry elements:

D_{5d}	I	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	1	1	1	-1	R_z	
E_{1g}	2	a	b	0	2	a	b	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	b	a	0	2	b	a	0		$(x^2 - y^2, xy)$
A_{1u}	1	1	1	1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	1	T_z	
E_{1u}	2	a	b	0	-2	-a	-b	0	(T_x, T_y)	
E_{2u}	2	b	a	0	-2	-b	-a	0		

$a = 2 \cos 2\pi/5 = \exp(2\pi i/5) + \exp(-2\pi i/5)$ $b = 2 \cos 4\pi/5 = \exp(4\pi i/5) + \exp(-4\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A_{1g}	A_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	E_{1u}	E_{2u}
A_{1g}								
A_{2g}								
E_{1g}								
E_{2g}								
A_{1u}								
A_{2u}								
E_{1u}								
E_{2u}								

(Missing information)

Raman:

	A_{1g}	A_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	E_{1u}	E_{2u}
A_{1g}								
A_{2g}								
E_{1g}								
E_{2g}								
A_{1u}								
A_{2u}								
E_{1u}								
E_{2u}								

(Missing information)

Symmetry elements: $5C_2$, C_5, $5\sigma_v$, σ_h

D_{5h}	I	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
A_1'	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	1	-1	1	1	1	-1	R_z	
E_1'	2	a	b	0	2	a	b	0	(T_x, T_y)	
E_2'	2	b	a	0	2	b	a	0		$(x^2 - y^2, xy)$
A_1''	1	1	1	1	-1	-1	-1	-1		
A_2''	1	1	1	-1	-1	-1	-1	1	T_z	
E_1''	2	a	b	0	-2	-a	-b	0	(R_x, R_y)	(xz, yz)
E_2''	2	b	a	0	-2	-b	-a	0		

$a = 2 \cos 2\pi/5 = \exp(2\pi i/5) + \exp(-2\pi i/5)$ $b = 2 \cos 4\pi/5 = \exp(4\pi i/5) + \exp(-4\pi i/5)$

Selection rules, forbidden vibrations

Infrared:

	A_1'	A_2'	E_1'	E_2'	A_1''	A_2''	E_1''	E_2''
A_1'								
A_2'								
E_1'								
E_2'								
A_1''								
A_2''								
E_1''								
E_2''								

(Missing information)

Raman:

	A_1'	A_2'	E_1'	E_2'	A_1''	A_2''	E_1''	E_2''
A_1'								
A_2'								
E_1'								
E_2'								
A_1''								
A_2''								
E_1''								
E_2''								

(Missing information)

Symmetry elements:

D_{6d}	I	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2S_{12}^5$	C_2	$6C_2'$	$6\sigma_d$		
A_1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1	1	1	-1		
B_2	1	-1	1	-1	1	-1	1	-1	1	T_z	
E_1	2	$\sqrt{3}$	1	0	-1	$-\sqrt{3}$	-2	0	0	(T_x, T_y)	
E_2	2	1	-1	-2	-1	1	2	0	0		$(x^2 - y^2, xy)$
E_3	2	0	-2	0	2	0	-2	0	0		
E_4	2	-1	-1	2	-1	-1	2	0	0		
E_5	2	$-\sqrt{3}$	1	0	-1	$\sqrt{3}$	-2	0	0	(R_x, R_y)	(xz, yz)

Selection rules, forbidden vibrations

Infrared:

	A_1	A_2	B_1	B_2	E_1	E_2	E_3	E_4	E_5
A_1									
A_2									
B_1									
B_2									
E_1									
E_2									
E_3									
E_4									
E_5									

(Missing information)

Raman:

	A_1	A_2	B_1	B_2	E_1	E_2	E_3	E_4	E_5
A_1									
A_2									
B_1									
B_2									
E_1									
E_2									
E_3									
E_4									
E_5									

(Missing information)

Symmetry elements:

S_8	I	S_8^1	C_4	S_8^3	C_2	S_8^5	C_4^3	S_8^7		
A	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1	1	-1	1	-1	T_z	
E_1	1	ε	i	$-\varepsilon^*$	-1	-ε	-i	ε^*	(T_x, T_y) (R_x, R_y)	
	1	ε^*	-i	-ε	-1	$-\varepsilon^*$	i	ε		
E_2	1	i	-1	-i	1	i	-1	-i		$(x^2 - y^2, xy)$
	1	-i	-1	i	1	-i	-1	i		
E_3	1	$-\varepsilon^*$	-i	ε	-1	ε^*	i	-ε		(xz, yz)
	1	-ε	i	ε^*	-1	ε	-i	$-\varepsilon^*$		

$\varepsilon = \exp(2\pi i/8)$ $\varepsilon^* = \exp(-2\pi i/8)$ $i = \exp(4\pi i/8)$

Selection rules, forbidden vibrations

Infrared:

	A	B	E_1	E_2	E_3
A					
B					
E_1					
E_2					
E_3					

(Missing information)

Raman:

	A	B	E_1	E_2	E_3
A					
B					
E_1					
E_2					
E_3					

(Missing information)

Symmetry elements: C_∞, $\infty\sigma_v$

$C_{\infty v}$	I	$2C_\infty^{\varphi}$	$2C_\infty^{2\varphi}$	$2C_\infty^{3\varphi}$	...	$\infty\sigma_v$		
$A_1 = \Sigma^+$	1	1	1	1	...	1	T_z	$x^2 + y^2, z^2$
$A_2 = \Sigma^-$	1	1	1	1	...	-1	R_z	
$E_1 = \Pi$	2	2 cos φ	2 cos 2φ	2 cos 3φ	...	0	(T_x, T_y) (R_x, R_y)	$(x^2 - y^2, xy, xz, yz)$
$E_2 = \Delta$	2	2 cos 2φ	2 cos 2×2φ	2 cos 3×2φ	...	0		
$E_3 = \Phi$	2	2 cos 3φ	2 cos 2×3φ	2 cos 3×3φ	...	0		
...	...	...	...	...	...	...		

Selection rules, forbidden vibrations

Infrared:

Σ^-, Δ, Φ, ...

Raman:

Σ^-, Φ, ...

Symmetry elements: C_∞, $\infty\sigma_v$, σ_h

$C_{\infty v}$	I	$2C_\infty^\varphi$	$2C_\infty^{2\varphi}$	$2C_\infty^{3\varphi}$	...	σ_h	∞C_2	$\infty\sigma_v$	$2S_\infty^\varphi$	$2S_\infty^{2\varphi}$	...	S_2		
$A_{1g} = \Sigma_g^+$	1	1	1	1	...	1	1	1	1	1	...	1		$x^2 + y^2, z^2$
$A_{1u} = \Sigma_u^+$	1	1	1	1	...	-1	-1	1	-1	-1	...	-1	T_z	
$A_{2g} = \Sigma_g^-$	1	1	1	1	...	1	-1	-1	1	1	...	1	R_z	
$A_{2u} = \Sigma_u^-$	1	1	1	1	...	-1	1	-1	-1	-1	...	-1		
$E_{1g} = \Pi_g$	2	a	b	c	...	-2	0	0	-a	-b	...	2	(R_x, R_y)	(xz, yz)
$E_{1u} = \Pi_u$	2	a	b	c	...	2	0	0	a	b	...	-2	(T_x, T_y)	
$E_{2g} = \Delta_g$	2	b	d	e	...	2	0	0	b	d	...	2		$(x^2 - y^2, xy, xz, yz)$
$E_{2u} = \Delta_u$	2	b	d	e	...	-2	0	0	-b	-d	...	-2		
$E_{3g} = \Phi_g$	2	c	e	f	...	-2	0	0	-c	-d	...	2		
$E_{3u} = \Phi_u$	2	c	e	f	...	2	0	0	c	d	...	-2		
...	...	...	...	...	...	...	...	...	...	...	...	...		

a = 2 cos φ b = 2 cos 2φ c = 2 cos 3φ d = 2 cos 4φ e = 2 cos 6φ f = 2 cos 9φ

Selection rules, forbidden vibrations

Infrared:

$\Sigma_g^+, \Sigma_g^-, \Sigma_u^-, \Pi_g, \Delta_g, \Delta_u, \Phi_g, \Phi_u$

Raman:

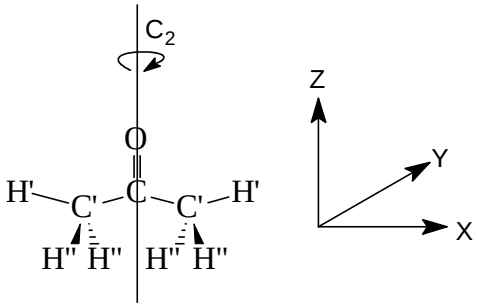
$\Sigma_u^+, \Sigma_g^-, \Sigma_u^-, \Pi_u, \Delta_u, \Phi_g, \Phi_u$

How to make an Adams - Newton analysis

1. Select the highest possible symmetry of the molecule and determine the point group by the scheme on page 3 and the space group by the table on page 4. Put the molecule in a right-hand cartesian coordinate system, with the highest rotation axis paralell to the z-axis.
2. Determine the total number of vibrations (3n - 6, 3n - 5 for linear molecules) in the molecule.
3. Determine and fill in the number and type of equivalent (with regard to symmetry) atoms.
4. Fill in the corresponding Wyckoff sites as taken from the table on page 4.
5. Look up the corresponding point group in the tables. From the Adams - Newton table No. 1 (3rd table on the page, following the selection rules) fill in the symmetry species and the number of vibrations. See the example below. The values for the degenerate groups are written as is and represents the observed number of vibrations, but are multiplied by 2 (for E) and by 3 (for F) to get the total degree of freedom.
6. Sum up the columns, subtract the rotational and translational vibrations (as taken from the character table). The total number of remaining vibrations should equal the total number of vibrations calculated under point 1.
7. Determine the number of infrared and Raman active modes by applying the selection rules (taken from the character table and/or the selection rules tables).

Example: *Acetone*

Molecule:	*Acetone*
Point group:	C_{2v}
Space group:	*25*
Total number of vibrations:	*3 × 10 - 6 = 24*



Equivalent coordinates	Wyckoff sites	A_1	A_2	B_1	B_2	Comments
O	*1A*	*1*	*0*	*1*	*1*	O on the C_2 axis → Wyckoff site A
C	*1A*	*1*	*0*	*1*	*1*	C on the C_2 axis → Wyckoff site A
2C'	*2E*	*2*	*1*	*2*	*1*	2 equivalent C' on the xz mirror plane → Wyckoff site E
2H'	*2E*	*2*	*1*	*2*	*1*	2 equivalent H' on the xz mirror plane → Wyckoff site E
4H"	*4I*	*3*	*3*	*3*	*3*	4 equivalent H" in unique positions → Wyckoff site I
- Rotational freedom		-	*1*	*1*	*1*	R_x, R_y and R_z in the character table
- Translational freedom		*1*	-	*1*	*1*	T_x, T_y and T_z in the character table
Γ_{total} = *24*		*8*	*4*	*7*	*5*	Total number of vibrations
IR active modes, Σ = *20*		*8*	-	*7*	*5*	A_2 is not infrared active, see the selection rules
Raman active modes, Σ = *24*		*8*	*4*	*7*	*5*	No forbidden vibrations, see the selection rules

Species containing x^2, y^2 and/or z^2 are Raman active and polarized.
Species containing other combinations of x, y and z are Raman active and depolarized.
Species containing the translations (T_x, T_y and T_z) are IR active.

Adams - Newton analysis

Molecule:
Point group:
Space group:
Total number of vibrations:

Equivalent coordinates	Wyckoff sites												
- Rotational freedom													
- Translational freedom													
Γ_{total}													
IR active modes, Σ =													
Raman active modes, Σ =													