Vibration
Spectroscopy

— Tables for Factor Group and
Point Group Analysis

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Introduction

Table I and Table II can be used for the application of point group analysis for molecules with any listed in Table I (32 point groups). The Table I is based on crystallographic **Wyckoff sites** of atoms in the molecule.

For the missing 23 point groups we have constructed character tables with special **Valli-Mink (VM)** sites which are listed in Table Ia.

Table II contains of the characters for 32 point group based on Wyckoff sites of the atoms in the molecule. In Table IIa we gave the characters of additional 23 molecular point groups not included in Table II.

The **32 crystallographic point groups** which can be treated by Adams-Newton method.

C_1 (1, P1), C_S (6, Pm), $C_i \equiv S_2$ (2, P$\bar{1}$), C_2 (3, P2), C_3 (143, P3), C_4 (75, P4), C_6 (168, P6), D_2 (16, P222), D_3 (149, P312), D_4 (89, P422), D_6 (177, P622), C_{2v} (25, Pmm2), C_{3v} (156, P3m1), C_{4v} (99, P4mm), C_{6v} (183, P6mm), C_{2h} (10, P2/m), C_{4h} (83, P4/m), C_{6h} (175, P6/m), D_{2h} (47, Pmmm), D_{3h} (187, P$\bar{6}$m2), D_{4h} (123, P4/mmm), D_{6h} (191, P6/mmm), D_{2d} (111, P$\bar{4}$2m), D_{3d} (162, P$\bar{3}$1m), S_4 (81, P$\bar{4}$), S_6 (147, P$\bar{3}$), T (195, P23), T_d (215, P$\bar{4}$3m), T_h (200, Pm3), O (207, P432) and O_h (221, Pm3m) which had been summarized by M. Valli in 1995.

In the **first part** of the Tables the above 32 "crystallographic" point groups are presented.

The missing **23 molecular point groups** are: D_{4d}, C_5, D_5, C_{5v}, C_{5h}, D_{5h}, D_{5d}, D_{6d}, C_7, D_7, C_{7v}, C_{7h}, D_{7h}, D_{7d}, C_8, D_8, C_{8v}, C_{8h}, D_{8h}, D_8, S_8, $C_{\infty v}$ and $D_{\infty h}$.

The missing very unique and special point groups, the icosahedral I, I_h, and spherical SU_2 and R_3 are not included in this treatments.

In the **second part** above point groups are discussed.

FIRST PART

Determination of Point Group

Molecule

Linear? Y / N

D∞h ← Y — i ? — N → C∞v

Two or more Cₙ(n>2)? Y / N

i ? Y / N

Iₕ ← Y — C₅ ? — N → Oₕ

T_d

‡ Y

Cₙ ? Y

Dₙₕ ← Y — σₕ?

N

Dₙd ← Y — nσ_d? — N → Dₙ

Cₛ ← Y — σ ? — N

Cᵢ ← Y — i ? — N → C₁

Cₙₕ ← Y — σₕ? — N

Cₙᵥ ← Y — nσᵥ? — N

S₂ₙ ← Y — S₂ₙ? — N → Cₙ

‡ Select Cₙ with highest n.
Then, is nC₂ perpendicular to Cₙ?
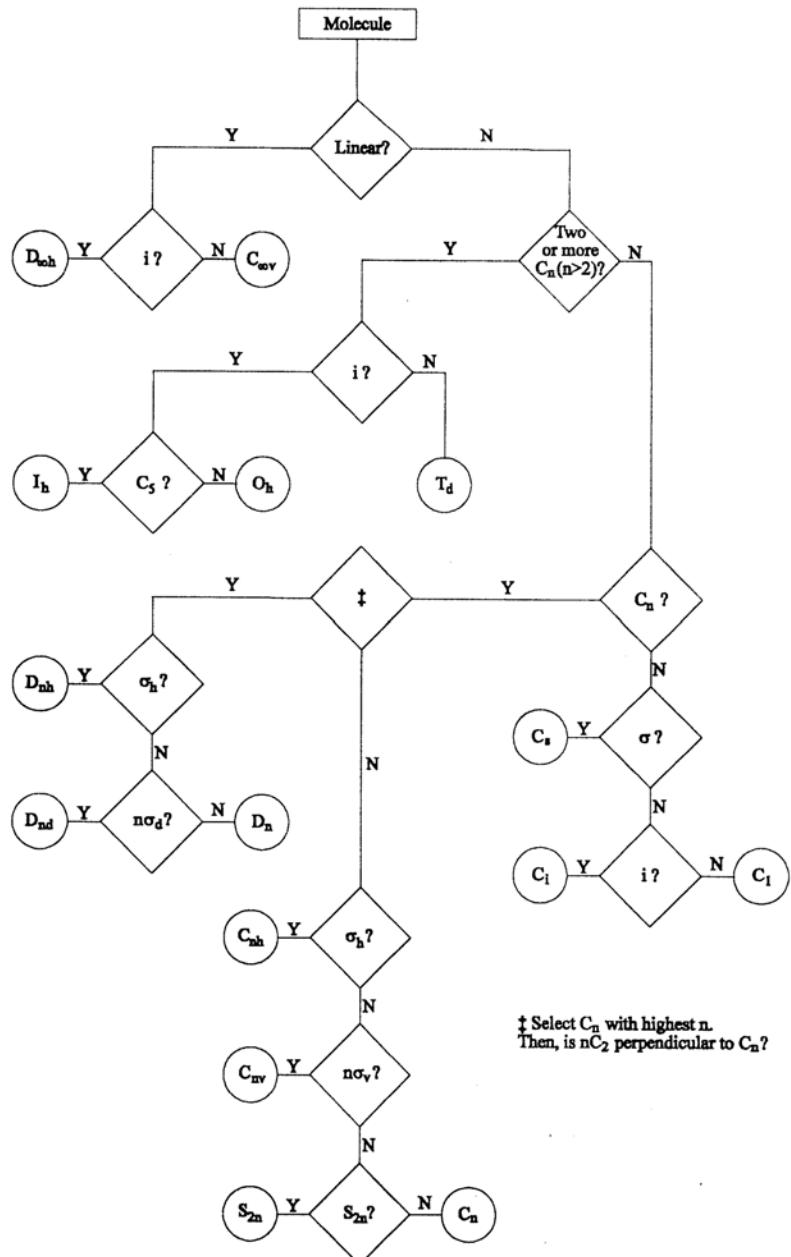
Table I

Point group	Space group	Allowed sites and their Wyckoff notation							
C_1	1	C_1 - A							
C_i	2	C_i - A	C_1 - I						
C_2	3	C_2 - A	C_1 - E						
C_s	6	C_s - A	C_1 - C						
C_{2h}	10	C_{2h} - A	C_2 - I	C_s - M	C_1 - O				
D_2	16	D_2 - A	$C_2(x)$ - I	$C_2(y)$ - M	$C_2(z)$ - Q	C_1 - U			
C_{2v}	25	C_{2v} - A	$C_s(zx)$ - E	$C_s(yz)$ - G	C_1 - I				
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 - ∞
C_4	75	C_4 - A	C_1 - D						
S_4	81	S_4 - A	C_1 - H						
C_{4h}	83	C_{4h} - A	C_4 - G	C_s - J	C_1 - L				
D_4	89	D_4 - A	C_4 - G	$C_2(C_2'')$ - J	$C_2(C_2')$ - L	C_1 - P			
C_{4v}	99	C_{4v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - G				
D_{2d}	111	D_{2d} - A	C_{2v} - G	$C_2(C_2')$ - I	C_s - N	C_1 - O			
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
C_3	143	C_3 - A	C_1 - D						
S_6	147	S_6 - A	C_1 - G						
D_3	149	D_3 - A	C_3 - G	C_2 - J	C_1 - L				
C_{3v}	156	C_{3v} - A	C_s - D	C_1 - E					
D_{3d}	162	D_{3d} - A	C_{3v} - E	C_2 - I	C_s - K	C_1 - L			
C_6	168	C_6 - A	C_1 - D						
C_{3h}	174	C_{3h} - A	C_3 - G	C_s - J	C_1 - L				
C_{6h}	175	C_{6h} - A	C_6 - E	C_s - J	C_1 - L				
D_6	177	D_6 - A	C_6 - E	$C_2(C_2')$ - J	$C_2(C_2'')$ - L	C_1 - N			
C_{6v}	183	C_{6v} - A	$C_s(\sigma_d)$ - D	$C_s(\sigma_v)$ - E	C_1 - F				
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_{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
T	195	T - A	C_3 - E	C_2 - F	C_1 - J				
T_h	200	T_h - A	C_3 - I	C_{2v} - E	C_s - J	C_1 - L			
O	207	O - A	C_4 - E	C_3 - G	$C_2(C_2')$ - I	C_1 - K			
T_d	215	T_d - A	C_{3v} - E	C_{2v} - F	C_s - I	C_1 - J			
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	

TABLE II

C_1 1 C_1

Symmetry elements: I

C_1	I
A	1

Selection rules, forbidden vibrations

Infrared:

	A
A	

(None)

Raman:

	A
A	

(None)
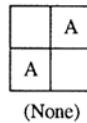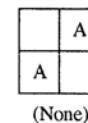
	C_1	Rotatory
	A	A
Wyckoff		
1A	3	3

	Vector
	A
Wyckoff	
1A	1

Symmetry elements: I, 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)

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

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

Symmetry elements: I, $C_2(z)$

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		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: I, $\sigma(xy)$

C_s	I	$\sigma(xy)$		
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)

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

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

Symmetry elements: I, $C_2(z)$, $\sigma_h(xy)$, 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

Wyckoff	C_{2h}				Rotatory			
	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

Wyckoff	Vector			
	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: $I, C_2(z), C_2(y), C_2(x)$

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)

Wyckoff	D_2				Rotatory			
	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

Wyckoff	Vector			
	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: I, $C_2(z)$, $\sigma_v(xz)$, $\sigma_v(yz)$

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)

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

Wyckoff	Vector			
	A	B_1	B_2	B_3
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, σ(xy), σ(xz), σ(yz), i, C_2(z), C_2(y), C_2(x)

$D_{2h} = V_h$	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.

Wyckhoff	D$_{2h}$								Rotatory							
	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

Wyckoff	Vector							
	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: I, C_4^1, C_2, C_4^3

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		

$$i = -1^{\frac{1}{2}}$$

Selection rules, forbidden vibrations

Infrared:

	A	B	E
A			
B			
E			

(Missing information)

Raman:

	A	B	E
A			
B			
E			

(Missing information)

	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: I, $S_4{}^1$, C_2, $S_4{}^3$

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			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_4^1, C_2, C_4^3, i, S_4^3, σ_h, S_4^1

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		

$i = -1^{\frac{1}{2}}$

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)

Wyckhoff	C_{4h}						Rotatory					
	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.

Wyckoff	Vector					
	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: I, $2C_4$, C_2, $2C_2'$, $2C_2''$

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)

Wyckoff	D_4					Rotatory				
	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.

Wyckoff	Vector				
	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: I, $2C_4(z)$, C_2, $2\sigma_v$, $2\sigma_d$

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					

Wyckoff	C_{4v}					Rotatory				
	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

Cont.

Wyckoff	Vector				
	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: I, $2S_4(z)$, $S_4^2 \equiv C_2''$, $2C_2$, $2\sigma_d$

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					

Wyckoff	D_{2d}					Rotatory				
	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.

Wyckoff	Vector				
	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, $2C_4(z)$, C_2'', $2C_2$, $2C_2'$, σ_h, $2\sigma_v$, $2\sigma_d$, i

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.

Wyckoff	D$_{4h}$										Rotatory									
	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

Wyckoff	Vector									
	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

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Symmetry elements: $I, C_3{}^1, C_3{}^2$

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)

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

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

Symmetry elements: I, $C_3{}^1$, $C_3{}^2$, i, $S_6{}^5$, $S_6{}^1$

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	$-\varepsilon$	$-\varepsilon^*$	T_x, T_y	
	1	ε^*	ε	-1	$-\varepsilon^*$	$-\varepsilon$		

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

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				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: I, $2C_3$, $3C_2$

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)

Wyckoff	D_3			Rotatory		
	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

Wyckoff	Vector		
	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: I, $C_3(z)$, $3\sigma_v$

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			

Wyckoff	C_{3v}			Rotatory		
	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

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

Symmetry elements: I, $2S_6(z)$, $2S_6^2 \equiv 2C_3$, $S_6^3 \equiv S_2 \equiv i$, $3C_2$, $3\sigma_d$

$D_{3d} \equiv S_{6v}$	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_{1g}	A_{1u}	A_{2g}	A_{2u}	E_g	E_u
A_{1g}	n	x	x		x	
A_{1u}	x	n		x		x
A_{2g}	x		n	x	x	
A_{2u}		x	x	e		x
E_g	x		x		n	
E_u		x		x		e

Raman:

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

	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.

Wyckoff	Vector					
	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: I, C_6^1, C_3^1, C_2, C_3^2, C_6^5

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	$-\varepsilon$	ε^*	T_x, T_y, R_x, R_y	xz, yz
	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε		
E_2	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		$x^2 - y^2, xy$
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon$		

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

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)

Wyckoff	C_6				Rotatory			
	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

Wyckoff	Vector			
	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: I, C_3, σ_h, S_3

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}				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_6^1, 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

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	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	-1	$-\varepsilon$	ε^*	R_x, R_y	xz, yz
	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε		
E_{2g}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		x^2-y^2, xy
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$		
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	$-\varepsilon$	ε^*	-1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	T_x, T_y	
	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε	-1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$		
E_{2u}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	-1	ε^*	ε	-1	ε^*	ε		
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	-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.

Symmetry elements: 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

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	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	-1	$-\varepsilon$	ε^*	R_x, R_y	xz, yz
	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε		
E_{2g}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		$x^2 - y^2$, xy
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$		
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	$-\varepsilon$	ε^*	-1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	T_x, T_y	
	1	ε^*	$-\varepsilon$	-1	$-\varepsilon^*$	ε	-1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$		
E_{2u}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	-1	ε^*	ε	-1	ε^*	ε		
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	-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.

Symmetry elements: I, $2C_6$, $2C_3$, C_2, $3C_2'$, $3C_2''$

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)

Wyckoff	D_6						Rotatory					
	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.

Wyckoff	Vector					
	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: I, $2C_6$, $2C_3$, C_2, $3\sigma_v$, $3\sigma_d$

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)

Wyckoff	D_{6v}						Rotatory					
	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.

Wyckoff	Vector					
	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: I, $2C_3(z)$, $3C_2$, σ_h, $2S_3$, $3\sigma_v$

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''						

Wyckoff	D_{6v}						Rotatory					
	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.

Wyckoff	Vector					
	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, $2C_6(z)$, $2C_6^2 \equiv 2C_3$, $C_6^3 \equiv C_2''$, $3C_2$, $3C_2'$, σ_h, $3\sigma_v$, $3\sigma_d$, $2S_6$, $2S_3$, $S_6^3 \equiv S_2 \equiv i$

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	x	o

Cont.

Wyckoff	D_{6h}												Rotatory											
	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

Wyckoff	Vector											
	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: I, $4C_3$, $4C_3^2$, $3C_2$

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

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

Selection rules, forbidden vibrations

Infrared:

	A	E	F
A			
E			
F			

(Missing information)

Raman:

	A	E	F
A			
E			
F			

(Missing information)

	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,

T			
A_g			$x^2 + y^2 + z^2$
A_u			
E_g			$x^2 + y^2 - 2z^2,\ x^2 - y^2$
E_u			
F_g		R_x, R_y, R_z	xy, yz, xz
F_u		T_x, T_y, T_z	

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)

Wyckoff	T_h						Rotatory					
	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.

Wyckoff	Vector					
	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: I, 8C$_3$, 3C$_2$, 6C$_4$, 6C$_2$'

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)

Wyckoff	O					Rotatory				
	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.

Wyckoff	Vector				
	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: $I, 8C_3, 6\sigma_d, 6S_4, 3S_4^2 \equiv 3C_2$

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			1	
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			1	
F_2		x			

Wyckoff	T_d					Rotatory				
	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.

Wyckoff	Vector				
	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, $8C_3$, $6C_2$, $6C_4$, $3C_4^2$, i, $6S_4$, $8S_6$, $3\sigma_h$, $6\sigma_d$

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		

<div align="center">Selection rules, forbidden vibrations</div>

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>		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

<div align="center">*Cont.*</div>

Wyckoff	O_h										Rotatory									
	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

Wyckoff	Vector									
	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

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	symmetric and antisymmetric with respect to a center of symmetry
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
prime and double prime (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

Adams - Newton table 1

Adams - Newton table 3

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, $\Sigma =$														
Raman active modes, $\Sigma =$														

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 2 and the space group by the table on page 3.

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 regards to symmetry) atoms.

4. Fill in the corresponding Wyckoff sites as taken from the table on page 3.

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.

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 the selection rules tables).

Example: *Acetone*

Molecule:	Acetone
Point group:	C_{2v}
Space group:	25
Total number of vibrations:	$3 \times 10 - 6 = 24$
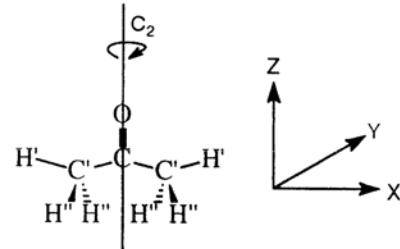
Equivalent coordinates	Wyckoff sites	A_1	A_2	B_1	B_2	Comments
O	A	1	0	1	1	O on the C_2 axis => Wyckoff site A
C	A	1	0	1	1	C on the C_2 axis => Wyckoff site A
2C'	E	2	1	2	1	2 equivalent C' on the xz mirror plane => Wyckoff site E
2H'	E	2	1	2	1	2 equivalent H' on the xz mirror plane => Wyckoff site E
4H"	I	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
$\Gamma_{total} = 24$		8	4	7	5	Total number of vibrations
IR active modes, $\Sigma = 20$		8	-	7	5	A_2 is not infrared active, see the selection rules
Raman active modes, $\Sigma = 24$		8	4	7	5	No forbidden vibrations, see the selection rules

SECOND PART

Character tables for chemically important point groups

Nonaxial groups: $C_1{}^a$ C_s C_i
(*Binary groups*)

C$_n$ groups: C_2 C_3 C_4 *$C_5{}^b$* C_6 *C_7*   *C_8*
(*Cyclic groups*)

D$_n$ groups: D_2 D_3 D_4 *D_5* D_6 *D_7*   *D_8*
(*Dihedral groups*)

C$_{nv}$ groups: C_{2v} C_{3v} C_{4v} *C_{5v}* C_{6v} *C_{7v}*   *C_{8v}*
(*Cnical groups*)

C$_{nh}$ groups C_{2h} C_{3h} C_{4h} *C_{5h}* C_{6h} *C_{7h}*   *C_{8h}*

D$_{nh}$ group: D_{2h} D_{3h} *D_{4h}*   *D_{5h}* D_{6h} *D_{7h}*   *D_{8h}*
(*Prismatic groups*)

D$_{nd}$ groups: D_{2d} D_{3d} D_{4d} *D_{5d}*   *D_{6d}*   *D_{7d}*   *D_{8d}*
(*Antiprizmatic groups*)

S$_n$ groups: S_4 S_6 *S_8*
(*Rotation-Reflection groups*)

Cubic groups: T T_h T_d O O_h
(*Terahedral/Cubic groups*)

Linear groups: *$C_{\infty V}$* *$D_{\infty V}$*
(*Cylindrical groups*)

Icosahedral groups^c: *I*   *Ih*

Spherical groups: *SU_2*   *R_3*

----

a 32 molecular point groups existing among 230 crystallographic space groups and can be obtained in Adams-Newton tables (recently black color).

b 23 point groups marked in red (and italics letters) are not existing in crystal structures. Their so called VM sites and characters were developed by the authors.

c The very rare and unique icosahedral and spherical groups are not discussed (marked in blue and not bold letters)

Table Ia

Point group	Sugg. space group	Allowed sites and their suggested VM notations							
D_{4d}	A1	D_{4d}-A	C_{2v}-B	C'_2-C	C_s-D	C_1-E			
C_5	A2	C_5-A	C_1-B	C_1-C	C_1-D	C_1-E			
C_{5v}	A3	C_{5v}-A	$C_s(\sigma_V)$-B	C_1-C	C_1-D	C_1-E			
C_{5h}	A4	C_{5h}-A	C_5-B	$C_s(\sigma_V)$-C	C_1-D				
D_5	A5	D_5-A	C_5-B	C_2-C	C_1-D	C_1-E	C_1-F		
D_{5h}	A6	D_{5h}-A	C_5-B	$C_{2v}(C_2)$-C	$C_s(\sigma_h)$-D	$C_s(\sigma_v)$-E	C_1-F		
D_{5d}	A7	D_{5d}-A	C_5-B	$C_{2v}(C_2)$-C	$C_s(\sigma_d)$-D	C_1-E			
D_{6d}	A8	D_{6d}-A	C_6-B	C''_2-C	$C_s(\sigma_d)$-D	C_1-E			
S_8	A9	S_8-A	C_1-B	C_1-C					
C_7	A10	C_7-A	C_1-B	C_1-C	C_1-D	C_1-E			
C_{7v}	A11[a]								
C_{7h}	A12								
D_7	A13								
D_{7h}	A14	D_{7h}-A	C_7-B	$C_{2v}(C_2)$-C	$C_s(\sigma_h)$-D	$C_s(\sigma_v)$-E	C_1-F		
D_{7d}	A15[a]								
C_8	A16								
C_{8v}	A17								
C_{8h}	A18								
D_8	A19								
D_{8h}	A20	D_{8h}-A	C_{8v}-B	$C_{2v}(C''_2)$-C	$C_{2v}(C'_2)$-D	$C_s(\sigma_h)$-E	$C_s(\sigma_d)$-F	$C_s(\sigma_v)$-G	C_1-H
D_{8d}	A21								
$C_{\infty v}$	A22	C_∞-2A[b]	C_∞-3A	C_∞-4A	C_∞-5A	C_∞-6A	C_∞-7A	C_∞-8A	C_∞-9A
			σ_v-3B	σ_v-4B	σ_v-5B	σ_v-6B	σ_v-7B	σ_v-8B	σ_v-9B
			C_∞-3[a]	C_∞-4A	C_∞-5A	C_∞-6A	C_∞-7A	C_∞-8A	C_∞-9A
$D_{\infty h}$	A23	C_∞-2A[b]	σ_v-3B	σ_v-4B	σ_v-5B	σ_v-6B	σ_v-7B	σ_v-8B	σ_v-9B

[a] The missing point group are under developments; [b] The letter **A** refers to sites of C_∞ axis and letter **B** to the sites of σ_v planes. The **B** sites are used for determination of species of linear bending modes. The figures near **A** and **B** represent the number of atoms in the linear molecule (e,g. for acetylene it is 4).

For illustration the characters of D4h point group discussed in PART I is shown below.

D₄ₕ   123   D₄ₕ
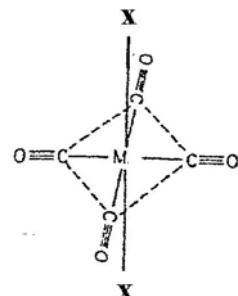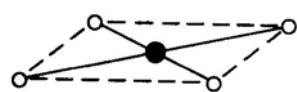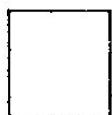
Regular square   Square planar structure   *trans*-substituted octahedron

Typical complexes: MX_4^{2-} (M=Pd, Pt, X=Cl, Br, I); AuX_4^- (X=Cl, Br, I), XeF_4, ClF_4^-, BrF_4^-, IF_4^- ; $M(CN)_4^{2-}$ (Ni, Pd, Pt), $Au(CN)_4^-$; $Pt(CN)_4X_2$ (X=Cl, Br, I); *trans*-$M(CO)_4L_2$ (M= Cr, Mo, W, L= PPh_3).

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.

Wyckoff	D$_{4h}$										Rotatory									
	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

Wyckoff	Vector									
	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

D_{4d} A1 D_{4d}
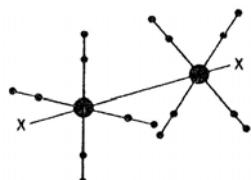
Staggered squares   **$Fe_2(CO)_8I_2$**   **IF_8^-**   **$Mn_2(CO)_{10}$**
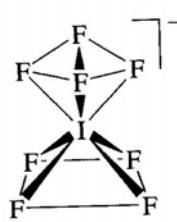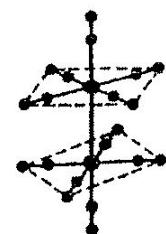
Other molecules with D_{4d} symmetry: CrO_8^{3-}, TeF_8^{2-}

Symmetry elements: I, $2S_8(z)$, $2S_8^2 = 2C_4$, $2S_8^3$, $2S_8^4 = C_2''$, $4C_2$, $4\sigma_d$

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			

D_{4d}

VM Sites	A_1	A_2	B_1	B_2	E_1	E_2	E_3
1A	0	0	0	1	1	0	0
2B	1	0	0	1	2	0	0
8C	1	2	1	2	3	3	3
8D	2	1	1	2	3	3	3
16E	3	3	3	3	6	6	6

Vector (D_{4d})

VM Sites	A_1	A_2	B_1	B_2	E_1	E_2	E_3
1A	1	0	0	0	0	0	0
2B	1	0	0	1	0	0	0
8C	1	0	1	0	1	1	1
8D	1	0	0	1	1	1	1
16E	1	1	1	1	2	2	2
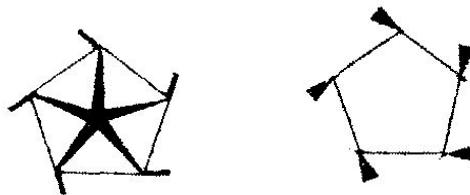
Non planar structures (e.g. $C_5(OH)_5$)

Symmetry elements: $I, C_5{}^1, C_5{}^2, C_5{}^3, C_5{}^4$

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)

C5

VM Sites	A_1	E_1	E_2
1A	1	1	0
5B	3	3	3
10C	6	6	6
15D	9	9	9

Vector (C5)

VM Sites	A_1	E_1	E_2
1A	1	0	0
5B	1	1	1
10C	2	2	2
15D	3	3	3

C_{5v} A3 C_{5v}
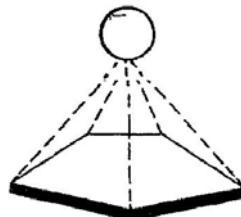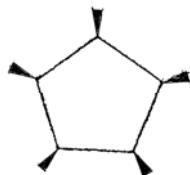
Non planar structures   **Cp-metal complexes**

Symmetry elements: $I, C_5^1, C_5^2, C_5^3, C_5^4$

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)

C_{5v}

VM Sites	A_1	A_2	E_1	E_2
1A	1	0	1	0
5B	2	1	3	3
10C	4	2	6	6
15D	5	4	9	9
20E	7	5	12	12

Vector (C_{5v})

VM Sites	A_1	A_2	E_1	E_2
1A	1	0	0	0
5B	1	0	1	1
10C	1	1	2	2
15D	2	1	3	3
20E	2	2	4	4
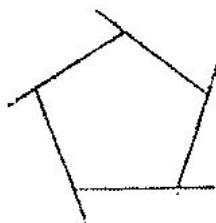
Planar structure (e.g. planar $C_5(OH)_5$)

Symmetry elements: 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

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)

C$_{5h}$

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	E$_3$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''	E$_3$''
1A	0	1	0	1	0	0	0	0	0	0
2B	1	0	0	1	0	0	1	1	0	0
7C	1	0	2	2	2	1	1	1	1	1
14D	2	1	4	4	4	2	1	2	2	2
14E	2	1	3	3	3	1	2	3	3	3
28F	3	3	6	6	6	3	3	6	6	6

Vector (C$_{5h}$)

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	E$_3$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''	E$_3$''
1A	1	0	0	0	0	0	0	0	0	0
2B	1	0	0	0	0	0	1	0	0	0
7C	1	0	1	1	1	0	0	0	0	0
14D	1	0	2	2	0	1	0	2	0	0
14E	1	0	1	1	1	0	1	1	1	1
28F	1	1	2	2	2	1	1	2	2	2

$$\mathbf{D_5} \qquad \mathbf{A5} \qquad \mathbf{D_5}$$
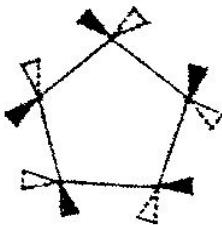
Model structure

Symmetry elements: I, $2C_5$, $2C_5^2$, $5C_2$

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)

D$_5$

VM Sites	A$_1$	A$_2$	E$_1$	E$_2$
1A	0	1	1	0
2B	1	1	2	0
5C	1	2	3	3
10D	3	3	6	6
15E	4	5	9	9
20F	5	7	12	12

Vector (D$_5$)

VM Sites	A$_1$	A$_2$	E$_1$	E$_2$
1A	1	0	0	0
2B	1	1	0	0
5C	1	0	1	1
10D	1	1	2	2
15E	2	1	3	3
20F	3	1	4	4
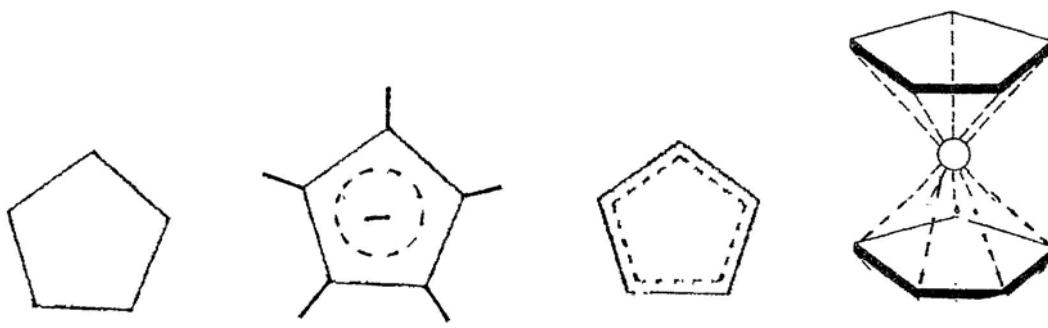
Regular pentagon   **Cp^- anion**   **Eclipsed sandwich**   **Rutenocene**

Otrher molecules with D_{5h} symmetry: I F_7, ReF_7, P_5^-, $UO_2F_5^{3-}$

Symmetry elements: I, $2C_5$, $2C_5^2$, $5C_2$, σ_h, $2S_5$, $2S_5^3$, $5\sigma_v$

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)

D$_{5h}$

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''
1A	0	0	1	0	0	1	0	0
2B	1	0	1	0	0	1	1	0
5C	1	0	2	0	1	1	1	0
10D	2	1	4	4	2	1	2	2
10E	2	1	3	3	1	2	3	3
20F	3	3	6	6	3	3	6	6

Vector (D$_{5h}$)

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''
1A	1	0	0	0	0	0	0	0
2B	1	0	0	0	0	1	0	0
5C	1	0	1	1	0	0	0	0
10D	1	0	2	2	1	0	0	0
10E	1	0	1	1	0	1	1	1
20F	1	1	2	2	1	1	2	2
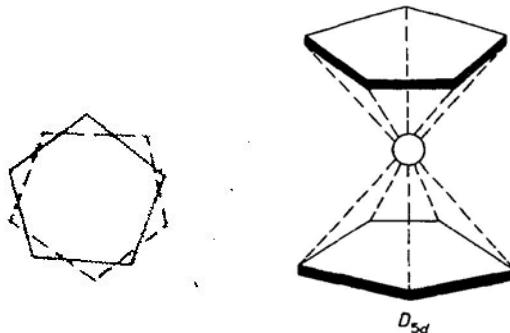
Staggered sandwich   Ferrocene type sandwich complexes

Symmetry elements: I, $2C_5$, $2C_5^z$, $5C_2$, i, $2S_{10}^5$, $2S_{10}$, $5\sigma_d$

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)

D$_{5d}$

VM Sites	A$_{1g}$	A$_{2g}$	E$_{1g}$	E$_{2g}$	A$_{1u}$	A$_{2u}$	E$_{1u}$	E$_{2u}$
1A	0	0	0	0	0	1	1	0
2B	1	0	1	0	0	1	1	0
10C	1	2	3	3	1	1	3	3
10D	2	1	3	3	1	2	3	3
20E	3	3	6	6	3	3	6	6

Vector (D$_{5d}$)

VM Sites	A$_{1g}$	A$_{2g}$	E$_{1g}$	E$_{2g}$	A$_{1u}$	A$_{2u}$	E$_{1u}$	E$_{2u}$
1A	1	0	0	0	0	0	0	0
2B	1	0	0	0	0	1	0	0
10C	1	0	1	1	1	0	1	1
10D	1	0	1	1	0	1	1	1
20E	1	1	2	2	1	1	2	2
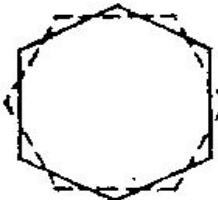
Staggered di-benzene sandwich

Symmetry elements: I, $2S_{12}$, $2C_6$, $2S_4$, $2C_3$, $2S_{12}^3$, C_2, $6C_2'$, $6\sigma_d$

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)

D$_{6d}$

VM Sites	A$_1$	A$_2$	B$_1$	B$_2$	E$_1$	E$_2$	E$_3$	E$_4$	E$_5$
1A	0	0	0	1	1	0	0	0	0
2B	1	0	0	1	2	0	0	0	0
6C	1	0	0	1	2	1	2	1	2
12D	1	2	1	2	3	3	3	3	3
12E	2	1	1	2	3	3	3	3	3
24F	3	3	3	3	6	6	6	6	6

Vector (D$_{6d}$)

VM Sites	A$_1$	A$_2$	B$_1$	B$_2$	E$_1$	E$_2$	E$_3$	E$_4$	E$_5$
1A	1	0	0	0	0	0	0	0	0
2B	1	0	0	1	0	0	0	0	0
6C	3	0	0	3	0	0	0	0	0
12D	1	0	1	0	1	1	1	1	1
12E	1	0	0	1	1	1	1	1	1
24F	1	1	1	1	2	2	2	2	2

S_8 A9 S_8
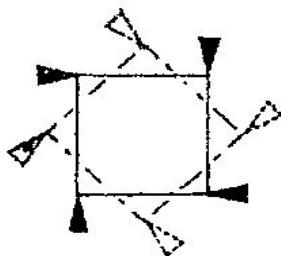
Model structure

Symmetry elements: I, S_8^1, C_4, S_8^3, C_2, S_8^5, C_4^3, S_8^7

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	$-\varepsilon$	$-i$	ε^*	T_x, T_y, R_x, R_y	
	1	ε^*	$-i$	$-\varepsilon$	-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	$-\varepsilon$		xz, yz
	1	$-\varepsilon$	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)

S$_8$

VM Sites	A	B	E$_1$	E2	E3
1A	0	1	1	0	0
4B	1	1	2	2	1
8C	3	3	3	3	3

Vector (S$_8$)

VM Sites	A	B	E$_1$	E2	E3
1A	1	0	0	0	0
4B	1	1	1	0	0
8C	1	1	1	1	1
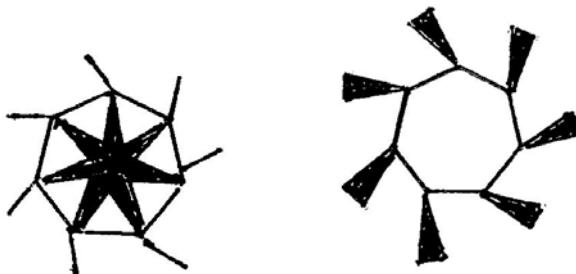
Non planar model structures

Symmetry elements: I, C_7, C_7^2, C_7^3, C_7^4, C_7^5, C_7^6

C_7	E	C_7	C_7^2	C_7^3	C_7^4	C_7^5	C_7^6		
A	1	1	1	1	1	1	1	T_z, R_z	$x^2 + y^2, z^2$
E_1	1	ε	ε^2	ε^3	ε^{*3}	ε^{*2}	ε^*	$T(x, y)$	(xz, yz)
	1	ε^*	ε^{*2}	ε^{*3}	ε^3	ε^2	ε	(R_x, R_y)	
E_2	1	ε^2	ε^{*3}	ε^*	ε	ε^3	ε^{*2}		$(x^2 - y^2, xy$
	1	ε^{*2}	ε^3	ε	ε^*	ε^{*3}	ε^2		
E_3	1	ε^3	ε^*	ε^2	ε^{*2}	ε	ε^{*3}		
	1	ε^{*3}	ε	ε^{*2}	ε^2	ε^*	ε^3		

$$\varepsilon = \exp(2\pi i/7) = 1/7 \qquad \varepsilon^* = \exp(-2\pi i/7)$$

Selection rules, forbidden vibrations

Infrared:

	A	E_1	E_2	E_3
A				
E_1				
E_2				
E_3				

(Missing information)

Raman:

	A	E_1	E_2	E_3
A				
E_1				
E_2				
E_3				

(Missing information)

C_7

VM Sites	A_1	E_1	E2	E3
1A	1	1	0	0
7B	3	3	3	3
14C	6	6	6	6
21D	9	9	9	9
28E	12	12	12	12

Vectors (C_7)

VM Sites	A_1	E_1	E2	E3
1A	1	0	0	0
7B	1	1	1	1
14C	2	2	2	2
21D	3	3	3	3
28E	4	4	4	4
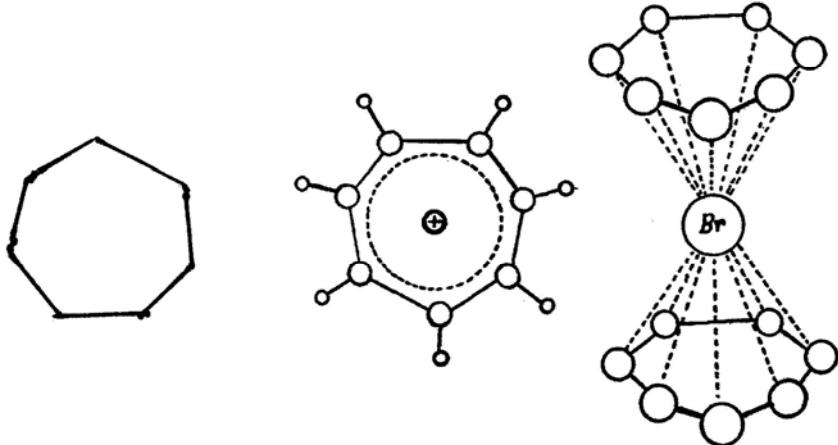
Regular heptagon   Tropylium ion, C$_7$H$_7^+$ Sandwich complex

Symmetry elements: I, 2C$_7$, 2C$_7^2$, 7C$_2$', σ_h, 2S$_7$, 2S$_7^3$, 2S$_7^5$, 7σ_v

D$_{7h}$	E	2C$_7$	2(C$_7$)^2	2(C$_7$)^3	7C'$_2$	σ_h	2S$_7$	2(S$_7$)^5	2(S$_7$)^3	7σ_v		
A'$_1$	+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	-1	R$_z$	-
E'$_1$	+2	+2cos(2π/7)	+2cos(4π/7)	+2cos(6π/7)	0	+2	+2cos(2π/7)	+2cos(4π/7)	+2cos(6π/7)	0	(x, y)	-
E'$_2$	+2	+2cos(4π/7)	+2cos(6π/7)	+2cos(2π/7)	0	+2	+2cos(4π/7)	+2cos(6π/7)	+2cos(2π/7)	0	-	(x^2-y^2, xy)
E'$_3$	+2	+2cos(6π/7)	+2cos(2π/7)	+2cos(4π/7)	0	+2	+2cos(6π/7)	+2cos(2π/7)	+2cos(4π/7)	0	-	-
A''$_1$	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-
A''$_2$	+1	+1	+1	+1	-1	-1	-1	-1	-1	+1	T$_z$	-
E''$_1$	+2	+2cos(2π/7)	+2cos(4π/7)	+2cos(6π/7)	0	-2	-2cos(2π/7)	-2cos(4π/7)	-2cos(6π/7)	0	(R$_x$, R$_y$)	(xz, yz)
E''$_2$	+2	+2cos(4π/7)	+2cos(6π/7)	+2cos(2π/7)	0	-2	-2cos(4π/7)	-2cos(6π/7)	-2cos(2π/7)	0	-	-
E''$_3$	+2	+2cos(6π/7)	+2cos(2π/7)	+2cos(4π/7)	0	-2	-2cos(6π/7)	-2cos(2π/7)	-2cos(4π/7)	0	-	-

Selection rules, forbidden vibrations

D$_{7h}$

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	E$_3$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''	E$_3$''
1A	0	0	0	1	0	0	1	0	0	0
2B	1	0	0	1	0	0	1	1	0	0
7C	1	0	2	2	2	1	1	1	1	1
14D	2	1	4	4	4	2	1	2	2	2
14E	2	1	3	3	3	1	2	3	3	3
28F	3	3	6	6	6	3	3	6	6	6

Vector (D$_{7h}$)

VM Sites	A$_1$'	A$_1$''	E$_1$'	E$_2$'	E$_3$'	A$_2$'	A$_2$''	E$_1$''	E$_2$''	E$_3$''
1A	1	0	0	0	0	0	0	0	0	0
2B	1	0	0	0	0	0	1	0	0	0
7C	1	0	1	1	1	0	0	0	0	0
14D	1	0	2	2	0	1	0	2	0	0
14E	1	0	1	1	1	0	1	1	1	1
28F	1	1	2	2	2	1	1	2	2	2

Regular octagon   **$C_8H_8^{2-}$ dianion**   **Eclipsed sandwich**   **Sandwich complex**

Complexes with D_{8h} symmetry: $(C_8H_8)_2Th$, $(C_8H_8)_2Pa$, $(C_8H_8)_2U$, $(C_8H_8)_2Np$, $(C_8H_8)_2Pu$
All are octahapto, η^8-C_8H_8 complexes.

Symmetry elements: I, $2C_8$, $2(C_8)^3$, $2C_4$, $C_2(z)$, $4C_2'$, $4C_2''$, i, $2(S_8)^3$, $2S_8$, $2S_4$, σ_h, $4\sigma_v$, $4\sigma_d$

D_{8h}	I	$2C_8$	$2(C_8)^3$	$2C_4$	$C_2(z)$	$4C_2'$	$4C_2''$	i	$2(S_8)^3$	$2S_8$	$2S_4$	σ_h	$4\sigma_v$	$4\sigma_d$		
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2
A_{2g}	+1	+1	+1	+1	+1	-1	-1	+1	+1	+1	+1	+1	-1	-1	R_z	-
B_{1g}	+1	-1	-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	-1	+1	-	-
E_{1g}	+2	$+(2)^{1/2}$	$-(2)^{1/2}$	0	-2	0	0	+2	$+(2)^{1/2}$	$-(2)^{1/2}$	0	-2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	+2	0	0	-2	+2	0	0	+2	0	0	-2	+2	0	0	-	(x^2-y^2, xy)
E_{3g}	+2	$-(2)^{1/2}$	$+(2)^{1/2}$	0	-2	0	0	+2	$-(2)^{1/2}$	$+(2)^{1/2}$	0	-2	0	0	-	-
A_{1u}	+1	+1	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-1	-1	-	-
A_{2u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-1	-1	+1	+1	T_z	-
B_{1u}	+1	-1	-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	+1	-1	-	-
E_{1u}	+2	$+(2)^{1/2}$	$-(2)^{1/2}$	0	-2	0	0	-2	$-(2)^{1/2}$	$+(2)^{1/2}$	0	+2	0	0	T_{xy}	-
E_{2u}	+2	0	0	-2	+2	0	0	-2	0	0	+2	-2	0	0		-
E_{3u}	+2	$-(2)^{1/2}$	$+(2)^{1/2}$	0	-2	0	0	-2	$+(2)^{1/2}$	$-(2)^{1/2}$	0	+2	0	0	-	-

Selection rules, forbidden vibrations

Infrared: **Raman:**

D$_{8h}$

VM Sites	A$_{1g}$	A$_{2g}$	B$_{1g}$	B$_{2g}$	E$_{1g}$	E$_{2g}$	E$_{3g}$	A$_{1u}$	A$_{2u}$	B$_{1u}$	B$_{2u}$	E$_{1u}$	E$_{2u}$	E$_{3u}$
1A	0	0	0	0	0	0	0	0	1	0	0	1	0	0
2B	1	0	0	0	1	0	0	0	1	0	0	1	0	0
8C	1	1	1	1	1	2	1	0	1	1	0	2	1	2
8D	1	1	1	1	1	2	1	0	1	0	1	2	1	2
16E	2	2	2	2	2	4	2	1	1	1	1	4	2	4
16F	2	1	1	2	3	3	3	1	2	2	1	3	3	3
16G	2	1	2	1	3	3	3	1	2	1	2	3	3	3
32H	3	3	3	3	6	6	6	3	3	3	3	6	6	6

Vectors (D$_{8h}$)

VM Sites	A$_{1g}$	A$_{2g}$	B$_{1g}$	B$_{2g}$	E$_{1g}$	E$_{2g}$	E$_{3g}$	A$_{1u}$	A$_{2u}$	B$_{1u}$	B$_{2u}$	E$_{1u}$	E$_{2u}$	E$_{3u}$
1A	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2B	1	0	0	0	0	0	0	0	1	0	0	0	0	0
8C	1	0	0	1	1	0	0	0	0	0	0	1	1	0
8D	1	0	1	0	1	0	0	0	0	0	0	1	1	0
16E	1	1	1	1	0	1	1	0	0	0	0	2	1	1
16F	1	0	0	1	1	1	1	0	1	1	0	1	1	1
16G	1	0	1	0	1	1	1	0	1	0	1	1	1	1
32H	1	1	1	1	2	2	2	1	1	1	1	2	6	6

Types of linear molecules with $C_{\infty v}$ symmetry: CO, OCS, HCN, HCNO, Cl-C≡C-H, H-C≡C-C≡N, X-C≡C- C≡C –CN (X=H, Cl,Br, I), H-C≡C- C≡C- C≡C –CN (cyano triacetylene) etc.

Symmetry elements: I, $2C_\infty{}^\varphi$, $2C_\infty{}^{2\varphi}$, $2C_\infty{}^{3\varphi}$,…, $\infty\sigma_v$

$C_{\infty v}$	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	$2\cos\varphi$	$2\cos 2\varphi$	$2\cos 3\varphi$	...	0	T_x, T_y, R_x, R_y	xz, yz
$E_2 = \Delta$	2	$2\cos 2\varphi$	$2\cos 2\times2\varphi$	$2\cos 3\times2\varphi$	...	0		x^2-y^2, xy
$E_3 = \Phi$	2	$2\cos 3\varphi$	$2\cos 2\times3\varphi$	$2\cos 3\times3\varphi$	...	0		
...	...	...	...	...	...	...		

$C_{\infty v}$

VM Sites (A) N^0 of atoms	A_1 (Σ^+)	E_1 (Π)	E_2 (Δ)
1A	0	0	0
2A	1	0	0
3A	2	1	0
4A	3	2	0
5A	4	3	0
6A	5	4	0
7A	6	5	0
8A	7	6	0
9A	8	7	0
…	…	...	…

Vectors (C∞v) for stretching modes

VM Sites (A)	A_1
N^0 of atoms	(Σ^+)
Stretchings	
2A	1
3A	2
4A	3
5A	4
6A	5
7A	6
8A	7
9A	8
...	...

Vectors (C∞v) for linear bending modes

Linear bendings		
VM Sites (B)	E_1	E_2
N^0 of atoms	(Π)	(Δ)
3B	1	0
4B	2	0
5B	3	0
6B	4	0
7B	5	0
8B	6	0
9B	7	0
...	...	...

Types of linear molecules with $D_{\infty h}$ symmetry: H_2, O_2, HF_2^-, CO_2, NCCN, H-C≡C-H, H-B=N-H, H-N=C=C=N-H, N≡C-C≡C-C≡N, H-C≡C- C≡C –H (diacetylene), H-C≡C- C≡C-C≡C –C-H (triacetylene), O=C=C=C=C=C=O (carbon oxide) etc.

Symmetry elements: I, $2C_\infty^\varphi$, $2C_\infty^{2\varphi}$, $2C_\infty^{3\varphi}$,…, $\infty\sigma_h$, ∞C_2 , $\infty\sigma_v$, $2S_\infty^\varphi$, $2S_\infty^{2\varphi}$, … , $S2 \equiv i$

$D_{\infty h}$	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
$E_{2u} = \Delta_u$	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∞h

VM Sites (A) N^0 of atoms	A_{1g} (Σ_g^+)	A_{1u} (Σ_u^+)	E_{1g} (Π_g)	E_{2g} (Δ_g)	E_{1u} (Π_u)
1A	0	0	0	0	0
2A	1	0	0	0	0
3A	1	1	0	0	1
4A	2	1	1	0	1
5A	2	2	1	0	2
6A	3	2	2	0	2
7A	3	3	3	0	3
8A	4	3	3	0	3
9A	4	4	3	0	4
...	...	...	...	...	...

Vectors (D∞h) for stretching modes

VM Sites (A) N^0 of atoms	Stretching modes	
	A_{1g} (Σ_g^+)	A_{1u} (Σ_u^+)
2A	1	0
3A	1	1
4A	2	1
5A	2	2
6A	3	2
7A	3	3
8A	4	3
9A	4	4
...	...	...

Vectors ($D_{\infty h}$) for linear bending modes

VM Sites (B) N^0 of atoms	Linear bending modes		
	E_{1g} (Π_g)	E_{2g} (Δ_g)	E_{1u} (Π_u)
3B	0	0	1
4B	1	0	1
5B	1	0	2
6B	2	0	2
7B	2	0	3
8B	3	0	3
9B	3	0	4
...	...	...	...