

1.30: Appendix B- Point Groups

Non axial groups

$$\begin{array}{c|c} C_1 & E \\ \hline A_1 & 1 \end{array} \quad (1.30.1)$$

$$\begin{array}{c|c|c|c} C_s & E & \sigma_h & \\ \hline A & 1 & 1 & x, y, R_z \\ A' & 1 & -1 & z, R_x, R_y \end{array} \quad \begin{array}{c} x^2, y^2, z^2, xy \\ yz, xz \end{array} \quad (1.30.2)$$

$$\begin{array}{c|c|c|c} C_i & E & i & \\ \hline A_g & 1 & 1 & R_x, R_y, R_z \\ A_u & 1 & -1 & x, y, z \end{array} \quad \begin{array}{c} x^2, y^2, z^2, xy, xz, yz \\ x, y, z \end{array} \quad (1.30.3)$$

C_n groups

$$\begin{array}{c|c|c|c} C_2 & E & C_2 & \\ \hline A & 1 & 1 & z, R_z \\ B & 1 & -1 & x, y, R_x, R_y \end{array} \quad \begin{array}{c} x^2, y^2, z^2, xy \\ yz, xz \end{array} \quad (1.30.4)$$

$$\begin{array}{c|c|c|c|c} C_3 & E & C_3 & C_3^2 & \\ \hline A & 1 & 1 & 1 & x, R_z \\ E & \begin{Bmatrix} 1 & c & c^* \\ 1 & c^* & c \end{Bmatrix} & & & x, y, R_x, R_y \end{array} \quad \begin{array}{c} c = e^{2\pi/3} \\ x^2 + y^2, z^2 \\ x^2 - y^2, xy, xz, yz \end{array} \quad (1.30.5)$$

$$\begin{array}{c|c|c|c|c|c} C_4 & E & C_4 & C_2 & C_4^3 & \\ \hline A & 1 & 1 & 1 & 1 & z, R_z \\ B & 1 & -1 & 1 & -1 & \\ E & \begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix} & & & & x, y, R_x, R_y \end{array} \quad \begin{array}{c} x^2 + y^2, z^2 \\ x^2 - y^2, xy \\ yz, xz \end{array} \quad (1.30.6)$$

C_{nv} groups

$$\begin{array}{c|c|c|c|c|c} C_{2v} & E & C_2 & \sigma_v(xz) & \sigma'_v(yz) & \\ \hline A_1 & 1 & 1 & 1 & 1 & z \\ A_2 & 1 & 1 & -1 & -1 & R_z \\ B_1 & 1 & -1 & 1 & -1 & x, R_y \\ B_2 & 1 & -1 & -1 & 1 & y, R_x \end{array} \quad \begin{array}{c} x^2, y^2, z^2 \\ xy \\ xz \\ yz \end{array} \quad (1.30.7)$$

$$\begin{array}{c|c|c|c|c} C_{3v} & E & 2C_3 & 3\sigma_v & \\ \hline A_1 & 1 & 1 & 1 & z \\ A_2 & 1 & 1 & -1 & R_z \\ E & 2 & -1 & 0 & x, y, R_x, R_y \end{array} \quad \begin{array}{c} x^2 + y^2, z^2 \\ x^2 - y^2, xy, xz, yz \end{array} \quad (1.30.8)$$

C_{nh} groups

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

(1.30.9)

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5		$c = e^{2\pi/3}$
A	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E	$\left\{ \begin{array}{cccccc} 1 & c & c^* & 1 & c & c^* \\ 1 & c^* & c & 1 & c^* & c \end{array} \right\}$						x, y	$x^2 - y^2, xy$
A'	1	1	1	-1	-1	-1	z	
E'	$\left\{ \begin{array}{cccccc} 1 & c & c^* & -1 & -c & -c^* \\ 1 & c^* & c & -1 & -c^* & -c \end{array} \right\}$						R_x, R_y	xz, yz

(1.30.10)

D_n groups

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

(1.30.11)

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

(1.30.12)

D_{nh} groups

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

(1.30.13)

D_{nd} groups

D_{2d}	E	$2S_4$	C_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	z	xy
E	2	0	-2	0	0	x, y, R_x, R_y	xy, yz

(1.30.14)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	-1	1	1	-1	R_z	
E_g	2	-1	0	2	-1	0	R_x, R_y	$x^2 - y^2, xy, xz, yz$
A_{1u}	1	1	1	-1	-1	-1		
A_{2u}	1	1	-1	-1	-1	1	z	
E_u	2	-1	0	-2	1	0	x, y	

(1.30.15)

$C_{\infty v}$ and $D_{\infty h}$

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

(1.30.16)

S_n groups

S_4	E	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1	z	$x^2 - y^2, xy$
E	$\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$				x, y, R_x, R_y	xz, yz

(1.30.17)

S_6	E	C_3	C_3^2	i	S_6^5	S_6		$c = e^{2\pi/3}$
A_g	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_g	$\begin{Bmatrix} 1 & c & c^* & 1 & c & c^* \\ 1 & c^* & c & 1 & c^* & c \end{Bmatrix}$						R_x, R_y	$x^2 - y^2, xy, xz, yz$
A_u	1	1	1	-1	-1	-1	z	
E_u	$\begin{Bmatrix} 1 & c & c^* & -1 & -c & -c^* \\ 1 & c^* & c & -1 & -c^* & -c \end{Bmatrix}$						x, y	

(1.30.18)

Cubic groups

T	E	$4C_3$	$4C_3^2$	$3C_2$		$c = e^{2\pi/3}$
A	1	1	1	1		$x^2 + y^2, z^2$
E	$\begin{Bmatrix} 1 & c & c^* & 1 \\ 1 & c^* & c & 1 \end{Bmatrix}$					$2z^2 - x^2 - y^2, x^2 - y^2$
T	3	0	0	-1	R_x, R_y, R_z, x, y, z	xy, xz, yz

(1.30.19)

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$2z^2 - x^2 - y^2, x^2 - y^2$
T_1	3	0	-1	1	-1	R_x, R_y, R_z	
T_2	3	0	-1	-1	1	x, y, z	xy, xz, yz

(1.30.20)

Direct product tables

For the point groups O and T_d (and O_h)

	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2		A_1	E	T_2	T_1
E			$A_1 + A_2 + E$	$T_1 + T_2$	$T_1 + T_2$
T_1				$A_1 + E + T_1 + T_2$	$A_2 + E + T_1 + T_2$
T_2					$A_1 + E + T_1 + T_2$

(1.30.21)

For the point groups D_4 , C_{4v} , D_{2d} (and $D_{4h} = D_4 \otimes C_i$)

	A_1	A_2	B_1	B_2	E
A_1	A_1	A_2	B_1	B_2	E
A_2		A_1	B_2	B_1	E
B_1			A_1	A_2	E
B_2				A_1	E
E					$A_1 + A_2 + B_1 + B_2$

(1.30.22)

For the point groups D_3 and C_{3v}

	A_1	A_2	E
A_1	A_1	A_2	E
A_2		A_1	E
E			$A_1 + A_2 + E$

(1.30.23)

For the point groups D_6 , C_{6v} and D_{3h}^*

	A_1	A_2	B_1	B_2	E_1	E_2
A_1	A_1	A_2	B_1	B_2	E_1	E_2
A_2		A_1	B_2	B_1	E_1	E_2
B_1			A_1	A_2	E_2	E_1
B_2				A_1	E_2	E_1
E_1					$A_1 + A_2 + E_2$	$B_1 + B_2 + E_1$
E_2						$A_1 + A_2 + E_2$

(1.30.24)

* in D_{3h} make the following changes in the above table

In table	In D_{3h}
A_1	A'_1
A_2	A'_2
B_1	A''_1
B_2	A''_2
E_1	E''
E_2	E'

(1.30.25)

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