

## 1.30: Appendix B- Point Groups

### Non axial groups

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

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

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

### $C_n$ groups

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

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

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

### $C_{nv}$ groups

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

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

### $C_{nh}$ groups

$C_{2h}$	$E$	$C_2$	$i$	$\sigma_h$		
$A_g$	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)

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

(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

$D_{2h}$	$E$	$C_2(z)$	$C_2(y)$	$C_2(x)$	$i$	$\sigma_{xy}$	$\sigma(xz)$	$\sigma(yz)$		
$A_g$	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	$R_z$	$x^2 + y^2, z^2$
$A_{2g}$	1	1	-1	1	1	-1		
$E_g$	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 $D_{\infty h}$

$D_{\infty h}$	$E$	$2C_{\infty}^{\Phi}$	$\dots$	$\infty\sigma_v$	$i$	$2S_{\infty}^{\Phi}$	$\dots$	$\infty C_2$		
$\Sigma_g^+$	1	1	$\dots$	1	1	1	$\dots$	1	$R_z$	$x^2 + y^2, z^2$
$\Sigma_g^-$	1	1	$\dots$	-1	1	1	$\dots$	-1		
$\Pi_g$	2	$2\cos\Phi$	$\dots$	0	2	$-2\cos\Phi$	$\dots$	0	$R_x, R_y$	$xz, yz$
$\Delta_g$	2	$2\cos 2\Phi$	$\dots$	0	2	$2\cos 2\Phi$	$\dots$	0		$x^2 - y^2, xy$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$		
$\Sigma_u^+$	1	1	$\dots$	1	-1	-1	$\dots$	-1	$z$	
$\Sigma_u^-$	1	1	$\dots$	-1	-1	-1	$\dots$	1		
$\Pi_u$	2	$2\cos\Phi$	$\dots$	0	-2	$2\cos\Phi$	$\dots$	0	$x, y$	
$\Delta_u$	2	$2\cos 2\Phi$	$\dots$	0	-2	$-2\cos 2\Phi$	$\dots$	0		
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$		

(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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