

# Appendix VIII: Character Tables for Some of the More Common Point Groups

Character tables are given in this appendix for the following point groups: (1) the groups which correspond to the 32 crystal classes (see Table 8-14), (2) groups containing 5-fold axes that may be needed to describe the symmetries of certain molecules or complex ions, and (3) the infinite groups  $C_{\infty v}$  and  $D_{\infty h}$  that are appropriate to linear structures.

Some comment on the notation for the irreducible representations (symmetry species) is necessary, as certain variations will be found in the literature. Molecular spectroscopists usually designate one-dimensional symmetry species by A or B, two-dimensional species by E, and three-dimensional species by F or T. Some authors prefer lower-case letters to capitals. The symmetry or antisymmetry of a given species with respect to the generating rotation operation distinguishes A and B. Subscripts 1 and 2 are used on A and B according to the symmetry with respect to rotation about a  $C_2$  axis perpendicular to the generating axis. Symmetry with respect to inversion is indicated by a subscript g or u (see Section 4.4.2), while a prime or double prime identifies species that are, respectively, symmetric or antisymmetric with respect to a horizontal plane. Finally numerical subscripts are used to distinguish various doubly and triply degenerate species.

For linear molecules or ions the symbols are usually those derived from the term symbols for the electronic states of diatomic and other linear molecules. A capital Greek letter  $\Sigma$ ,  $\Pi$ ,  $\Delta$ ,  $\Phi$ , ... is used, corresponding to  $\lambda = 0, 1, 2, 3, \dots$ , where  $\lambda$  is the quantum number for rotation about the molecular axis. For  $\Sigma$  species a superscript + or - is added to indicate the symmetry with respect to a plane that contains the molecular axis.

The components of the translation and rotation vectors are given as  $T_x$ ,  $T_y$ ,  $T_z$  and  $R_x$ ,  $R_y$ ,  $R_z$ , respectively. The components of the polarizability tensor appear as linear combinations such as  $\alpha_{xx} + \alpha_{yy}$ , etc., that have the symmetry of the indicated irreducible representation.

**Table 1** Character tables for the cyclic groups,  $G_n$  ( $n = 2, 3, 4, 5, 6$ ).

$G_2$	$E$	$C_2$					
A	1	1	$T_z, R_z$	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$			
B	1	-1	$T_x, T_y, R_x, R_y$	$\alpha_{yz}, \alpha_{zx}$			
$G_3$	$E$	$C_3$	$C_3^2$				
A	1	1	1	$T_z, R_z$			
E	$\left\{ \begin{array}{l} 1 \\ \varepsilon \\ 1 \end{array} \right.$	$\left. \begin{array}{l} \varepsilon^\star \\ \varepsilon \\ \varepsilon \end{array} \right\}$		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$			
			$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{zx})$			
$G_4$	$E$	$C_4$	$C_2$	$C_4^3$			
A	1	1	1	1			
B	1	-1	1	-1			
E	$\left\{ \begin{array}{l} 1 \\ i \\ 1 \end{array} \right.$	$\left. \begin{array}{l} -1 \\ -i \\ -1 \end{array} \right\}$		$T_z, R_z$			
			$(T_x, T_y), (R_x, R_y)$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$			
				$\alpha_{xx} - \alpha_{yy}, \alpha_{zz}$			
				$(\alpha_{yz}, \alpha_{zx})$			
$G_5$	$E$	$C_5$	$C_5^2$	$C_5^3$	$C_5^4$		$\varepsilon = \exp(2\pi i/5)$
A	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$E_1$	$\left\{ \begin{array}{l} 1 \\ \varepsilon \\ 1 \end{array} \right.$	$\left. \begin{array}{l} \varepsilon^2 \\ \varepsilon^{2\star} \\ \varepsilon^2 \end{array} \right\}$	$\left. \begin{array}{l} \varepsilon^{2\star} \\ \varepsilon^2 \\ \varepsilon \end{array} \right\}$		$T_z, R_z$	$(T_x, T_y), (R_x, R_y)$	$\alpha_{yz}, \alpha_{zx}$
$E_2$	$\left\{ \begin{array}{l} 1 \\ \varepsilon^2 \\ 1 \end{array} \right.$	$\left. \begin{array}{l} \varepsilon^\star \\ \varepsilon \\ \varepsilon^2 \end{array} \right\}$	$\left. \begin{array}{l} \varepsilon \\ \varepsilon^\star \\ \varepsilon^2 \end{array} \right\}$				$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$G_6$	$E$	$C_6$	$C_3$	$C_2$	$C_3^2$	$C_6^5$	
A	1	1	1	1	1	1	$T_z, R_z$
B	1	-1	1	-1	1	-1	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$E_1$	$\left\{ \begin{array}{l} 1 \\ \varepsilon \\ 1 \end{array} \right.$	$\left. \begin{array}{l} -\varepsilon^\star \\ -\varepsilon \\ -\varepsilon \end{array} \right\}$	$\left. \begin{array}{l} -1 \\ -\varepsilon \\ -1 \end{array} \right\}$	$\left. \begin{array}{l} -\varepsilon \\ -\varepsilon^\star \\ -\varepsilon \end{array} \right\}$	$\left. \begin{array}{l} \varepsilon^\star \\ \varepsilon \\ \varepsilon \end{array} \right\}$		$(T_x, T_y), (R_x, R_y)$
$E_2$	$\left\{ \begin{array}{l} 1 \\ -\varepsilon^\star \\ 1 \end{array} \right.$	$\left. \begin{array}{l} -\varepsilon \\ -\varepsilon^\star \\ -\varepsilon \end{array} \right\}$	$\left. \begin{array}{l} 1 \\ 1 \\ 1 \end{array} \right\}$	$\left. \begin{array}{l} -\varepsilon^\star \\ -\varepsilon \\ -\varepsilon \end{array} \right\}$	$\left. \begin{array}{l} -\varepsilon \\ -\varepsilon^\star \\ -\varepsilon \end{array} \right\}$		$(\alpha_{yz} - \alpha_{zx})$
							$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

**Table 2** Character tables for the dihedral groups,  $\mathcal{D}_n$  ( $n = 2, 3, 4, 5, 6$ ).

$\mathcal{D}_2 = \mathcal{P}$	$E$	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
B <sub>1</sub>	1	1	-1	-1	$T_z, R_z$	$\alpha_{xy}$
B <sub>2</sub>	1	-1	1	-1	$T_y, R_y$	$\alpha_{zx}$
B <sub>3</sub>	1	-1	-1	1	$T_x, R_x$	$\alpha_{yz}$

  

$\mathcal{D}_3$	$E$	$2C_3$	$3C'_2$			
A <sub>1</sub>	1	1	1			$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2</sub>	1	1	-1		$T_z, R_z$	
E	2	-1	0	$(T_x, T_y), (R_x, R_y)$		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{zx})$

  

$\mathcal{D}_4$	$E$	$2C_4$	$C_2$	$2C'_2$	$2C''_2$		
A <sub>1</sub>	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2</sub>	1	1	1	-1	-1		
B <sub>1</sub>	1	-1	1	1	-1	$T_z, R_z$	$\alpha_{xx} - \alpha_{yy}$
B <sub>2</sub>	1	-1	1	-1	1		$\alpha_{xy}$
E	2	0	-2	0	0	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{yz}, \alpha_{zx})$

  

$\mathcal{D}_5$	$E$	$2C_5$	$2C_5^2$	$5C'_2$			$\alpha = 72^\circ$
A <sub>1</sub>	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2</sub>	1	1	1	-1	-1		
E <sub>1</sub>	2	$2 \cos \alpha$	$2 \cos 2\alpha$	0		$T_z, R_z$	$(\alpha_{yz}, \alpha_{zx})$
E <sub>2</sub>	2	$2 \cos 2\alpha$	$2 \cos \alpha$	0		$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

  

$\mathcal{D}_6$	$E$	$2C_6$	$2C_3$	$C_2$	$3C'_2$	$3C''_2$		
A <sub>1</sub>	1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2</sub>	1	1	1	1	-1	-1	$T_z, R_z$	
B <sub>1</sub>	1	-1	1	-1	1	-1		
B <sub>2</sub>	1	-1	1	-1	-1	1		
E <sub>1</sub>	2	1	-1	-2	0	0	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{yz}, \alpha_{zx})$
E <sub>2</sub>	2	-1	-1	2	0	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

**Table 3** Character tables for the groups  $\mathcal{D}_{nh}(n = 2, 3, 4, 5, 6)$ .

$\mathcal{D}_{2h} = \mathcal{V}_h$	$E$	$C_2(z)$	$C_2(y)$	$C_2(x)$	$i$	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A <sub>g</sub>	1	1	1	1	1	1	1	1		$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
B <sub>1g</sub>	1	1	-1	-1	1	1	-1	-1	$R_z$	$\alpha_{xy}$
B <sub>2g</sub>	1	-1	1	-1	1	-1	1	-1	$R_y$	$\alpha_{zx}$
B <sub>3g</sub>	1	-1	-1	1	1	-1	-1	1	$R_x$	$\alpha_{yz}$
A <sub>u</sub>	1	1	1	1	-1	-1	-1	-1		
B <sub>1u</sub>	1	1	-1	-1	-1	-1	1	1	$T_z$	
B <sub>2u</sub>	1	-1	1	-1	-1	1	-1	1	$T_y$	
B <sub>3u</sub>	1	-1	-1	1	-1	1	1	-1	$T_x$	

$\mathcal{D}_{3h}$	$E$	$2C_3$	$3C'_2$	$\sigma_h$	$2S_3$	$3\sigma_v$			
A'_1	1	1	1	1	1	1			$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A'_2	1	1	-1	1	1	-1	$R_z$		
E'	2	-1	0	2	-1	0	( $T_x, T_y$ )		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
A''_1	1	1	1	-1	-1	-1			
A''_2	1	1	-1	-1	-1	1	$T_z$		
E''	2	-1	0	-2	1	0	( $R_x, R_y$ )		$(\alpha_{yx}, \alpha_{zx})$

$\mathcal{D}_{4h}$	$E$	$2C_4$	$C_2$	$2C'_2$	$2C''_2$	$i$	$2S_4$	$\sigma_h$	$2\sigma_v$	$2\sigma_d$	
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1	
A <sub>2g</sub>	1	1	1	-1	-1	1	1	1	-1	-1	$R_z$
B <sub>1g</sub>	1	-1	1	1	-1	1	-1	1	1	-1	
B <sub>2g</sub>	1	-1	1	-1	1	1	1	-1	1	-1	
E <sub>g</sub>	2	0	-2	0	0	2	0	-2	0	0	( $R_x, R_y$ )
A <sub>1u</sub>	1	1	1	1	1	-1	-1	-1	-1	-1	
A <sub>2u</sub>	1	1	1	-1	-1	-1	-1	-1	1	1	$T_z$
B <sub>1u</sub>	1	-1	1	1	-1	-1	1	-1	-1	1	
B <sub>2u</sub>	1	-1	1	-1	1	-1	1	-1	1	-1	
E <sub>u</sub>	2	0	-2	0	0	-2	0	2	0	0	( $T_x, T_y$ )

$\mathcal{D}_{5h}$	$E$	$2C_5$	$2C_5^2$	$5C'_2$	$\sigma_h$	$2S_5$	$2S_5^3$	$5\sigma_v$		$\alpha = 72^\circ$
A'_1	1	1	1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A'_2	1	1	1	-1	1	1	1	-1	$R_z$	$\alpha_{zz}$
E'_1	2	$2 \cos \alpha$	$2 \cos 2\alpha$	0	2	$2 \cos \alpha$	$2 \cos 2\alpha$	0	( $T_x, T_y$ )	
E'_2	2	$2 \cos 2\alpha$	$2 \cos \alpha$	0	2	$2 \cos 2\alpha$	$2 \cos \alpha$	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
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	$2 \cos \alpha$	$2 \cos 2\alpha$	0	-2	$-2 \cos \alpha$	$-2 \cos 2\alpha$	0	( $R_x, R_y$ )	$(\alpha_{yz}, \alpha_{zx})$
E''_2	2	$2 \cos 2\alpha$	$2 \cos \alpha$	0	-2	$-2 \cos 2\alpha$	$-2 \cos \alpha$	0		

**Table 3** (Continued).

$\mathcal{D}_{6h}$	$E$	$2C_6$	$2C_3$	$C_2$	$3C'_2$	$3C''_2$	$i$	$2S_3$	$2S_6$	$\sigma_h$	$3\sigma_d$	$3\sigma_v$	
$A_{1g}$	1	1	1	1	1	1	1	1	1	1	1	1	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$A_{2g}$	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	
$B_{2g}$	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1	
$E_{1g}$	2	1	-1	-2	0	0	2	1	-1	-2	0	0	$(R_x, R_y)$
$E_{2g}$	2	-1	-1	2	0	0	2	-1	-1	2	0	0	$(\alpha_{yz}, \alpha_{zx})$ $(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$A_{1u}$	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	$T_z$
$B_{1u}$	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	
$E_{1u}$	2	1	-1	-2	0	0	-2	-1	1	2	0	0	$(T_x, T_y)$
$E_{2u}$	2	-1	-1	2	0	0	-2	1	1	-2	0	0	

**Table 4** Character tables for the groups  $S_n$  ( $n = 2, 4, 6, 8$ ).

$S_2 \equiv \mathcal{G}_i$	$E$	$i$								
$A_g$	1	1	$R_x, R_y, R_z$	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$						
$A_u$	1	-1	$T_x, T_y, T_z$	$\alpha_{yz}, \alpha_{zx}$						
$S_4$	$E$	$S_4$	$C_2$	$S_4^3$						
$A$	1	1	1	1	$R_z$					
$B$	1	-1	1	-1	$T_z$					
$E$	$\{ 1 \}$	$i$	-1	$-i$	$(T_x, T_y), (R_x, R_y)$					
	$\{ 1 \}$	$-i$	-1	$i$	$(\alpha_{yz}, \alpha_{zx})$					
$S_6$	$E$	$C_3$	$C_3^2$	$i$	$S_6^5$	$S_6$		$\varepsilon = \exp(2\pi i/3)$		
$A_g$	1	1	1	1	1	1	$R_z$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$		
$E_g$	$\{ 1 \}$	$\varepsilon$	$\varepsilon^\star$	1	$\varepsilon$	$\varepsilon^\star$	$(R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{zx})$		
$A_u$	1	1	1	-1	-1	-1	$T_z$			
$E_u$	$\{ 1 \}$	$\varepsilon$	$\varepsilon^\star$	-1	$-\varepsilon$	$-\varepsilon^\star$	$(T_x, T_y)$			
	$\{ 1 \}$	$\varepsilon^\star$	$\varepsilon$	-1	$-\varepsilon^\star$	$-\varepsilon$				
$S_8$	$E$	$S_8$	$C_4$	$S_8^3$	$C_2$	$S_8^5$	$C_4^3$	$S_8^7$		$\varepsilon = \exp(2\pi i/8)$
$A$	1	1	1	1	1	1	1	1	$R_z$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$B$	1	-1	1	-1	1	-1	1	-1	$T_z$	
$E_1$	$\{ 1 \}$	$\varepsilon$	$i$	$-\varepsilon^\star$	-1	$-\varepsilon$	$-i$	$\varepsilon^\star$	$(T_x, T_y)$	
$E_2$	$\{ 1 \}$	$\varepsilon^\star$	$-i$	$-\varepsilon$	-1	$-\varepsilon^\star$	$i$	$\varepsilon$		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$E_3$	$\{ 1 \}$	$-\varepsilon^\star$	$-i$	$\varepsilon$	-1	$\varepsilon^\star$	$i$	$-\varepsilon$	$(R_x, R_y)$	$(\alpha_{yz}, \alpha_{zx})$
	$\{ 1 \}$	$-\varepsilon$	$i$	$\varepsilon^\star$	-1	$\varepsilon$	$-i$	$-\varepsilon^\star$		

**Table 5** Character tables for the groups  $G_{nh}$  ( $n = 1, 2, 3, 4, 5, 6$ ).

$G_{1h} \equiv G'_S$	$E$	$\sigma_h$										
A'	1	1	$T_x, T_y, R_z$	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$								
A''	1	-1	$T_z, R_x, R_y$	$\alpha_{yz}, \alpha_{zx}$								
$G_{2h}$	$E$	$C_2$	$i$	$\sigma_h$								
A <sub>g</sub>	1	1	1	1								
B <sub>g</sub>	1	-1	1	-1								
A <sub>u</sub>	1	1	-1	-1								
B <sub>u</sub>	1	-1	-1	1								
R <sub>z</sub>												
$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$												
$\alpha_{yz}, \alpha_{zx}$												
$G_{3h}$	$E$	$C_3$	$C_3^2$	$\sigma_h$	$S_3$	$S_3^5$			$\varepsilon = \exp(2\pi i/3)$			
A'	1	1	1	1	1	1	$R_z$		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$			
E'	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon \end{cases}$	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon \end{cases}$	$(T_x, T_y)$			$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$			
A''	1	1	1	-1	-1	-1	$T_z$					
E''	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon \end{cases}$	$\begin{cases} -1 & -\varepsilon \\ -1 & -\varepsilon^2 \star \end{cases}$	$\begin{cases} -\varepsilon \\ -\varepsilon \end{cases}$	$\begin{cases} -\varepsilon^2 \star \\ -\varepsilon \end{cases}$	$(R_x, R_y)$			$(\alpha_{yz}, \alpha_{zx})$			
$G_{4h}$	$E$	$C_4$	$C_2$	$C_4^3$	$i$	$S_4^3$	$\sigma_h$	$S_4$				
A <sub>g</sub>	1	1	1	1	1	1	1	1	$R_z$			
B <sub>g</sub>	1	-1	1	-1	1	-1	1	-1	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$			
E <sub>g</sub>	$\begin{cases} 1 & i \\ 1 & -i \end{cases}$	$\begin{cases} -1 & -i \\ 1 & i \end{cases}$	$\begin{cases} 1 & i \\ 1 & -i \end{cases}$	$\begin{cases} -1 & -i \\ -1 & i \end{cases}$	$\begin{cases} 1 & i \\ 1 & -i \end{cases}$	$\begin{cases} -1 & -i \\ -1 & i \end{cases}$	$(R_x, R_y)$		$\alpha_{xx} - \alpha_{yy}, \alpha_{xy}$			
A <sub>u</sub>	1	1	1	1	-1	-1	-1	-1	$T_z$			
B <sub>u</sub>	1	-1	1	-1	-1	1	-1	1				
E <sub>u</sub>	$\begin{cases} 1 & i \\ 1 & -i \end{cases}$	$\begin{cases} -1 & -i \\ 1 & i \end{cases}$	$\begin{cases} 1 & -i \\ 1 & i \end{cases}$	$\begin{cases} -1 & -i \\ -1 & i \end{cases}$	$\begin{cases} 1 & -i \\ 1 & i \end{cases}$	$\begin{cases} 1 & i \\ 1 & -i \end{cases}$	$(T_x, T_y)$					
$G_{5h}$	$E$	$C_5$	$C_5^2$	$C_5^3$	$C_5^4$	$\sigma_h$	$S_5$	$S_5^7$	$S_5^3$	$S_5^9$		$\varepsilon = \exp(2\pi i/5)$
A'	1	1	1	1	1	1	1	1	1	1	$R_z$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
E'_1	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \end{cases}$	$\begin{cases} \varepsilon \star \\ \varepsilon \end{cases}$	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$(T_z, T_y)$					
E'_2	$\begin{cases} 1 & \varepsilon^2 \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon \end{cases}$	$\begin{cases} \varepsilon \star \\ \varepsilon \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \end{cases}$	$\begin{cases} 1 & \varepsilon^2 \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} 1 & \varepsilon^2 \\ 1 & \varepsilon^2 \star \end{cases}$						$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
A''	1	1	1	1	-1	-1	-1	-1	-1	-1	$T_z$	
E''_1	$\begin{cases} 1 & \varepsilon \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \end{cases}$	$\begin{cases} \varepsilon \star \\ \varepsilon \end{cases}$	$\begin{cases} -1 & -\varepsilon \\ -1 & -\varepsilon^2 \star \end{cases}$	$\begin{cases} -\varepsilon \\ -\varepsilon^2 \star \end{cases}$	$(R_x, R_y)$					$(\alpha_{yz} + \alpha_{zx})$
E''_2	$\begin{cases} 1 & \varepsilon^2 \\ 1 & \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \star \end{cases}$	$\begin{cases} \varepsilon \star \\ \varepsilon \end{cases}$	$\begin{cases} \varepsilon^2 \star \\ \varepsilon^2 \end{cases}$	$\begin{cases} -1 & -\varepsilon^2 \\ -1 & -\varepsilon^2 \star \end{cases}$	$\begin{cases} -\varepsilon^2 \star \\ -\varepsilon^2 \end{cases}$	$(T_x, T_y)$					$(\alpha_{yz} + \alpha_{zx})$

**Table 5** (Continued).

$G_{6h}$	$E$	$C_6$	$C_3$	$C_2$	$C_3^2$	$C_6^5$	$i$	$S_3^5$	$S_6^5$	$\sigma_h$	$S_6$	$S_3$		$\varepsilon = \exp(2\pi i/6)$	
$A_g$	1	1	1	1	1	1	1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$	
$B_g$	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1			
$E_{1g}$	{	1	$\varepsilon$	$-\varepsilon^\star$	-1	$-\varepsilon$	$\varepsilon^\star$	1	$\varepsilon$	$-\varepsilon^\star$	-1	$-\varepsilon$	$\varepsilon^\star$	{}	$(R_x, R_y)$
$E_{2g}$	{	1	$-\varepsilon^\star$	$-\varepsilon$	1	$-\varepsilon^\star$	$-\varepsilon$	1	$-\varepsilon^\star$	$-\varepsilon$	1	$-\varepsilon^\star$	$-\varepsilon$	{}	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$A_u$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1			
$B_u$	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1			
$E_{1u}$	{	1	$\varepsilon$	$-\varepsilon^\star$	-1	$-\varepsilon$	$\varepsilon^\star$	-1	$-\varepsilon$	$\varepsilon^\star$	1	$\varepsilon$	$-\varepsilon^\star$	{}	$(T_x, T_y)$
$E_{2u}$	{	1	$-\varepsilon^\star$	$-\varepsilon$	1	$-\varepsilon^\star$	$-\varepsilon$	-1	$\varepsilon^\star$	$\varepsilon$	-1	$\varepsilon^\star$	$\varepsilon$	{}	

**Table 6** Character tables for the groups  $G_{nv}$  ( $n = 2, 3, 4, 5, 6$ ).

$G_{2v}$	$E$	$C_2$	$\sigma_v(xz)$	$\sigma_v(yz)$			
$A_1$	1	1	1	1		$T_z$	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
$A_2$	1	1	-1	-1		$R_z$	$\alpha_{xy}$
$B_1$	1	-1	1	-1		$T_x, R_y$	$\alpha_{zx}$
$B_2$	1	-1	-1	1		$T_y, R_x$	$\alpha_{yz}$
$G_{3v}$	$E$	$2C_3$	$3\sigma_v$				
$A_1$	1	1	1			$T_z$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$A_2$	1	1	-1			$R_z$	
$E$	2	-1	0			$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{zx})$
$G_{4v}$	$E$	$2C_4$	$C_2$	$2\sigma_v$	$2\sigma_d$		
$A_1$	1	1	1	1	1		$T_x$
$A_2$	1	1	1	-1	-1		$R_z$
$B_1$	1	-1	1	1	-1		
$B_2$	1	-1	1	-1	1		
$E$	2	0	-2	0	0		$(T_x, T_y), (R_x, R_y)$
$G_{5v}$	$E$	$2C_5$	$2C_5^2$	$5\sigma_v$			$\alpha = 72^\circ$
$A_1$	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$A_2$	1	1	1	-1	-1		
$E_1$	2	$2 \cos \alpha$	$2 \cos 2\alpha$	0			$(\alpha_{yz}, \alpha_{zx})$
$E_2$	2	$2 \cos 2\alpha$	$2 \cos \alpha$	0			$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$G_{6v}$	$E$	$2C_6$	$2C_3$	$C_2$	$3\sigma_v$	$3\sigma_d$	
$A_1$	1	1	1	1	1	1	
$A_2$	1	1	1	1	-1	-1	
$B_1$	1	-1	1	-1	1	-1	
$B_2$	1	-1	1	-1	-1	1	
$E_1$	2	1	-1	-2	0	0	
$E_2$	2	-1	-1	2	0	0	
							$(\alpha_{yz}, \alpha_{zx})$
							$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

**Table 7** Character tables for the groups,  $\mathcal{D}_{nd}$  ( $n = 2, 3, 4, 5, 6$ ).

$\mathcal{D}_{2d} = \mathcal{P}_d$	$E$	$2S_4$	$C_2$	$2C'_2$	$2\sigma_d$			
A <sub>1</sub>	1	1	1	1	1			$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2</sub>	1	1	1	-1	-1		$R_z$	$\alpha_{xx} - \alpha_{yy}$
B <sub>1</sub>	1	-1	1	1	-1			$\alpha_{xy}$
B <sub>2</sub>	1	-1	1	-1	1		$T_z$	$(\alpha_{yz}, \alpha_{zx})$
E	2	0	-2	0	0	$(T_x, T_y)$	$(R_x, R_y)$	

  

$\mathcal{D}_{3d}$	$E$	$2C_3$	$3C_2$	$i$	$2S_6$	$3\sigma_d$		
A <sub>1g</sub>	1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2g</sub>	1	1	-1	1	1	-1	$R_z$	
E <sub>g</sub>	2	-1	0	2	-1	0	$(R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{zx})$
A <sub>1u</sub>	1	1	1	-1	-1	-1		
A <sub>2u</sub>	1	1	-1	-1	-1	1	$T_z$	
E <sub>u</sub>	2	-1	0	-2	1	0	$(T_x, T_y)$	

  

$\mathcal{D}_{4d}$	$E$	$2S_8$	$2C_4$	$2S_8^3$	$C_2$	$4C'_2$	$4\sigma_d$		
A <sub>1</sub>	1	1	1	1	1	1	1		
A <sub>2</sub>	1	1	1	1	1	-1	-1	$R_z$	
B <sub>1</sub>	1	-1	1	-1	1	1	-1		
B <sub>2</sub>	1	-1	1	-1	1	-1	1	$T_z$	
E <sub>1</sub>	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	$(T_x, T_y)$	
E <sub>2</sub>	2	0	-2	0	2	0	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E <sub>3</sub>	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0	$(R_x, R_y)$	$(\alpha_{yz}, \alpha_{zx})$

  

$\mathcal{D}_{5d}$	$E$	$2C_5$	$2C_5^2$	$5C_2$	$i$	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$	$\alpha = 72^\circ$
A <sub>1g</sub>	1	1	1	1	1	1	1	1	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A <sub>2g</sub>	1	1	1	-1	1	1	1	-1	$R_z$
E <sub>1g</sub>	2	$2\cos\alpha$	$2\cos 2\alpha$	0	2	$2\cos\alpha$	$2\cos 2\alpha$	0	$(R_x, R_y)$
E <sub>2g</sub>	2	$2\cos 2\alpha$	$2\cos\alpha$	0	2	$2\cos 2\alpha$	$2\cos\alpha$	0	$(\alpha_{yz}, \alpha_{zx})$
A <sub>1u</sub>	1	1	1	1	-1	-1	-1	-1	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
A <sub>2u</sub>	1	1	1	-1	-1	-1	-1	1	$T_z$
E <sub>1u</sub>	2	$2\cos\alpha$	$2\cos 2\alpha$	0	-2	$-2\cos\alpha$	$-2\cos 2\alpha$	0	$(T_x, T_y)$
E <sub>2u</sub>	2	$2\cos 2\alpha$	$2\cos\alpha$	0	-2	$-2\cos 2\alpha$	$-2\cos\alpha$	0	

  

$\mathcal{D}_{6d}$	$E$	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2S_{12}^5$	$C_2$	$6C'_2$	$6\sigma_d$		
A <sub>1</sub>	1	1	1	1	1	1	1	1	1	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$	
A <sub>2</sub>	1	1	1	1	1	1	1	-1	-1	$R_z$	
B <sub>1</sub>	1	-1	1	-1	1	-1	1	1	-1		
B <sub>2</sub>	1	-1	1	-1	1	-1	1	-1	1	$T_z$	
E <sub>1</sub>	2	$\sqrt{3}$	1	0	-1	$-\sqrt{3}$	-2	0	0	$(T_x, T_y)$	
E <sub>2</sub>	2	1	-1	-2	-1	1	2	0	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E <sub>3</sub>	2	0	-2	0	2	0	-2	0	0		
E <sub>4</sub>	2	-1	-1	2	-1	-1	2	0	0		
E <sub>5</sub>	2	$-\sqrt{3}$	1	0	-1	$\sqrt{3}$	-2	0	0	$(R_x, R_y)$	$(\alpha_{yz}, \alpha_{zx})$

**Table 8** Character tables for the cubic groups.

$\mathcal{T}$	$E$	$4C_3$	$4C_3^2$	$3C_2$	$i$	$4S_6$	$4S_6^5$	$3\sigma$	$\varepsilon = \exp(2\pi i/3)$
A	1	1	1	1					$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
E	{ 1 1 1 } $\varepsilon$ $\varepsilon^\star$	$\varepsilon^\star$	1	{ 1 1 1 } $\varepsilon$					$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T \equiv F$	3	0	0	-1		T, R			$(\alpha_{xy}, \alpha_{yz}, \alpha_{zx})$

  

$\mathcal{T}_h$	$E$	$4C_3$	$4C_3^2$	$3C_2$	$i$	$4S_6$	$4S_6^5$	$3\sigma$	$\varepsilon = \exp(2\pi i/3)$
$A_g$	1	1	1	1	1	1	1	1	$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
$E_g$	{ 1 1 1 } $\varepsilon$ $\varepsilon^\star$	$\varepsilon^\star$	1	1	1	$\varepsilon^\star$	$\varepsilon$	1	$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T_g \equiv F_g$	3	0	0	-1	3	0	0	-1	R
$A_u$	1	1	1	1	-1	-1	-1	-1	
$E_u$	{ 1 1 1 } $\varepsilon$ $\varepsilon^\star$	$\varepsilon^\star$	1	-1	-1	$-\varepsilon^\star$	$-\varepsilon$	-1	
$T_u \equiv F_u$	3	0	0	-1	-3	0	0	1	T

  

$\mathcal{T}_d$	$E$	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	$i$	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$	$\varepsilon = \exp(2\pi i/3)$
$A_1$	1	1	1	1	1						$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
$A_2$	1	1	1	-1	-1						
E	2	-1	2	0	0						$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T_1 \equiv F_1$	3	0	-1	1	-1		R				
$T_2 \equiv F_2$	3	0	-1	-1	1		T				$(\alpha_{xy}, \alpha_{yz}, \alpha_{zx})$

  

$\mathcal{O}_h$	$E$	$8C_3$	$3C_2$	$6C_4$	$6C'_2$	$i$	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$	$\varepsilon = \exp(2\pi i/3)$
$A_{1g}$	1	1	1	1	1	1	1	1	1	1	$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
$A_{2g}$	1	1	1	-1	-1	1	1	1	-1	-1	
$E_g$	2	-1	2	0	0	2	-1	2	0	0	$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T_{1g} \equiv F_{1g}$	3	0	-1	1	-1	3	0	-1	1	-1	R
$T_{2g} \equiv F_{2g}$	3	0	-1	-1	1	3	0	-1	-1	1	$(\alpha_{xy}, \alpha_{yz}, \alpha_{zx})$
$A_{1u}$	1	1	1	1	1	-1	-1	-1	-1	-1	
$A_{2u}$	1	1	1	-1	-1	-1	-1	-1	1	1	
$E_u$	2	-1	2	0	0	-2	1	-2	0	0	
$T_{1u} \equiv F_{1u}$	3	0	-1	1	-1	-3	0	1	-1	1	T
$T_{2u} \equiv F_{2u}$	3	0	-1	-1	1	-3	0	1	1	-1	

**Table 9** Character tables for the icosahedral groups.

$\mathcal{G}$	$E$	$12C_5$	$12C_3^2$	$20C_3$	$15C_2$		
A	1	1	1	1	1		$\alpha_{zz} + \alpha_{yy} + \alpha_{zz}$
$T_1 \equiv F_1$	3	$\frac{1+\sqrt{5}}{2}$	$\frac{1-\sqrt{5}}{2}$	0	-1	$\mathbf{T}, \mathbf{R}$	
$T_2 \equiv F_2$	3	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$	0	-1		
G	4	-1	-1	1	0		
H	5	0	0	-1	1		$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy}, \alpha_{xy}, \alpha_{yz}, \alpha_{zx})$
$\mathcal{G}_h$	$E$	$12C_5$	$12C_3^2$	$20C_3$	$15C_2$	$i$	$12S_{10}$
$A_g$	1	1	1	1	1	1	1
$T_{1g} \equiv F_{1g}$	3	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	0	-1	3	$\frac{1}{2}(1-\sqrt{5})$
$T_{2g} \equiv F_{2g}$	3	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	0	-1	3	$\frac{1}{2}(1+\sqrt{5})$
$G_g$	4	-1	-1	1	0	4	-1
$H_g$	5	0	0	-1	1	5	0
							$12S_{10}^3$
							$20S_6$
							$15\sigma$
$A_u$	1	1	1	1	1	-1	-1
$T_{1u} \equiv F_{1u}$	3	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	0	-1	-3	$-\frac{1}{2}(1-\sqrt{5})$
$T_{2u} \equiv F_{2u}$	3	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	0	-1	-3	$-\frac{1}{2}(1+\sqrt{5})$
$G_u$	4	-1	-1	1	0	-4	1
$H_u$	5	0	0	-1	1	-5	0
							$\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz},$
							$\alpha_{xx} - \alpha_{yy}, \alpha_{xy},$
							$\alpha_{yz}, \alpha_{zx} \rangle$
							$\mathbf{T}$

**Table 10** Character tables for the infinite groups of linear structures.

$G_{\infty v}$	$E$	$2C_{\infty}^{\phi}$	...	$\infty\sigma_v$					
$A_1 \equiv \Sigma^+$	1	1	...	1					$\alpha_{zz} + \alpha_{yy}, \alpha_{zz}$
$A_2 \equiv \Sigma^-$	1	1	...	-1					$R_z$
$E_1 \equiv \Pi$	2	$2\cos\phi$	...	0	$(T_x, T_y), (R_x, R_y)$				$(\alpha_{yz}, \alpha_{zx})$
$E_2 \equiv \Delta$	2	$2\cos 2\phi$	...	0					$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$E_3 \equiv \Phi$	2	$2\cos 3\phi$	...	0					
...	...	...	...	...					

  

$G_{\infty h}$	$E$	$2C_{\infty}^{\phi}$	...	$\infty\sigma_v$	$i$	$2S_{\infty}^{\phi}$	...	$\infty C_2$		
$\Sigma_g^+$	1	1	...	1	1	1	...	1		
$\Sigma_g^-$	1	1	...	-1	1	1	...	-1	$R_z$	
$\Pi_g$	2	$2\cos\phi$	...	0	2	$-2\cos\phi$	...	0	$(R_z, R_y)$	$(\alpha_{yz}, \alpha_{zx})$
$\Delta_g$	2	$2\cos 2\phi$	...	0	2	$2\cos 2\phi$	...	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
...	...	...	...	...	...	...	...	...		
$\Sigma_u^+$	1	1	...	1	-1	-1	...	-1	$T_z$	
$\Sigma_u^-$	1	1	...	-1	-1	-1	...	1		
$\Pi_u$	2	$2\cos\phi$	...	0	-2	$2\cos\phi$	...	0	$(T_x, T_y)$	
$\Delta_u$	2	$2\cos 2\phi$	...	0	-2	$-2\cos 2\phi$	...	0		
...	...	...	...	...	...	...	...	...		