

Table A.2

C_i	I	i		
A_g	1	1	R_x, R_y, R_z	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}, \alpha_{xz}, \alpha_{yz}$
A_u	1	-1	T_x, T_y, T_z	

Table A.3

C_i	I	
A	1	All R, T, α

Table A.4

C_2	I	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	α_{yz}, α_{xz}

Table A.5

C_3	I	C_3	C_3^2		
A	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
E	$\begin{Bmatrix} 1 & \epsilon & \epsilon^* \\ 1 & \epsilon^* & \epsilon \end{Bmatrix}$			$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{yz}, \alpha_{xz})$

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

Table A.6

C_4	I	C_4	C_2	C_4^3		
A	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
B	1	-1	1	-1		$\alpha_{xx} - \alpha_{yy}, \alpha_{xy}$
E	$\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$				$(T_x, T_y), (R_x, R_y)$	$(\alpha_{yz}, \alpha_{xz})$

Table A.7

C_5	I	C_5	C_5^2	C_5^3	C_5^4		
A	1	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
E_1	$\begin{Bmatrix} 1 & \epsilon & \epsilon^2 & \epsilon^{2*} & \epsilon^* \\ 1 & \epsilon^* & \epsilon^2 & \epsilon^2 & \epsilon \end{Bmatrix}$					$(T_x, T_y), (R_x, R_y)$	$(\alpha_{yz}, \alpha_{xz})$
E_2	$\begin{Bmatrix} 1 & \epsilon^2 & \epsilon^* & \epsilon & \epsilon^{2*} \\ 1 & \epsilon^{2*} & \epsilon & \epsilon^* & \epsilon^2 \end{Bmatrix}$						$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

$$\epsilon = \exp(2\pi i/5), \epsilon^* = \exp(-2\pi i/5)$$

Table A.8

C_6	I	C_6	C_3	C_2	C_3^2	C_6^5		
A	1	1	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
B	1	-1	1	-1	1	-1		
E_1	$\begin{Bmatrix} 1 & \epsilon & -\epsilon^* & -1 & -\epsilon & \epsilon^* \\ 1 & \epsilon^* & -\epsilon & -1 & -\epsilon^* & \epsilon \end{Bmatrix}$						$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$
E_2	$\begin{Bmatrix} 1 & -\epsilon^* & -\epsilon & 1 & -\epsilon^* & -\epsilon \\ 1 & -\epsilon & -\epsilon^* & 1 & -\epsilon & -\epsilon^* \end{Bmatrix}$							$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

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

Table A.9

C_7	I	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	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
E_1	$\begin{Bmatrix} 1 & \epsilon & \epsilon^2 & \epsilon^3 & \epsilon^{3*} & \epsilon^{2*} & \epsilon^* \\ 1 & \epsilon^* & \epsilon^{2*} & \epsilon^{3*} & \epsilon^3 & \epsilon^2 & \epsilon \end{Bmatrix}$							$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$
E_2	$\begin{Bmatrix} 1 & \epsilon^2 & \epsilon^{3*} & \epsilon^* & \epsilon & \epsilon^3 & \epsilon^{2*} \\ 1 & \epsilon^{2*} & \epsilon^3 & \epsilon & \epsilon^* & \epsilon^{3*} & \epsilon^2 \end{Bmatrix}$								$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_3	$\begin{Bmatrix} 1 & \epsilon^3 & \epsilon^* & \epsilon^2 & \epsilon^{2*} & \epsilon & \epsilon^{3*} \\ 1 & \epsilon^{3*} & \epsilon & \epsilon^{2*} & \epsilon^2 & \epsilon^* & \epsilon^3 \end{Bmatrix}$								

$$\epsilon = \exp(2\pi i/7), \epsilon^* = \exp(-2\pi i/7)$$

Table A.10

C_8	I	C_8	C_4	C_8^3	C_2	C_8^5	C_4^3	C_8^7		
A	1	1	1	1	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
B	1	-1	1	-1	1	-1	1	-1		
E_1	$\begin{Bmatrix} 1 & \epsilon & i & -\epsilon^* & -1 & -\epsilon & -i & \epsilon^* \\ 1 & \epsilon^* & -i & -\epsilon & -1 & -\epsilon^* & i & \epsilon \end{Bmatrix}$								$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$
E_2	$\begin{Bmatrix} 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & -i & -1 & i & 1 & -i & -1 & i \end{Bmatrix}$									$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_3	$\begin{Bmatrix} 1 & -\epsilon^* & -i & \epsilon & -1 & \epsilon^* & i & -\epsilon \\ 1 & -\epsilon & i & \epsilon^* & -1 & \epsilon & -i & -\epsilon^* \end{Bmatrix}$									

$$\epsilon = \exp(2\pi i/8), \epsilon^* = \exp(-2\pi i/8)$$

Table A.11

C_{2v}	I	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	α_{xy}
B_1	1	-1	1	-1	T_x, R_y	α_{xz}
B_2	1	-1	-1	1	T_y, R_x	α_{yz}

Table A.12

C_{3v}	I	$2C_3$	$3\sigma_v$		
A_1	1	1	1	T_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	-1	R_z	
E	2	-1	0	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{xz}, \alpha_{yz})$

Table A.13

C_{4v}	I	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	T_z R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	-1	-1		
B_1	1	-1	1	1	-1	$(T_x, T_y), (R_x, R_y)$	$\alpha_{xx} - \alpha_{yy}$
B_2	1	-1	1	-1	1		α_{xy}
E	2	0	-2	0	0		$(\alpha_{xz}, \alpha_{yz})$

Table A.14

C_{5v}	I	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	T_z R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	-1		
E_1	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$
E_2	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

Table A.15

C_{6v}	I	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	T_z R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	1	-1	-1		
B_1	1	-1	1	-1	1	-1	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$
B_2	1	-1	1	-1	-1	1		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_1	2	1	-1	-2	0	0		
E_2	2	-1	-1	2	0	0		

Table A.16

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

Table A.17

D_2	I	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1	T_z, R_z T_y, R_y T_x, R_x	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
B_1	1	1	-1	-1		α_{xy}
B_2	1	-1	1	-1		α_{xz}
B_3	1	-1	-1	1		α_{yz}

Table A.18

D_3	I	$2C_3$	$3C_2$		
A_1	1	1	1	T_z, R_z $(T_x, T_y), (R_x, R_y)$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	-1		
E	2	-1	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{xz}, \alpha_{yz})$

Table A.19

D_4	I	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$		
A_1	1	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	-1	-1		
B_1	1	-1	1	1	-1		$\alpha_{xx} - \alpha_{yy}$
B_2	1	-1	1	-1	1		α_{xy}
E	2	0	-2	0	0	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$

Table A.20

D_5	I	$2C_5$	$2C_5^2$	$5C_2$		
A_1	1	1	1	1	T_z, R_z $(T_x, T_y), (R_x, R_y)$	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	-1		
E_1	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0		$(\alpha_{xz}, \alpha_{yz})$
E_2	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

Table A.21

D_6	I	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$		
A_1	1	1	1	1	1	1	T_z, R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_2	1	1	1	1	-1	-1		
B_1	1	-1	1	-1	1	-1		$(\alpha_{xz}, \alpha_{yz})$
B_2	1	-1	1	-1	-1	1		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_1	2	1	-1	-2	0	0	$(T_x, T_y), (R_x, R_y)$	
E_2	2	-1	-1	2	0	0		

Table A.22

C_{2h}	I	C_2	i	σ_h		
A_g	1	1	1	1	R_z R_x, R_y T_z T_x, T_y	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$
B_g	1	-1	1	-1		α_{xz}, α_{yz}
A_u	1	1	-1	-1		
B_u	1	-1	-1	1		

Table A.23

C_{3h}	I	C_3	C_3^2	σ_h	S_3	S_3^5		
A'	1	1	1	1	1	1	R_z T_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A''	1	1	1	-1	-1	-1		
E'	$\begin{Bmatrix} 1 & \epsilon & \epsilon^* \\ 1 & \epsilon^* & \epsilon \end{Bmatrix}$	ϵ	ϵ^*	1	ϵ	ϵ^*	(T_x, T_y)	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E''	$\begin{Bmatrix} 1 & \epsilon & \epsilon^* \\ 1 & \epsilon^* & \epsilon \end{Bmatrix}$	ϵ	ϵ^*	-1	$-\epsilon$	$-\epsilon^*$		$(\alpha_{xz}, \alpha_{yz})$

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

Table A.32

D_{2h}	I	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1	R_z	$\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_y	α_{xy}
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_x	α_{xz}
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	α_{yz}
A_u	1	1	1	1	-1	-1	-1	-1	T_z	
B_{1u}	1	1	-1	-1	-1	-1	1	1	T_y	
B_{2u}	1	-1	1	-1	-1	1	-1	1	T_y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	T_x	

Table A.33

D_{3h}	I	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A'_1	1	1	1	1	1	1	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A'_2	1	1	-1	1	1	-1	(T_x, T_y)	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E'	2	-1	0	2	-1	0		
A''_1	1	1	1	-1	-1	-1	T_z	
A''_2	1	1	-1	-1	-1	1	(R_x, R_y)	$(\alpha_{xz}, \alpha_{yz})$
E''	2	-1	0	-2	1	0		

Table A.34

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

Table A.35

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	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A'_2	1	1	1	-1	1	1	1	-1	(T_x, T_y)	
E'_1	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E'_2	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0		
A''_1	1	1	1	1	-1	-1	-1	-1	T_z	
A''_2	1	1	1	-1	-1	-1	-1	1	(R_x, R_y)	$(\alpha_{xz}, \alpha_{yz})$
E''_1	2	$2\cos 72^\circ$	$2\cos 144^\circ$	0	-2	$-2\cos 72^\circ$	$-2\cos 144^\circ$	0		
E''_2	2	$2\cos 144^\circ$	$2\cos 72^\circ$	0	-2	$-2\cos 144^\circ$	$-2\cos 72^\circ$	0		

Table A.36

D_{6h}	I	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1		
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	(R_x, R_y)	$(\alpha_{xz}, \alpha_{yz})$
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0		
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0		
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	T_z	
A_{2u}	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_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1	(T_x, T_y)	
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0		
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0		

Table A.37

$D_{\infty h}$	I	$2C_\infty^\phi$	$\dots$	$\infty\sigma_v$	i	$2S_\infty^\phi$	$\dots$	∞C_2		
$A_{1g} \equiv \Sigma_g^+$	1	1	$\dots$	1	1	1	$\dots$	1	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$A_{2g} \equiv \Sigma_g^-$	1	1	$\dots$	-1	1	1	$\dots$	-1	(R_x, R_y)	$(\alpha_{xz}, \alpha_{yz})$
$E_{1g} \equiv \Pi_g$	2	$2\cos\phi$	$\dots$	0	2	$-2\cos\phi$	$\dots$	0		$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
$E_{2g} \equiv \Delta_g$	2	$2\cos 2\phi$	$\dots$	0	2	$2\cos 2\phi$	$\dots$	0		
$E_{3g} \equiv \Phi_g$	2	$2\cos 3\phi$	$\dots$	0	2	$-2\cos 3\phi$	$\dots$	0		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$		
$A_{2u} \equiv \Sigma_u^+$	1	1	$\dots$	1	-1	-1	$\dots$	-1	T_z	
$A_{1u} \equiv \Sigma_u^-$	1	1	$\dots$	-1	-1	-1	$\dots$	1	(T_x, T_y)	
$E_{1u} \equiv \Pi_u$	2	$2\cos\phi$	$\dots$	0	-2	$2\cos\phi$	$\dots$	0		
$E_{2u} \equiv \Delta_u$	2	$2\cos 2\phi$	$\dots$	0	-2	$-2\cos 2\phi$	$\dots$	0		
$E_{3u} \equiv \Phi_u$	2	$2\cos 3\phi$	$\dots$	0	-2	$2\cos 3\phi$	$\dots$	0		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$		

Table A.38

S_4	I	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
B	1	-1	1	-1	T_z	$\alpha_{xx} - \alpha_{yy}, \alpha_{xy}$
E	$\begin{Bmatrix} 1 & i \\ 1 & -i \end{Bmatrix}$	$\begin{Bmatrix} i & -1 \\ -i & -1 \end{Bmatrix}$	$\begin{Bmatrix} -1 & -i \\ -1 & i \end{Bmatrix}$	$\begin{Bmatrix} -i & 1 \\ i & 1 \end{Bmatrix}$	$(T_x, T_y), (R_x, R_y)$	$(\alpha_{xz}, \alpha_{yz})$

Table A.39

S_6	I	C_3	C_3^2	i	S_6^5	S_6		
A_g	1	1	1	1	1	1	R_z	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
E_g	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} 1 & \epsilon \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	(R_x, R_y)	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy}), (\alpha_{xz}, \alpha_{yz})$
A_u	1	1	1	-1	-1	-1	T_z	
E_u	$\begin{Bmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} \epsilon & 1 \\ \epsilon^* & 1 \end{Bmatrix}$	$\begin{Bmatrix} \epsilon^* & \epsilon \\ 1 & \epsilon^* \end{Bmatrix}$	$\begin{Bmatrix} -1 & -\epsilon \\ -\epsilon^* & -1 \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon & -\epsilon^* \\ -\epsilon^* & -\epsilon \end{Bmatrix}$	$\begin{Bmatrix} -\epsilon^* & -\epsilon \\ -1 & -\epsilon^* \end{Bmatrix}$	(T_x, T_y)	

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

Table A.40

S_8	I	S_8	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	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
B	1	-1	1	-1	1	-1	1	-1	T_z	
E_1	$\begin{Bmatrix} 1 & \epsilon & i & -\epsilon^* & -1 & -\epsilon & -i & \epsilon^* \end{Bmatrix}$								$(T_x, T_y), (R_x, R_y)$	
E_2	$\begin{Bmatrix} 1 & i & -1 & -i & 1 & i & -1 & -i \end{Bmatrix}$									$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_3	$\begin{Bmatrix} 1 & -\epsilon^* & -i & \epsilon & -1 & \epsilon^* & i & -\epsilon \end{Bmatrix}$									$(\alpha_{xz}, \alpha_{yz})$

$$\epsilon = \exp(2\pi i/8), \epsilon^* = \exp(-2\pi i/8)$$

Table A.41

T_d	I	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
A_2	1	1	1	-1	-1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
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_x, R_y, R_z)	
$T_2 \equiv F_2$	3	0	-1	-1	1	(T_x, T_y, T_z)	$(\alpha_{xy}, \alpha_{xz}, \alpha_{yz})$

Table A.42

T	I	$4C_3$	$4C_3^2$	$3C_2$		
A	1	1	1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
E	$\begin{Bmatrix} 1 & \epsilon & \epsilon^* & 1 \end{Bmatrix}$					$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T \equiv F$	3	0	0	-1	$(T_x, T_y, T_z), (R_x, R_y, R_z)$	$(\alpha_{xy}, \alpha_{xz}, \alpha_{yz})$

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

Table A.43

O_h	I	$8C_3$	$6C_2$	$6C_4$	$3C_2' (= 3C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
A_{2g}	1	1	-1	-1	1	1	-1	-1	1	-1		$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
E_g	2	-1	0	0	2	2	0	-1	2	0		$(\alpha_{xz}, \alpha_{yz}, \alpha_{xy})$
$T_{1g} \equiv F_{1g}$	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
$T_{2g} \equiv F_{2g}$	3	0	1	-1	-1	3	-1	0	-1	1		$(\alpha_{xx}, \alpha_{yy}, \alpha_{zz})$
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
A_{2u}	1	1	-1	-1	1	-1	1	1	1	1		$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
E_u	2	-1	0	0	2	-2	0	1	-2	0		$(\alpha_{xz}, \alpha_{yz}, \alpha_{xy})$
$T_{1u} \equiv F_{1u}$	3	0	-1	1	-1	-3	-1	0	1	1	(T_x, T_y, T_z)	
$T_{2u} \equiv F_{2u}$	3	0	1	-1	-1	-3	1	0	1	-1		$(\alpha_{xx}, \alpha_{yy}, \alpha_{zz})$

Table A.44

O	I	$8C_3$	$6C_2$	$6C_4$	$3C_2' (= 3C_4^2)$		
A_1	1	1	1	1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
A_2	1	1	-1	-1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
E	2	-1	0	0	2		$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$T_1 \equiv F_1$	3	0	-1	1	-1	$(T_x, T_y, T_z), (R_x, R_y, R_z)$	
$T_2 \equiv F_2$	3	0	1	-1	-1		$(\alpha_{xy}, \alpha_{xz}, \alpha_{yz})$

Table A.45

K_h	I	$\infty C_n^k \dots$	$\infty S_n^k \dots$	i		
S_6	1	1	1	1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
S_6	1	1	-1	-1		$\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
P_6	3	$1 + 2\cos\phi$	$1 - 2\cos\phi$	1	(R_x, R_y, R_z)	
P_6	3	$1 + 2\cos\phi$	$-1 + 2\cos\phi$	-1	(T_x, T_y, T_z)	
D_6	5	$1 + 2\cos\phi + 2\cos 2\phi$	$1 - 2\cos\phi + 2\cos 2\phi$	1		$(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy}, \alpha_{xy}, \alpha_{xz}, \alpha_{yz})$
D_u	5	$1 + 2\cos\phi + 2\cos 2\phi$	$-1 + 2\cos\phi - 2\cos 2\phi$	-1		
F_g	7	$1 + 2\cos\phi + 2\cos 2\phi + 2\cos 3\phi$	$1 - 2\cos\phi + 2\cos 2\phi - 2\cos 3\phi$	1		
F_u	7	$1 + 2\cos\phi + 2\cos 2\phi + 2\cos 3\phi$	$-1 + 2\cos\phi - 2\cos 2\phi + 2\cos 3\phi$	-1		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$		

Convenis d'orientació d'eixos

- 1) orige al cdm
- 2) eix z e's l'eix principal
 - si hi ha mes d'ú, el que passe per mes atòms
 - Pel major nombre d'enllaços en cas de dubte
- 3) En molècules planes x es perpendicular al eix molecular a no ser que coincideixi amb z segons el conveni anterior