Appendix A
Character Tables

Contents

Character tables were introduced to chemistry through the pioneering work of Robert Mulliken [1]. The book on "Chemical Applications of Group Theory" by F. Albert Cotton has been instrumental in disseminating their use in chemistry [2]. Atkins, Child, and Phillips [3] produced a handy pamphlet of the point group character tables.[1]

[1] In the tables the columns on the right list representative coordinate functions that transform according to the corresponding irrep. The symbols R_x, R_y, R_z stand for rotations about the Cartesian directions.

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A.1 Finite Point Groups

C_1 and the Binary Groups C_s, C_i, C_2

C_1	$\hat{E}$
A	1

C_s	$\hat{E}$	$\hat{\sigma}_h$		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz

C_i	$\hat{E}$	$\hat{\imath}$		
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, yz, xz, xy$
A_u	1	-1	x, y, z	

C_2	$\hat{E}$	$\hat{C}_2^z$		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	-1	x, y, R_x, R_y	yz, xz

The Cyclic Groups C_n ($n = 3, 4, 5, 6, 7, 8$)

C_3	$\hat{E}$	$\hat{C}_3$	$\hat{C}_3^2$	$\epsilon = \exp(2\pi i/3)$	
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E {	1	ϵ	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(yz, xz)$
	1	$\bar{\epsilon}$	ϵ		

C_4	$\hat{E}$	$\hat{C}_4$	$\hat{C}_2$	$\hat{C}_4^3$		
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 {	1	i	-1	$-i$	$(x, y)(R_x, R_y)$	(yz, xz)
	1	$-i$	-1	i		

C_5		$\hat{E}$	$\hat{C}_5$	$\hat{C}_5^2$	$\hat{C}_5^3$	$\hat{C}_5^4$	$\epsilon = \exp(2\pi i/5)$	
A		1	1	1	1	1	z, R_z	x^2+y^2, z^2
E_1	{	1	ϵ	ϵ^2	$\bar{\epsilon}^2$	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	(yz, xz)
		1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	ϵ^2	ϵ		
E_2	{	1	ϵ^2	$\bar{\epsilon}$	ϵ	$\bar{\epsilon}^2$		(x^2-y^2, xy)
		1	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}$	ϵ^2		

C_6		$\hat{E}$	$\hat{C}_6$	$\hat{C}_3$	$\hat{C}_2$	$\hat{C}_3^2$	$\hat{C}_6^5$	$\epsilon = \exp(2\pi i/6)$	
A		1	1	1	1	1	1	z, R_z	x^2+y^2, z^2
B		1	-1	1	-1	1	-1		
E_1	{	1	ϵ	$-\bar{\epsilon}$	-1	$-\epsilon$	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	(yz, xz)
		1	$\bar{\epsilon}$	$-\epsilon$	-1	$-\bar{\epsilon}$	ϵ		
E_2	{	1	$-\bar{\epsilon}$	$-\epsilon$	1	$-\bar{\epsilon}$	$-\epsilon$		(x^2-y^2, xy)
		1	$-\epsilon$	$-\bar{\epsilon}$	1	$-\epsilon$	$-\bar{\epsilon}$		

C_7		$\hat{E}$	$\hat{C}_7$	$\hat{C}_7^2$	$\hat{C}_7^3$	$\hat{C}_7^4$	$\hat{C}_7^5$	$\hat{C}_7^6$	$\epsilon = \exp(2\pi i/7)$	
A		1	1	1	1	1	1	1	z, R_z	x^2+y^2, z^2
E_1	{	1	ϵ	ϵ^2	ϵ^3	$\bar{\epsilon}^3$	$\bar{\epsilon}^2$	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	(yz, xz)
		1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	$\bar{\epsilon}^3$	ϵ^3	ϵ^2	ϵ		
E_2	{	1	ϵ^2	$\bar{\epsilon}^3$	$\bar{\epsilon}$	ϵ	ϵ^3	$\bar{\epsilon}^2$		(x^2-y^2, xy)
		1	$\bar{\epsilon}^2$	ϵ^3	ϵ	$\bar{\epsilon}$	$\bar{\epsilon}^3$	ϵ^2		
E_3	{	1	ϵ^3	$\bar{\epsilon}$	ϵ^2	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}^3$		$[x(x^2-3y^2),$
		1	$\bar{\epsilon}^3$	ϵ	$\bar{\epsilon}^2$	ϵ^2	$\bar{\epsilon}$	ϵ^3		$y(3x^2-y^2)]$

C_8		$\hat{E}$	$\hat{C}_8$	$\hat{C}_4$	$\hat{C}_2$	$\hat{C}_4^3$	$\hat{C}_8^3$	$\hat{C}_8^5$	$\hat{C}_8^7$	$\epsilon = \exp(2\pi i/8)$	
A		1	1	1	1	1	1	1	1	z, R_z	x^2+y^2, z^2
B		1	-1	1	1	1	-1	-1	-1		
E_1	{	1	ϵ	i	-1	$-i$	$-\bar{\epsilon}$	$-\epsilon$	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	(yz, xz)
		1	$\bar{\epsilon}$	$-i$	-1	i	$-\epsilon$	$-\bar{\epsilon}$	ϵ		
E_2	{	1	i	-1	1	-1	$-i$	i	$-i$		(x^2-y^2, xy)
		1	$-i$	-1	1	-1	i	$-i$	i		
E_3	{	1	$-\epsilon$	i	-1	$-i$	$\bar{\epsilon}$	ϵ	$-\bar{\epsilon}$		$[x(x^2-3y^2),$
		1	$-\bar{\epsilon}$	$-i$	-1	i	ϵ	$\bar{\epsilon}$	$-\epsilon$		$y(3x^2-y^2)]$

The Dihedral Groups D_n (n = 2, 3, 4, 5, 6)

D_2	$\hat{E}$	$\hat{C}_2^z$	$\hat{C}_2^y$	$\hat{C}_2^x$		
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

D_3	$\hat{E}$	$2\hat{C}_3$	$3\hat{C}_2$		
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	−1	z, R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(xz, yz)(x^2-y^2, xy)$

D_4	$\hat{E}$	$2\hat{C}_4$	$\hat{C}_2\ (=\hat{C}_4^2)$	$2\hat{C}_2'$	$2\hat{C}_2''$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	−1	−1	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	$(x, y)(R_x, R_y)$	(xz, yz)

D_5	$\hat{E}$	$2\hat{C}_5$	$2\hat{C}_5^2$	$5\hat{C}_2'$		
A_1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	−1	z, R_z	
E_1	2	$2\cos(2\pi/5)$	$2\cos(4\pi/5)$	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	$2\cos(4\pi/5)$	$2\cos(2\pi/5)$	0		(x^2-y^2, xy)

D_6	$\hat{E}$	$2\hat{C}_6$	$2\hat{C}_3$	$\hat{C}_2$	$3\hat{C}_2'$	$3\hat{C}_2''$		
A_1	1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	1	−1	−1	z, R_z	
B_1	1	−1	1	−1	1	−1		$x(x^2-3y^2)$
B_2	1	−1	1	−1	−1	1		$y(3x^2-y^2)$
E_1	2	1	−1	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		(x^2-y^2, xy)

The Conical Groups C_{nv} ($n = 2, 3, 4, 5, 6$)

C_{2v}	$\hat{E}$	$\hat{C}_2^z$	$\hat{\sigma}_v^{xz}$	$\hat{\sigma}_v^{yz}$		
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

C_{3v}	$\hat{E}$	$2\hat{C}_3$	$3\hat{\sigma}_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

C_{4v}	$\hat{E}$	$2\hat{C}_4$	$\hat{C}_2$	$2\hat{\sigma}_v$	$2\hat{\sigma}_d$		
A_1	1	1	1	1	1	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	$(x, y)(R_x, R_y)$	(xz, yz)

C_{5v}	$\hat{E}$	$2\hat{C}_5$	$2\hat{C}_5^2$	$5\hat{\sigma}_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	R_z	
E_1	2	$2\cos(2\pi/5)$	$2\cos(4\pi/5)$	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	$2\cos(4\pi/5)$	$2\cos(2\pi/5)$	0		$(x^2 - y^2, xy)$

C_{6v}	$\hat{E}$	$2\hat{C}_6$	$2\hat{C}_3$	$\hat{C}_2$	$3\hat{\sigma}_v$	$3\hat{\sigma}_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	−1		$x(x^2 - 3y^2)$
B_2	1	−1	1	−1	−1	1		$y(3x^2 - y^2)$
E_1	2	1	−1	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

The C_{nh} Groups ($n = 2, 3, 4, 5, 6$)

C_{2h}	$\hat{E}$	$\hat{C}_2^z$	$\hat{\imath}$	$\hat{\sigma}_h$		
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	

C_{3h}	$\hat{E}$	$\hat{C}_3$	$\hat{C}_3^2$	$\hat{\sigma}_h$	$\hat{S}_3$	$\hat{S}_3^2$	$\epsilon = \exp(2\pi i/3)$	
A'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E'	1	ϵ	$\bar{\epsilon}$	1	ϵ	$\bar{\epsilon}$	(x, y)	$(x^2 - y^2, xy)$
	1	$\bar{\epsilon}$	ϵ	1	$\bar{\epsilon}$	ϵ		
A''	1	1	1	−1	−1	−1	z	
E''	1	ϵ	$\bar{\epsilon}$	−1	$-\epsilon$	$-\bar{\epsilon}$	(R_x, R_y)	(xz, yz)
	1	$\bar{\epsilon}$	ϵ	−1	$-\bar{\epsilon}$	$-\epsilon$		

C_{4h}	$\hat{E}$	$\hat{C}_4$	$\hat{C}_2$	$\hat{C}_4^3$	$\hat{\imath}$	$\hat{S}_4^3$	$\hat{\sigma}_h$	$\hat{S}_4$		
A_g	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
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)	(yz, xz)
	1	$-i$	−1	i	1	$-i$	−1	i		
A_u	1	1	1	1	−1	−1	−1	−1	z	
B_u	1	−1	1	−1	−1	1	−1	1		
E_u	1	i	−1	$-i$	−1	$-i$	1	i	(x, y)	
	1	$-i$	−1	i	−1	i	1	$-i$		

C_{5h}	$\hat{E}$	$\hat{C}_5$	$\hat{C}_5^2$	$\hat{C}_5^3$	$\hat{C}_5^4$	$\hat{\sigma}_h$	$\hat{S}_5$	$\hat{S}_5^7$	$\hat{S}_5^3$	$\hat{S}_5^9$	$\epsilon = \exp(2\pi i/5)$	
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	$\bar{\epsilon}^2$	$\bar{\epsilon}$	1	ϵ	ϵ^2	$\bar{\epsilon}^2$	$\bar{\epsilon}$	(x, y)	
	1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	ϵ^2	ϵ	1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	ϵ^2	ϵ		
E_2'	1	ϵ^2	$\bar{\epsilon}$	ϵ	$\bar{\epsilon}^2$	1	ϵ^2	$\bar{\epsilon}$	ϵ	$\bar{\epsilon}^2$		$(x^2 - y^2, xy)$
	1	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}$	ϵ^2	1	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}$	ϵ^2		
A''	1	1	1	1	1	−1	−1	−1	−1	−1	z	
E_1''	1	ϵ	ϵ^2	$\bar{\epsilon}^2$	$\bar{\epsilon}$	−1	$-\epsilon$	$-\epsilon^2$	$-\bar{\epsilon}^2$	$-\bar{\epsilon}$	(R_x, R_y)	(xz, yz)
	1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	ϵ^2	ϵ	−1	$-\bar{\epsilon}$	$-\bar{\epsilon}^2$	$-\epsilon^2$	$-\epsilon$		
E_2''	1	ϵ^2	$\bar{\epsilon}$	ϵ	$\bar{\epsilon}^2$	−1	$-\epsilon^2$	$-\bar{\epsilon}$	$-\epsilon$	$-\bar{\epsilon}^2$		
	1	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}$	ϵ^2	−1	$-\bar{\epsilon}^2$	$-\epsilon$	$-\bar{\epsilon}$	$-\epsilon^2$		

C_{6h}	$\hat{E}$	$\hat{C}_6$	$\hat{C}_3$	$\hat{C}_2$	$\hat{C}_3^2$	$\hat{C}_6^5$	$\hat{\imath}$	$\hat{S}_3^5$	$\hat{S}_6^5$	$\hat{\sigma}_h$	$\hat{S}_6$	$\hat{S}_3$	$\epsilon = \exp(2\pi i/6)$	
A_g	1	1	1	1	1	1	1	1	1	1	1	1	R_z	x^2+y^2, z^2
B_g	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		
E_{1g}	1	ϵ	$-\bar{\epsilon}$	-1	$-\epsilon$	$\bar{\epsilon}$	1	ϵ	$-\bar{\epsilon}$	-1	$-\epsilon$	$\bar{\epsilon}$	(R_x, R_y)	(yz, xz)
	1	$\bar{\epsilon}$	$-\epsilon$	-1	$-\bar{\epsilon}$	ϵ	1	$\bar{\epsilon}$	$-\epsilon$	-1	$-\bar{\epsilon}$	ϵ		
E_{2g}	1	$-\bar{\epsilon}$	$-\epsilon$	1	$-\bar{\epsilon}$	$-\epsilon$	1	$-\bar{\epsilon}$	$-\epsilon$	1	$-\bar{\epsilon}$	$-\epsilon$		
	1	$-\epsilon$	$-\bar{\epsilon}$	1	$-\epsilon$	$-\bar{\epsilon}$	1	$-\epsilon$	$-\bar{\epsilon}$	1	$-\epsilon$	$-\bar{\epsilon}$		
A_u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	z	x^2+y^2, z^2
B_u	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		
E_{1u}	1	ϵ	$-\bar{\epsilon}$	-1	$-\epsilon$	$\bar{\epsilon}$	-1	$-\epsilon$	$\bar{\epsilon}$	1	ϵ	$-\bar{\epsilon}$	(x, y)	
	1	$\bar{\epsilon}$	$-\epsilon$	-1	$-\bar{\epsilon}$	ϵ	-1	$-\bar{\epsilon}$	ϵ	1	$\bar{\epsilon}$	$-\epsilon$		
E_{2u}	1	$-\bar{\epsilon}$	$-\epsilon$	1	$-\bar{\epsilon}$	$-\epsilon$	-1	$\bar{\epsilon}$	ϵ	-1	$\bar{\epsilon}$	ϵ		
	1	$-\epsilon$	$-\bar{\epsilon}$	1	$-\epsilon$	$-\bar{\epsilon}$	-1	ϵ	$\bar{\epsilon}$	-1	ϵ	$\bar{\epsilon}$		

The Rotation–Reflection Groups S_{2n} ($n = 2, 3, 4$)

S_4	$\hat{E}$	$\hat{S}_4$	$\hat{C}_2$	$\hat{S}_4^3$		
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	1	i	-1	$-i$	$(x, y)(R_x, R_y)$	(xz, yz)
	1	$-i$	-1	i		

S_6	$\hat{E}$	$\hat{C}_3$	$\hat{C}_3^2$	$\hat{\imath}$	$\hat{S}_6^5$	$\hat{S}_6$	$\epsilon = \exp(2\pi i/3)$	
A_g	1	1	1	1	1	1	R_z	x^2+y^2, z^2
E_g	1	ϵ	$\bar{\epsilon}$	1	ϵ	$\bar{\epsilon}$	(R_x, R_y)	$(x^2-y^2, xy)(yz, xz)$
	1	$\bar{\epsilon}$	ϵ	1	$\bar{\epsilon}$	ϵ		
A_u	1	1	1	-1	-1	-1	z	
E_u	1	ϵ	$\bar{\epsilon}$	-1	$-\epsilon$	$-\bar{\epsilon}$	(x, y)	
	1	$\bar{\epsilon}$	ϵ	-1	$-\bar{\epsilon}$	$-\epsilon$		

S_8	$\hat{E}$	$\hat{S}_8$	$\hat{C}_4$	$\hat{S}_8^3$	$\hat{C}_2$	$\hat{S}_8^5$	$\hat{C}_4^3$	$\hat{S}_8^7$	$\epsilon = \exp(2\pi i/8)$	
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	z	
E_1	1	ϵ	i	$-\bar{\epsilon}$	-1	$-\epsilon$	$-i$	$\bar{\epsilon}$	$(x, y)(R_x, R_y)$	
	1	$\bar{\epsilon}$	$-i$	$-\epsilon$	-1	$-\bar{\epsilon}$	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	$-\bar{\epsilon}$	$-i$	ϵ	-1	$\bar{\epsilon}$	i	$-\epsilon$		(xz, yz)
	1	$-\epsilon$	i	$\bar{\epsilon}$	-1	ϵ	$-i$	$-\bar{\epsilon}$		

The Prismatic Groups D_{nh} ($n = 2, 3, 4, 5, 6, 8$)

D_{2h}	$\hat{E}$	$\hat{C}_2^z$	$\hat{C}_2^y$	$\hat{C}_2^x$	$\hat{\imath}$	$\hat{\sigma}_{xy}$	$\hat{\sigma}_{xz}$	$\hat{\sigma}_{yz}$		
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		xyz
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	

D_{3h}	$\hat{E}$	$2\hat{C}_3$	$3\hat{C}_2$	$\hat{\sigma}_h$	$2\hat{S}_3$	$3\hat{\sigma}_v$		
A'_1	1	1	1	1	1	1		x^2+y^2, z^2
A'_2	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	(x^2-y^2, xy)
A''_1	1	1	1	−1	−1	−1		
A''_2	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	$\hat{E}$	$2\hat{C}_4$	$\hat{C}_2$	$2\hat{C}'_2$	$2\hat{C}''_2$	$\hat{\imath}$	$2\hat{S}_4$	$\hat{\sigma}_h$	$2\hat{\sigma}_v$	$2\hat{\sigma}_d$		
A_{1g}	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	R_z	
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1		x^2-y^2
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1		xy
E_g	2	0	−2	0	0	2	0	−2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	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	(x, y)	

D_{5h}	$\hat{E}$	$2\hat{C}_5$	$2\hat{C}_5^2$	$5\hat{C}_2$	$\hat{\sigma}_h$	$2\hat{S}_5$	$2\hat{S}_5^3$	$5\hat{\sigma}_v$	$\alpha = \cos(2\pi/5)$	$\beta = \cos(4\pi/5)$
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	2α	2β	0	2	2α	2β	0	(x, y)	
E'_2	2	2β	2α	0	2	2β	2α	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	z	
E''_1	2	2α	2β	0	−2	-2α	-2β	0	(R_x, R_y)	
E''_2	2	2β	2α	0	−2	-2β	-2α	0		(xz, yz)

D_{6h}	$\hat{E}$	$2\hat{C}_6$	$2\hat{C}_3$	$\hat{C}_2$	$3\hat{C}_2'$	$3\hat{C}_2''$	$\hat{\imath}$	$2\hat{S}_3$	$2\hat{S}_6$	$\hat{\sigma}_h$	$3\hat{\sigma}_d$	$3\hat{\sigma}_v$	
A_{1g}	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	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	$(R_x, R_y)(xz, yz)$
E_{2g}	2	−1	−1	2	0	0	2	−1	−1	2	0	0	(x^2-y^2, 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	z
B_{1u}	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	$x(x^2-3y^2)$
B_{2u}	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1	$y(3x^2-y^2)$
E_{1u}	2	1	−1	−2	0	0	−2	−1	1	2	0	0	(x, y)
E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0	

D_{8h}	$\hat{E}$	$2\hat{C}_8$	$2\hat{C}_8^3$	$2\hat{C}_4$	$\hat{C}_2$	$4\hat{C}_2'$	$4\hat{C}_2''$	$\hat{\imath}$	$2\hat{S}_8^3$	$2\hat{S}_8$	$2\hat{S}_4$	$\hat{\sigma}_h$	$4\hat{\sigma}_v$	$4\hat{\sigma}_d$
A_{1g}	1	1	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	−1	−1
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	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0
E_{2g}	2	0	0	−2	2	0	0	2	0	0	−2	2	0	0
E_{3g}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	2	$-\sqrt{2}$	$\sqrt{2}$	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
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	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	−2	$-\sqrt{2}$	$\sqrt{2}$	0	2	0	0
E_{2u}	2	0	0	−2	2	0	0	−2	0	0	2	−2	0	0
E_{3u}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	−2	$\sqrt{2}$	$-\sqrt{2}$	0	2	0	0

The Antiprismatic Groups D_{nd} ($n = 2, 3, 4, 5, 6$)

D_{2d}	$\hat{E}$	$2\hat{S}_4$	$\hat{C}_2$	$2\hat{C}_2'$	$2\hat{\sigma}_d$		
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	$(x, y)(R_x, R_y)$	(xz, yz)

D_{3d}	$\hat{E}$	$2\hat{C}_3$	$3\hat{C}_2$	$\hat{\imath}$	$2\hat{S}_6$	$3\hat{\sigma}_d$		
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)	

D_{4d}	$\hat{E}$	$2\hat{S}_8$	$2\hat{C}_4$	$2\hat{S}_8^3$	$\hat{C}_2$	$4\hat{C}_2'$	$4\hat{\sigma}_d$		
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	z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(x, 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)	(xz, yz)

D_{5d}	$\hat{E}$	$2\hat{C}_5$	$2\hat{C}_5^2$	$5\hat{C}_2$	$\hat{\imath}$	$2\hat{S}_{10}^3$	$2\hat{S}_{10}$	$5\hat{\sigma}_d$	$\alpha=\cos(2\pi/5)$	$\beta=\cos(4\pi/5)$
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	2α	2β	0	2	2α	2β	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	2β	2α	0	2	2β	2α	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	z	
E_{1u}	2	2α	2β	0	−2	-2α	-2β	0	(x, y)	
E_{2u}	2	2β	2α	0	−2	-2β	-2α	0		

D_{6d}	$\hat{E}$	$2\hat{S}_{12}$	$2\hat{C}_6$	$2\hat{S}_4$	$2\hat{C}_3$	$2\hat{S}_{12}^5$	$\hat{C}_2$	$6\hat{C}_2'$	$6\hat{\sigma}_d$		
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	z	
E_1	2	$\sqrt{3}$	1	0	−1	$-\sqrt{3}$	−2	0	0	(x, 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)

The Tetrahedral and Cubic Groups

T	$\hat{E}$	$4\hat{C}_3$	$4\hat{C}_3^2$	$3\hat{C}_2$	$\epsilon = \exp(2\pi i/3)$	
A	1	1	1	1		$x^2 + y^2 + z^2$
E	1	ϵ	$\bar{\epsilon}$	1		$(2z^2 - x^2 - y^2, x^2 - y^2)$
	1	$\bar{\epsilon}$	ϵ	1		
T	3	0	0	−1	$(R_x, R_y, R_z)(x, y, z)$	(xz, yx, xy)

T_d	$\hat{E}$	$8\hat{C}_3$	$3\hat{C}_2$	$6\hat{S}_4$	$6\hat{\sigma}_d$		
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)	(xz, yz, xy)

T_h	$\hat{E}$	$4\hat{C}_3$	$4\hat{C}_3^2$	$3\hat{C}_2$	$\hat{\imath}$	$4\hat{S}_6^5$	$4\hat{S}_6$	$3\hat{\sigma}_h$	$\epsilon = \exp(2\pi i/3)$	
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		
E_g	1	ϵ	$\bar{\epsilon}$	1	1	ϵ	$\bar{\epsilon}$	1		$(2z^2 - x^2 - y^2,$
	1	$\bar{\epsilon}$	ϵ	1	1	$\bar{\epsilon}$	ϵ	1		$x^2 - y^2)$
E_u	1	ϵ	$\bar{\epsilon}$	1	−1	$-\epsilon$	$-\bar{\epsilon}$	−1		
	1	$\bar{\epsilon}$	ϵ	1	−1	$-\bar{\epsilon}$	$-\epsilon$	−1		
T_g	3	0	0	−1	3	0	0	−1	(R_x, R_y, R_z)	(xz, yz, xy)
T_u	3	0	0	−1	−3	0	0	1	(x, y, z)	

O	$\hat{E}$	$6\hat{C}_4$	$3\hat{C}_2\ (= \hat{C}_4^2)$	$8\hat{C}_3$	$6\hat{C}_2$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	−1	1	1	−1		
E	2	0	2	−1	0		$(2z^2 - x^2 - y^2,$ $x^2 - y^2)$
T_1	3	1	−1	0	−1	$(R_x, R_y, R_z)(x, y, z)$	
T_2	3	−1	−1	0	1		(xz, yz, xy)

O_h	$\hat{E}$	$8\hat{C}_3$	$6\hat{C}_2$	$6\hat{C}_4$	$3\hat{C}_2$	$\hat{\imath}$	$6\hat{S}_4$	$8\hat{S}_6$	$3\hat{\sigma}_h$	$6\hat{\sigma}_d$		
A_{1g}	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		
E_g	2	−1	0	0	2	2	0	−1	2	0		$(2z^2-x^2-y^2,$ $x^2-y^2)$
T_{1g}	3	0	−1	1	−1	3	1	0	−1	−1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	−1	−1	3	−1	0	−1	1		(xz, yz, xy)
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	0	0	2	−2	0	1	−2	0		
T_{1u}	3	0	−1	1	−1	−3	−1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

The Icosahedral Groups

I	$\hat{E}$	$12\hat{C}_5$	$12\hat{C}_5^2$	$20\hat{C}_3$	$15\hat{C}_2$	$\phi=(1+\sqrt{5})/2$	
A	1	1	1	1	1		$x^2+y^2+z^2$
T_1	3	ϕ	$-\phi^{-1}$	0	−1	$(R_x, R_y, R_z)(x, y, z)$	
T_2	3	$-\phi^{-1}$	ϕ	0	−1		
G	4	−1	−1	1	0		
H	5	0	0	−1	1		$(2z^2-x^2-y^2,$ $x^2-y^2,$ (xz, yz, xy)

I_h	$\hat{E}$	$12\hat{C}_5$	$12\hat{C}_5^2$	$20\hat{C}_3$	$15\hat{C}_2$	$\hat{\imath}$	$12\hat{S}_{10}$	$12\hat{S}_{10}^3$	$20\hat{S}_6$	$15\hat{\sigma}$	$\phi=(1+\sqrt{5})/2$
A_g	1	1	1	1	1	1	1	1	1	1	$x^2+y^2+z^2$
T_{1g}	3	ϕ	$-\phi^{-1}$	0	−1	3	$-\phi^{-1}$	ϕ	0	−1	(R_x, R_y, R_z)
T_{2g}	3	$-\phi^{-1}$	ϕ	0	−1	3	ϕ	$-\phi^{-1}$	0	−1	
G_g	4	−1	−1	1	0	4	−1	−1	1	0	
H_g	5	0	0	−1	1	5	0	0	−1	1	$(2z^2-x^2-y^2,$ $x^2-y^2,$ $xz, yz, xy)$
A_u	1	1	1	1	1	−1	−1	−1	−1	−1	
T_{1u}	3	ϕ	$-\phi^{-1}$	0	−1	−3	ϕ^{-1}	$-\phi$	0	1	(x, y, z)
T_{2u}	3	$-\phi^{-1}$	ϕ	0	−1	−3	$-\phi$	ϕ^{-1}	0	1	
G_u	4	−1	−1	1	0	−4	1	1	−1	0	
H_u	5	0	0	−1	1	−5	0	0	1	−1	

A.2 Infinite Groups

Cylindrical Symmetry

C_∞	$\hat{E}$	$\hat{C}_2$	$\hat{C}_\phi$		
Σ	1	1	1	z	x^2+y^2, z^2
Π	1	-1	$\exp(i\phi)$	(x, y)	(xz, yz)
	1	-1	$\exp(-i\phi)$		
Δ	1	1	$\exp(2i\phi)$		(x^2-y^2, xy)
	1	1	$\exp(-2i\phi)$		
Φ	1	-1	$\exp(3i\phi)$		$[x(x^2-3y^2), y(3x^2-y^2)]$
	1	-1	$\exp(-3i\phi)$		

$C_{\infty v}$	$\hat{E}$	$\hat{C}_2$	$2\hat{C}_\phi$	$\infty\hat{\sigma}_v$		
Σ^+	1	1	1	1	z	x^2+y^2, z^2
Σ^-	1	1	1	-1	R_z	
Π	2	-2	$2\cos(\phi)$	0	$(x, y)(R_x, R_y)$	(xz, yz)
Δ	2	2	$2\cos(2\phi)$	0		(x^2-y^2, xy)
Φ	2	-2	$2\cos(3\phi)$	0		

$C_{\infty h}$	$\hat{E}$	$\hat{C}_2$	$\hat{C}_\phi$	$\hat{\imath}$	$\hat{S}_\phi$	$\hat{\sigma}_h$		
Σ_g	1	1	1	1	1	1		x^2+y^2, z^2
Π_g	1	-1	$\exp(i\phi)$	1	$-\exp(i\phi)$	-1		(xz, yz)
	1	-1	$\exp(-i\phi)$	1	$-\exp(-i\phi)$	-1		
Δ_g	1	1	$\exp(2i\phi)$	1	$\exp(2i\phi)$	1		(x^2-y^2, xy)
	1	1	$\exp(-2i\phi)$	1	$\exp(-2i\phi)$	1		
Φ_g	1	-1	$\exp(3i\phi)$	1	$-\exp(3i\phi)$	-1		
	1	-1	$\exp(-3i\phi)$	1	$-\exp(-3i\phi)$	-1		
Σ_u	1	1	1	-1	-1	-1	z	z^3
Π_u	1	-1	$\exp(i\phi)$	-1	$\exp(i\phi)$	1	(x, y)	(xz^2, yz^2)
	1	-1	$\exp(-i\phi)$	-1	$\exp(-i\phi)$	1		
Δ_u	1	1	$\exp(2i\phi)$	-1	$-\exp(2i\phi)$	-1		$((x^2-y^2)z,$
	1	1	$\exp(-2i\phi)$	-1	$-\exp(-2i\phi)$	-1		$xyz)$
Φ_u	1	-1	$\exp(3i\phi)$	-1	$\exp(3i\phi)$	1		
	1	-1	$\exp(-3i\phi)$	-1	$\exp(-3i\phi)$	1		

$D_{\infty h}$	$\hat{E}$	$\hat{C}_2^z$	$2\hat{C}_\phi$	$\infty\hat{\sigma}_v$	$\hat{\imath}$	$2\hat{S}_\phi$	$\infty\hat{C}_2^\perp$		
Σ_g^+	1	1	1	1	1	1	1		x^2+y^2, z^2
Σ_g^-	1	1	1	−1	1	1	−1	R_z	
Π_g	2	−2	$2\cos(\phi)$	0	2	$-2\cos(\phi)$	0	(R_x, R_y)	(xz, yz)
Δ_g	2	2	$2\cos(2\phi)$	0	2	$2\cos(2\phi)$	0		(x^2-y^2, xy)
Φ_g	2	−2	$2\cos(3\phi)$	0	2	$-2\cos(3\phi)$	0		
...									
Σ_u^+	1	1	1	1	−1	−1	−1	z	
Σ_u^-	1	1	1	−1	−1	−1	1		
Π_u	2	−2	$2\cos(\phi)$	0	−2	$2\cos(\phi)$	0	(x, y)	
Δ_u	2	2	$2\cos(2\phi)$	0	−2	$-2\cos(2\phi)$	0		
Φ_u	2	−2	$2\cos(3\phi)$	0	−2	$2\cos(3\phi)$	0		

Spherical Symmetry

$SO(3)$	$\hat{E}$	$\infty\hat{C}_\alpha^{\phi\theta}$		
S	1	1		$x^2+y^2+z^2$
P	3	$1+2\cos\alpha$	$(x, y, z)(R_x, R_y, R_z)$	
D	5	$1+2\cos\alpha+2\cos 2\alpha$		$(2z^2-x^2-y^2,$ $x^2-y^2, xz, yz, xy)$
...				
L	$2L+1$	$\frac{\sin(L+\frac{1}{2})\alpha}{sin\frac{1}{2}\alpha}$		

$O(3)$	$\hat{E}$	$\infty\hat{C}_\alpha^{\phi\theta}$	$\hat{\imath}$	$\infty\hat{\sigma}$	$\infty\hat{S}_\alpha^{\theta,\phi}$	
S_g	1	1	1	1	1	$x^2+y^2+z^2$
P_g	3	$1+2\cos\alpha$	3	−1	$1-2\cos\alpha$	(R_x, R_y, R_z)
D_g	5	$1+2\cos\alpha$ $+2\cos 2\alpha$	5	1	$1-2\cos\alpha$ $+2\cos 2\alpha$	d-orbitals
L_g	$2L+1$	$\frac{\sin(L+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha}$	$2L+1$	$(-1)^L$	$\frac{(-1)^L\cos(L+\frac{1}{2})\alpha}{\cos\frac{1}{2}\alpha}$	
...						
S_u	1	1	−1	−1	−1	
P_u	3	$1+2\cos\alpha$	−3	1	$-1+2\cos\alpha$	p-orbitals
D_u	5	$1+2\cos\alpha$ $+2\cos 2\alpha$	−5	−1	$-1+2\cos\alpha$ $-2\cos 2\alpha$	
L_u	$2L+1$	$\frac{\sin(L+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha}$	$-(2L+1)$	$(-1)^{L+1}$	$\frac{(-1)^{L+1}\cos(L+\frac{1}{2})\alpha}{\cos\frac{1}{2}\alpha}$	

Appendix B
Symmetry Breaking by Uniform Linear Electric and Magnetic Fields

Contents

B.1 Spherical Groups

G	B	E
T	C_3, C_2, C_1	C_3, C_2, C_1
T_d	S_4, C_3, C_2, C_s, C_1	C_{3v}, C_{2v}, C_s, C_1
T_h	S_6, C_{2h}, C_i	C_3, C_2, C_s, C_1
O	C_4, C_3, C_2, C_1	C_4, C_3, C_2, C_1
O_h	C_{4h}, S_6, C_{2h}, C_i	$C_{4v}, C_{3v}, C_{2v}, C_s, C_1$
I	C_5, C_3, C_2, C_1	C_5, C_3, C_2, C_1
I_h	S_{10}, S_6, C_{2h}, C_i	$C_{5v}, C_{3v}, C_{2v}, C_s, C_1$

B.2 Binary and Cylindrical Groups

The $\parallel$ notation refers to a field oriented along the principal cylindrical axis; in the $\perp$ direction several symmetry breakings are possible: C_2 symmetry implies that the field coincides with the $\hat{C}_2$ axis; a magnetic field perpendicular to a symmetry plane or an electric field in a symmetry plane will conserve at least C_s symmetry.

A.J. Ceulemans, *Group Theory Applied to Chemistry*, Theoretical Chemistry and Computational Modelling, DOI 10.1007/978-94-007-6863-5,

G	B		E	
	$\parallel$	$\perp$	$\parallel$	$\perp$
C_i	C_i		C_1	
C_s	C_1	C_s	C_s	C_1
C_2	C_2	C_1	C_2	C_1
C_n	C_n	C_1	C_n	C_1
D_n	C_n	C_2, C_1	C_n	C_2, C_1
C_{nv}	C_n	C_s, C_1	C_{nv}	C_s, C_1
C_{2nh}	C_{2nh}	C_i	C_{2n}	C_s
$C_{(2n+1)h}$	$C_{(2n+1)h}$	C_1	C_{2n+1}	C_s
S_{4n}	S_{4n}	C_1	C_{2n}	C_1
S_{4n+2}	S_{4n+2}	C_i	C_{2n+1}	C_1
D_{2nh}	C_{2nh}	C_{2h}, C_i	C_{2nv}	C_{2v}, C_s
$D_{(2n+1)h}$	$C_{(2n+1)h}$	C_2, C_s, C_1	$C_{(2n+1)v}$	C_2, C_s
D_{2nd}	S_{4n}	C_2, C_s, C_1	C_{2nv}	C_2, C_s, C_1
$D_{(2n+1)d}$	S_{4n+2}	C_{2h}, C_i	$C_{(2n+1)v}$	C_2, C_s, C_1

Appendix C
Subduction and Induction

Contents

C.1 Subduction $G \downarrow H$

C_{6v}	C_6	C_{3v}^v $2\hat{C}_3, 3\hat{\sigma}_v$	C_{3v}^d $2\hat{C}_3, 3\hat{\sigma}_d$	C_{2v}
A_1	A	A_1	A_1	A_1
A_2	A	A_2	A_2	A_2
B_1	B	A_1	A_2	B_1
B_2	B	A_2	A_1	B_2
E_1	E_1	E	E	$B_1 + B_2$
E_2	E_2	E	E	$A_1 + A_2$

A.J. Ceulemans, *Group Theory Applied to Chemistry*, Theoretical Chemistry and Computational Modelling, DOI 10.1007/978-94-007-6863-5,

D_{4h}	D_{2d} $\hat{C}_2^z, 2\hat{C}_2', 2\hat{\sigma}_d$	C_{4h}	C_{2v}^{zv} $\hat{C}_2^z, 2\hat{\sigma}_v$	C_{2v}^{zd} $\hat{C}_2^z, 2\hat{\sigma}_d$	C_{2v}' $\hat{C}_2', \hat{\sigma}_h, \hat{\sigma}_v$	C_{2v}'' $\hat{C}_2'', \hat{\sigma}_h, \hat{\sigma}_d$
A_{1g}	A_1	A_g	A_1	A_1	A_1	A_1
A_{2g}	A_2	A_g	A_2	A_2	B_1	B_1
B_{1g}	B_1	B_g	A_1	A_2	A_1	B_1
B_{2g}	B_2	B_g	A_2	A_1	B_1	A_1
E_g	E	E	$B_1 + B_2$	$B_1 + B_2$	$A_2 + B_2$	$A_2 + B_2$
A_{1u}	B_1	A_u	A_2	A_2	A_2	A_2
A_{2u}	B_2	A_u	A_1	A_1	B_2	B_2
B_{1u}	A_1	B_u	A_2	A_1	A_2	B_2
B_{2u}	A_2	B_u	A_1	A_2	B_2	A_2
E_u	E	E	$B_1 + B_2$	$B_1 + B_2$	$A_1 + B_1$	$A_1 + B_1$

D_{3d}	S_6	C_{3v}	C_{2h}
A_{1g}	A_g	A_1	A_g
A_{2g}	A_g	A_2	B_g
E_g	E_g	E	$A_g + B_g$
A_{1u}	A_u	A_2	A_u
A_{2u}	A_u	A_1	B_u
E_u	E_u	E	$A_u + B_u$

T_d	D_{2d}	C_{3v}	D_2	C_{2v}	S_4
A_1	A_1	A_1	A	A_1	A
A_2	B_1	A_2	A	A_2	B
E	$A_1 + B_1$	E	$2A$	$A_1 + A_2$	$A + B$
T_1	$A_2 + E$	$A_2 + E$	$B_1 + B_2 + B_3$	$A_2 + B_1 + B_2$	$A + E$
T_2	$B_2 + E$	$A_1 + E$	$B_1 + B_2 + B_3$	$A_1 + B_1 + B_2$	$B + E$

T_h	D_{2h}	S_6	C_{2v}	C_{2h}
A_g	A_g	A_g	A_1	A_g
A_u	A_u	A_u	A_2	A_u
E_g	$2A_g$	E_g	$2A_1$	$2A_g$
E_u	$2A_u$	E_u	$2A_2$	$2A_u$
T_g	$B_{1g} + B_{2g} + B_{3g}$	$A_g + E_g$	$A_2 + B_1 + B_2$	$A_g + 2B_g$
T_u	$B_{1u} + B_{2u} + B_{3u}$	$A_u + E_u$	$A_1 + B_1 + B_2$	$A_u + 2B_u$

O_h	T_d	D_{4h}	D_{3d}	T_h	D_{2h}^z	D_{2h}'
A_{1g}	A_1	A_{1g}	A_{1g}	A_g	A_g	A_g
A_{2g}	A_2	B_{1g}	A_{2g}	A_g	A_g	B_{1g}
E_g	E	$A_{1g}+B_{1g}$	E_g	E_g	$2A_g$	A_g+B_{1g}
T_{1g}	T_1	$A_{2g}+E_g$	$A_{2g}+E_g$	T_g	$B_{1g}+B_{2g}+B_{3g}$	$B_{1g}+B_{2g}+B_{3g}$
T_{2g}	T_2	$B_{2g}+E_g$	$A_{1g}+E_g$	T_g	$B_{1g}+B_{2g}+B_{3g}$	$A_g+B_{2g}+B_{3g}$
A_{1u}	A_2	A_{1u}	A_{1u}	A_u	A_u	A_u
A_{2u}	A_1	B_{1u}	A_{2u}	A_u	A_u	B_{1u}
E_u	E	$A_{1u}+B_{1u}$	E_u	E_u	$2A_u$	A_u+B_{1u}
T_{1u}	T_2	$A_{2u}+E_u$	$A_{2u}+E_u$	T_u	$B_{1u}+B_{2u}+B_{3u}$	$B_{1u}+B_{2u}+B_{3u}$
T_{2u}	T_1	$B_{2u}+E_u$	$A_{1u}+E_u$	T_u	$B_{1u}+B_{2u}+B_{3u}$	$A_u+B_{2u}+B_{3u}$

I_h	T_h	D_{5d}	D_{3d}	D_{2h}	C_{2v}
A_g	A_g	A_{1g}	A_{1g}	A_g	A_1
T_{1g}	T_g	$A_{2g}+E_{1g}$	$A_{2g}+E_g$	$B_{1g}+B_{2g}+B_{3g}$	$A_2+B_1+B_2$
T_{2g}	T_g	$A_{2g}+E_{2g}$	$A_{2g}+E_g$	$B_{1g}+B_{2g}+B_{3g}$	$A_2+B_1+B_2$
G_g	A_g+T_g	$E_{1g}+E_{2g}$	$A_{1g}+A_{2g}+E_g$	$A_g+B_{1g}+B_{2g}+B_{3g}$	$A_1+A_2+B_1+B_2$
H_g	E_g+T_g	$A_{1g}+E_{1g}+E_{2g}$	$A_{1g}+2E_g$	$2A_g+B_{1g}+B_{2g}+B_{3g}$	$2A_1+A_2+B_1+B_2$
A_u	A_u	A_{1u}	A_{1u}	A_u	A_2
T_{1u}	T_u	$A_{2u}+E_{1u}$	$A_{2u}+E_u$	$B_{1u}+B_{2u}+B_{3u}$	$A_1+B_1+B_2$
T_{2u}	T_u	$A_{2u}+E_{2u}$	$A_{2u}+E_u$	$B_{1u}+B_{2u}+B_{3u}$	$A_1+B_1+B_2$
G_u	A_u+T_u	$E_{1u}+E_{2u}$	$A_{1u}+A_{2u}+E_u$	$A_u+B_{1u}+B_{2u}+B_{3u}$	$A_1+A_2+B_1+B_2$
H_u	E_u+T_u	$A_{1u}+E_{1u}+E_{2u}$	$A_{1u}+2E_u$	$2A_u+B_{1u}+B_{2u}+B_{3u}$	$A_1+2A_2+B_1+B_2$

$SO(3)$ ℓ	I	O
0 (S)	A	A_1
1 (P)	T_1	T_1
2 (D)	H	$E + T_2$
3 (F)	$T_2 + G$	$A_2 + T_1 + T_2$
4 (G)	$G + H$	$A_1 + E + T_1 + T_2$
5	$T_1 + T_2 + H$	$E + 2T_1 + T_2$
6	$A + T_1 + G + H$	$A_1 + A_2 + E + T_1 + 2T_2$
7	$T_1 + T_2 + G + H$	$A_2 + E + 2T_1 + 2T_2$
8	$T_2 + G + 2H$	$A_1 + 2E + 2T_1 + 2T_2$
9	$T_1 + T_2 + 2G + H$	$A_1 + A_2 + E + 3T_1 + 2T_2$
10	$A + T_1 + T_2 + G + 2H$	$A_1 + A_2 + 2E + 2T_1 + 3T_2$
11	$2T_1 + T_2 + G + 2H$	$A_2 + 2E + 3T_1 + 3T_2$
12	$A + T_1 + T_2 + 2G + 2H$	$A_1 + \Gamma_{reg}$

C.2 Induction: $H \uparrow G$

Ascent in symmetry tables have been provided by Boyle [4]. Fowler and Quinn have listed the irreps that are induced by σ-, π-, and δ-type orbitals on molecular sites [5]. These tables are reproduced below. They are useful for the construction of cluster orbitals. Γ_{reg} always denotes the regular representation. Γ_σ corresponds to the positional representation. The mechanical representation is the sum $\Gamma_\sigma + \Gamma_\pi$.

G	H	$\frac{G}{H}$	Γ_σ	Γ_π	Γ_δ
D_2	C_2^z	2	$A + B_1$	$2B_2 + 2B_3$	$2\Gamma_\sigma$
D_3	C_2	3	$A_1 + E$	$2A_2 + 2E$	$2\Gamma_\sigma$
D_4	C_4	2	$A_1 + A_2$	$2E$	$2B_1 + 2B_2$
	C_2'	4	$A_1 + B_1 + E$	$2A_2 + 2B_2 + 2E$	$2\Gamma_\sigma$
	C_2''	4	$A_2 + B_2 + E$	$2A_2 + 2B_1 + 2E$	$2\Gamma_\sigma$
D_5	C_5	2	$A_1 + A_2$	$2E_1$	$2E_2$
	C_2	4	$A_1 + E_1 + E_2$	$2A_2 + 2E_1 + 2E_2$	$2\Gamma_\sigma$
D_6	C_6	6	$A_1 + A_2$	$2E_1$	$2E_2$
	C_2'	4	$A_1 + B_1 + E_1 + E_2$	$2A_2 + 2B_2 + 2E_1 + 2E_2$	$2\Gamma_\sigma$
	C_2''	4	$A_1 + B_2 + E_1 + E_2$	$2A_2 + 2B_1 + 2E_1 + 2E_2$	$2\Gamma_\sigma$
C_{2v}	C_s^{xz}	2	$A_1 + B_1$	Γ_{reg}	Γ_{reg}
C_{3v}	C_s	3	$A_1 + E$	Γ_{reg}	Γ_{reg}
C_{4v}	C_s^v	4	$A_1 + B_1 + E$	Γ_{reg}	Γ_{reg}
	C_s^d	4	$A_1 + B_2 + E$	Γ_{reg}	Γ_{reg}
C_{5v}	C_s	5	$A_1 + E_1 + E_2$	Γ_{reg}	Γ_{reg}
C_{6v}	C_s^v	6	$A_1 + B_1 + E_1 + E_2$	Γ_{reg}	Γ_{reg}
	C_s^d	6	$A_1 + B_2 + E_1 + E_2$	Γ_{reg}	Γ_{reg}
C_{2h}	C_2	2	$A_g + A_u$	$2B_g + 2B_u$	$2\Gamma_\sigma$
	C_s	2	$A_g + B_u$	Γ_{reg}	Γ_{reg}
C_{3h}	C_3	2	$A' + A''$	$E' + E''$	$E' + E''$
	C_s	3	$A' + E'$	Γ_{reg}	Γ_{reg}
C_{4h}	C_4	2	$A_g + A_u$	$E_g + E_u$	$2B_g + 2B_u$
	C_s	4	$A_g + B_g + E_u$	Γ_{reg}	Γ_{reg}
C_{5h}	C_5	2	$A' + A''$	$E_1' + E_1''$	$E_2' + E_2''$
	C_s	5	$A' + E_1' + E_2'$	Γ_{reg}	Γ_{reg}
C_{6h}	C_6	2	$A_g + A_u$	$E_{1g} + E_{1u}$	$E_{2g} + E_{2u}$
	C_s	6	$A_g + B_u + E_{2g}$ $+ E_{1u}$	Γ_{reg}	Γ_{reg}
S_4	C_2	2	$A + B$	$2E$	$2\Gamma_\sigma$
S_6	C_3	2	$A_g + A_u$	$E_g + E_u$	$E_g + E_u$

G	H	$\frac{\lvert G\rvert}{\lvert H\rvert}$	Γ_σ	Γ_π	Γ_δ
D_{2h}	C_{2v}^z	2	$A_g + B_{1u}$	$B_{2g} + B_{2u} + B_{3g} + B_{3u}$	$A_g + A_u + B_{1g} + B_{1u}$
	C_s^{xy}	4	$A_g + B_{1g} + B_{2u} + B_{3u}$	Γ_{reg}	Γ_{reg}
D_{3h}	C_{3v}	2	$A_1' + A_2''$	$E' + E''$	$E' + E''$
	C_{2v}	3	$A_1' + E'$	$A_1' + A_2'' + E' + E''$	$A_1' + A_1'' + E' + E''$
	C_s^v	6	$A_1' + A_2'' + E' + E''$	Γ_{reg}	Γ_{reg}
D_{4h}	C_{4v}	2	$A_{1g} + A_{2u}$	$E_g + E_u$	$B_{1g} + B_{1u} + B_{2g} + B_{2u}$
	C_{2v}'	4	$A_{1g} + B_{1g} + E_u$	$A_{2g} + A_{2u} + B_{2g} + B_{2u} + E_g + E_u$	$A_{1g} + A_{1u} + B_{1g} + B_{1u} + E_g + E_u$
	C_{2v}''	4	$A_{1g} + B_{2g} + E_u$	$A_{2g} + A_{2u} + B_{1g} + B_{1u} + E_g + E_u$	$A_{1g} + A_{1u} + B_{2g} + B_{2u} + E_g + E_u$
	C_s^h	8	$A_{1g} + A_{2g} + B_{1g} + B_{2g} + 2E_u$	Γ_{reg}	Γ_{reg}
	C_s^v	8	$A_{1g} + A_{2u} + B_{1g} + B_{2u} + E_g + E_u$	Γ_{reg}	Γ_{reg}
	C_s^d	8	$A_{1g} + A_{2u} + B_{1u} + B_{2g} + E_g + E_u$	Γ_{reg}	Γ_{reg}
D_{5h}	C_{5v}	2	$A_1' + A_2''$	$E_1' + E_1''$	$E_2' + E_2''$
	C_{2v}	5	$A_1' + E_1' + E_2'$	$A_2' + A_2'' + E_1' + E_1'' + E_2' + E_2''$	$A_1' + A_1'' + E_1' + E_1'' + E_2' + E_2''$
	C_s^h	10	$A_1' + A_2' + 2E_1' + 2E_2'$	Γ_{reg}	Γ_{reg}
	C_s^v	10	$A_1' + A_2'' + E_1' + E_1'' + E_2' + E_2''$	Γ_{reg}	Γ_{reg}
D_{6h}	C_{6v}	2	$A_{1g} + A_{2u}$	$E_{1g} + E_{1u}$	$E_{2g} + E_{2u}$
	C_{2v}'	6	$A_{1g} + B_{1u} + E_{1u} + E_{2g}$	$A_{2g} + A_{2u} + B_{2g} + B_{2u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$	$A_{1g} + A_{1u} + B_{1g} + B_{1u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$
	C_{2v}''	6	$A_{1g} + B_{2u} + E_{1u} + E_{2g}$	$A_{2g} + A_{2u} + B_{1g} + B_{1u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$	$A_{1g} + A_{1u} + B_{2g} + B_{2u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$
	C_s^h	12	$A_{1g} + A_{2g} + B_{1u} + B_{2u} + 2E_{1u} + 2E_{2g}$	Γ_{reg}	Γ_{reg}
	C_s^v	12	$A_{1g} + A_{2u} + B_{1g} + B_{2u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$	Γ_{reg}	Γ_{reg}
	C_s^d	12	$A_{1g} + A_{2u} + B_{1g} + B_{2u} + E_{1g} + E_{1u} + E_{2g} + E_{2u}$	Γ_{reg}	Γ_{reg}

G	H	$\frac{\lvert G\rvert}{\lvert H\rvert}$	Γ_σ	Γ_π	Γ_δ
D_{2d}	C_{2v}^z	2	A_1+B_2	$2E$	$A_1+A_2+B_1+B_2$
	C_2'	4	A_1+B_1+E	$2A_2+2B_2+2E$	$2\Gamma_\sigma$
	C_s	4	A_1+B_2+E	Γ_{reg}	Γ_{reg}
D_{3d}	C_{3v}	2	$A_{1g}+A_{2u}$	E_g+E_u	E_g+E_u
	C_2	6	$A_{1g}+A_{1u}+E_g+E_u$	$2A_{2g}+2A_{2u}$ $+2E_g+2E_u$	$2\Gamma_\sigma$
	C_s	6	$A_{1g}+A_{2u}+E_g+E_u$	Γ_{reg}	Γ_{reg}
D_{4d}	C_{4v}	2	A_1+B_2	E_1+E_3	$2E_2$
	C_2'	8	$A_1+B_1+E_1+E_2$ $+E_3$	$2A_2+2B_2+2E_1$ $+2E_2+2E_3$	$2\Gamma_\sigma$
	C_s	8	$A_1+B_2+E_1+E_2$ $+E_3$	Γ_{reg}	Γ_{reg}
D_{5d}	C_{5v}	2	$A_{1g}+A_{2u}$	$E_{1g}+E_{1u}$	$E_{2g}+E_{2u}$
	C_2	10	$A_{1g}+A_{1u}+E_{1g}$ $+E_{1u}+E_{2g}+E_{2u}$	$2A_{2g}+2A_{2u}+2E_{1g}$ $+2E_{1u}+2E_{2g}$ $+2E_{2u}$	$2\Gamma_\sigma$
	C_s	10	$A_{1g}+A_{2u}+E_{1g}$ $+E_{1u}+E_{2g}+E_{2u}$	Γ_{reg}	Γ_{reg}
D_{6d}	C_{6v}	2	A_1+B_2	E_1+E_5	E_2+E_4
	C_2'	12	$A_1+B_1+E_1+E_2$ $+E_3+E_4+E_5$	$2A_2+2B_2+2E_1$ $+2E_2+2E_3$ $+2E_4+2E_5$	$2\Gamma_\sigma$
	C_s	12	$A_1+B_2+E_1+E_2$ $+E_3+E_4+E_5$	Γ_{reg}	Γ_{reg}
T	C_3	4	$A+T$	$E+2T$	Γ_π
	C_2	6	$A+E+T$	$4T$	$2\Gamma_\sigma$
T_d	C_{3v}	4	A_1+T_2	$E+T_1+T_2$	Γ_π
	C_{2v}	6	A_1+E+T_2	$2T_1+2T_2$	A_1+A_2+2E $+T_1+T_2$
	C_s	12	$A_1+E+T_1+2T_2$	Γ_{reg}	Γ_{reg}
T_h	C_3	8	$A_g+A_u+T_g+T_u$	$E_g+E_u+2T_g+2T_u$	Γ_π
	C_{2v}	6	$A_g+E_g+T_u$	$2T_g+2T_u$	$A_g+A_u+E_g$ $+E_u+T_g+T_u$
	C_s	12	$A_g+E_g+T_g+2T_u$	Γ_{reg}	Γ_{reg}
O	C_4	6	A_1+E+T_1	$2T_1+2T_2$	$2A_2+2E+2T_2$
	C_3	8	$A_1+A_2+T_1+T_2$	$2E+2T_1+2T_2$	Γ_π
	C_2	12	$A_1+E+T_1+2T_2$	$2A_2+2E+4T_1+2T_2$	$2\Gamma_\sigma$

G	H	$\frac{\lvert G\rvert}{\lvert H\rvert}$	Γ_σ	Γ_π	Γ_δ
O_h	C_{4v}	6	$A_{1g}+E_g+T_{1u}$	$T_{1g}+T_{1u}+T_{2g}+T_{2u}$	$A_{2g}+A_{2u}+E_g+E_u+T_{2g}+T_{2u}$
	C_{3v}	8	$A_{1g}+A_{2u}+T_{1u}+T_{2g}$	$E_g+E_u+T_{1g}+T_{1u}+T_{2g}+T_{2u}$	Γ_π
	C_{2v}	12	$A_{1g}+E_g+T_{1u}+T_{2g}+T_{2u}$	$A_{2g}+A_{2u}+E_g+E_u+2T_{1g}+2T_{1u}+T_{2g}+T_{2u}$	$A_{1g}+A_{1u}+E_g+E_u+T_{1g}+T_{1u}+2T_{2g}+2T_{2u}$
	C_s^h	24	$A_{1g}+A_{2g}+2E_g+T_{1g}+2T_{1u}+T_{2g}+2T_{2u}$	Γ_{reg}	Γ_{reg}
	C_s^d	24	$A_{1g}+A_{2u}+E_g+E_u+T_{1g}+2T_{1u}+2T_{2g}+T_{2u}$	Γ_{reg}	Γ_{reg}
I	C_5	12	$A+T_1+T_2+H$	$2T_1+2G+2H$	$2T_2+2G+2H$
	C_3	20	$A+T_1+T_2+2G+H$	$2T_1+2T_2+2G+4H$	Γ_π
	C_2	30	$A+T_1+T_2+2G+3H$	$4T_1+4T_2+4G+4H$	$2\Gamma_\sigma$
I_h	C_{5v}	12	$A_g+T_{1u}+T_{2u}+H_g$	$T_{1g}+T_{1u}+G_g+G_u+H_g+H_u$	$T_{2g}+T_{2u}+G_g+G_u+H_g+H_u$
	C_{3v}	20	$A_g+T_{1u}+T_{2u}+G_g+G_u+H_g$	$T_{1g}+T_{1u}+T_{2g}+T_{2u}+G_g+G_u+2H_g+2H_u$	Γ_π
	C_{2v}	30	$A_g+T_{1u}+T_{2u}+G_g+G_u+2H_g+H_u$	$2T_{1g}+2T_{1u}+2T_{2g}+2T_{2u}+2G_g+2G_u+2H_g+2H_u$	$A_g+A_u+T_{1g}+T_{1u}+T_{2g}+T_{2u}+2G_g+2G_u+3H_g+3H_u$
	C_s	60	$A_g+T_{1g}+2T_{1u}+T_{2g}+2T_{2u}+2G_g+2G_u+3H_g+2H_u$	Γ_{reg}	Γ_{reg}

Appendix D
Canonical-Basis Relationships

The importance of canonical-basis relationships was demonstrated by Griffith in his monumental work on the theory of transition-metal ions [6]. The icosahedral basis sets were defined by Boyle and Parker [7].

D_3	$\mathbb{D}(C_3^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_x\rangle, \lvert E_y\rangle$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_4	$\mathbb{D}(C_4^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_x\rangle, \lvert E_y\rangle$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_5	$\mathbb{D}(C_5^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_{1x}\rangle, \lvert E_{1y}\rangle$	$\begin{pmatrix} \cos(2\pi/5) & -\sin(2\pi/5) \\ \sin(2\pi/5) & \cos(2\pi/5) \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\lvert E_{2x}\rangle, \lvert E_{2y}\rangle$	$\begin{pmatrix} \cos(4\pi/5) & -\sin(4\pi/5) \\ \sin(4\pi/5) & \cos(4\pi/5) \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_6	$\mathbb{D}(C_6^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_{1x}\rangle, \lvert E_{1y}\rangle$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\lvert E_{2x}\rangle, \lvert E_{2y}\rangle$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

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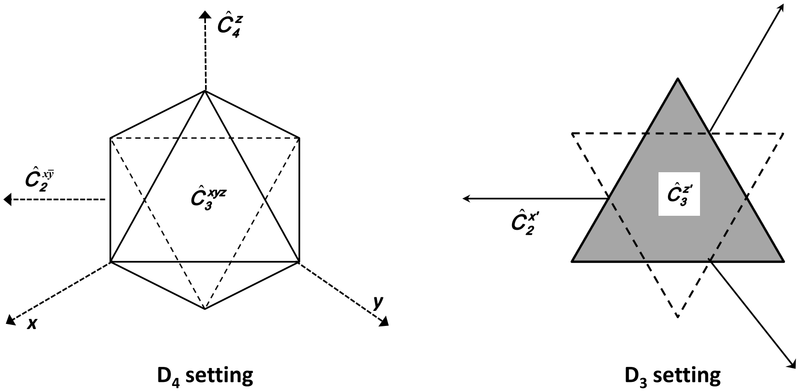


Fig. D.1 Octahedron with x, y, z coordinates in D_4 and D_3 setting

O (D_4 basis)	$\mathbb{D}(C_4^z)$	$\mathbb{D}(C_3^{xyz})$
$\|E_\theta\rangle, \|E_\epsilon\rangle$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
$\|T_{1x}\rangle, \|T_{1y}\rangle, \|T_{1z}\rangle$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\|T_{2\xi}\rangle, \|T_{2\eta}\rangle, \|T_{2\zeta}\rangle$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

(See Fig. D.1.) Transformation to trigonal basis set:

$$|E_\theta\rangle = d_{z^2} = \frac{1}{\sqrt{3}}(-d_{x'^2-y'^2} - \sqrt{2}d_{y'z'})$$

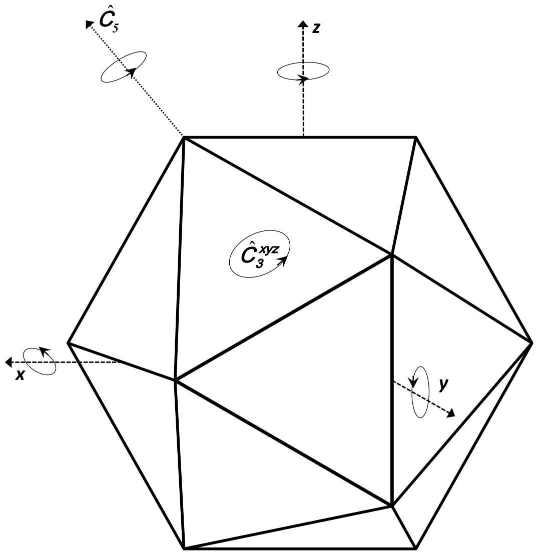
$$|E_\epsilon\rangle = d_{x^2-y^2} = \frac{1}{\sqrt{3}}(d_{x'y'} + \sqrt{2}d_{x'z'})$$

$$|T_{1a}\rangle = \frac{1}{\sqrt{3}}\big(|T_{1x}\rangle + |T_{1y}\rangle + |T_{1z}\rangle\big) = p_{z'}$$

$$|T_{1\theta}\rangle = \frac{1}{\sqrt{2}}\big(|T_{1x}\rangle - |T_{1y}\rangle\big) = p_{x'}$$

$$|T_{1\epsilon}\rangle = \frac{1}{\sqrt{6}}\big(|T_{1x}\rangle + |T_{1y}\rangle - 2|T_{1z}\rangle\big) = p_{y'}$$

Fig. D.2 Icosahedron with x, y, z coordinates in D_2 setting



$$|T_{2a}\rangle = \frac{1}{\sqrt{3}}\big(|T_{2\xi}\rangle + |T_{2\eta}\rangle + |T_{2\zeta}\rangle\big) = d_{z'^2}$$

$$|T_{2\theta}\rangle = \frac{1}{\sqrt{6}}\big(|T_{2\xi}\rangle + |T_{2\eta}\rangle - 2|T_{2\zeta}\rangle\big) = \frac{1}{\sqrt{3}}(\sqrt{2}d_{x'^2-y'^2} - d_{y'z'})$$

$$|T_{2\epsilon}\rangle = \frac{1}{\sqrt{2}}\big(|T_{2\eta}\rangle - |T_{2\xi}\rangle\big) = \frac{1}{\sqrt{3}}(-\sqrt{2}d_{x'y'} + d_{x'z'})$$

O (D_3 basis)	$\mathbb{D}(C_3^{z'})$	$\mathbb{D}(C_2^{x'})$
$\lvert E_\theta\rangle, \lvert E_\epsilon\rangle$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\lvert T_{1a}\rangle, \lvert T_{1\theta}\rangle, \lvert T_{1\epsilon}\rangle$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\lvert T_{2a}\rangle, \lvert T_{2\theta}\rangle, \lvert T_{2\epsilon}\rangle$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

I (D_2 basis, Fig. D.2)	$\mathbb{D}(C_5)$	$\mathbb{D}(C_3^{xyz})$	$\mathbb{D}(C_2^z)$
$\|T_{1x}\rangle, \|T_{1y}\rangle, \|T_{1z}\rangle$	$\frac{1}{2}\begin{pmatrix} 1 & -\phi & \phi^{-1} \\ \phi & \phi^{-1} & -1 \\ \phi^{-1} & 1 & \phi \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\|T_{2x}\rangle, \|T_{2y}\rangle, \|T_{2z}\rangle$	$\frac{1}{2}\begin{pmatrix} 1 & \phi^{-1} & -\phi \\ -\phi^{-1} & -\phi & -1 \\ -\phi & 1 & -\phi^{-1} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\|G_a\rangle, \|G_x\rangle, \|G_y\rangle,$ $\|G_z\rangle$	$\frac{1}{4}\begin{pmatrix} -1 & -\sqrt{5} & \sqrt{5} & \sqrt{5} \\ \sqrt{5} & -3 & -1 & -1 \\ \sqrt{5} & 1 & -1 & 3 \\ -\sqrt{5} & -1 & -3 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

I $\|H\theta\rangle, \|H\epsilon\rangle, \|H\xi\rangle, \|H\eta\rangle, \|H\zeta\rangle$		
$\mathbb{D}(C_5)$	$\mathbb{D}(C_3^{xyz})$	$\mathbb{D}(C_2^z)$
$\begin{pmatrix} -\frac{1}{4} & -\frac{\sqrt{3}}{4} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{8}} \\ -\frac{\sqrt{3}}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{\sqrt{8}} & 0 & -\frac{\sqrt{3}}{\sqrt{8}} \\ -\frac{1}{\sqrt{8}} & \frac{\sqrt{3}}{\sqrt{8}} & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{\sqrt{8}} & \frac{\sqrt{3}}{\sqrt{8}} & \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$

It is important to note that in the Boyle and Parker basis the $|H\theta\rangle$ and $|H\epsilon\rangle$ components do not denote components that transform like the functions d_{z^2} and $d_{x^2-y^2}$, but refer to linear combinations of these:

$$|H\theta\rangle = \sqrt{\frac{3}{8}}d_{z^2} + \sqrt{\frac{5}{8}}d_{x^2-y^2}$$

$$|H\epsilon\rangle = -\sqrt{\frac{5}{8}}d_{z^2} + \sqrt{\frac{3}{8}}d_{x^2-y^2}$$

Griffith has presented the subduction of spherical $|JM\rangle$ states to point-group canonical bases for the case of the octahedral group. Similar tables for subduction to the icosahedral canonical basis have been published by Qiu and Ceulemans [8]. Extensive tables of bases in terms of spherical harmonics for several branching schemes are also provided by Butler [9].

Appendix E
Direct-Product Tables

Extensive direct-product tables are provided by Herzberg [10]. Antisymmetrized and symmetrized parts of direct squares are indicated by braces and brackets, respectively.

D_3	A_1	A_2	E
A_1	A_1	A_2	E
A_2	A_2	A_1	E
E	E	E	$[A_1 + E] + \{A_2\}$

D_4	A_1	A_2	B_1	B_2	E
A_1	A_1	A_2	B_1	B_2	E
A_2	A_2	A_1	B_2	B_1	E
B_1	B_1	B_2	A_1	A_2	E
B_2	B_2	B_1	A_2	A_1	E
E	E	E	E	E	$[A_1 + B_1 + B_2] + \{A_2\}$

D_5	A_1	A_2	E_1	E_2
A_1	A_1	A_2	E_1	E_2
A_2	A_2	A_1	E_1	E_2
E_1	E_1	E_1	$[A_1 + E_2] + \{A_2\}$	$E_1 + E_2$
E_2	E_2	E_2	$E_1 + E_2$	$[A_1 + E_1] + \{A_2\}$

D_6	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_2	A_1	B_2	B_1	E_1	E_2
B_1	B_1	B_2	A_1	A_2	E_2	E_1
B_2	B_2	B_1	A_2	A_1	E_2	E_1
E_1	E_1	E_1	E_2	E_2	$[A_1 + E_2] + \{A_2\}$	$B_1 + B_2 + E_1$
E_2	E_2	E_2	E_1	E_1	$B_1 + B_2 + E_1$	$[A_1 + E_2] + \{A_2\}$

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T_d	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2	A_2	A_1	E	T_2	T_1
E	E	E	$[A_1 + E] + \{A_2\}$	$T_1 + T_2$	$T_1 + T_2$
T_1	T_1	T_2	$T_1 + T_2$	$[A_1 + E + T_2] + \{T_1\}$	$A_2 + E + T_1 + T_2$
T_2	T_2	T_1	$T_1 + T_2$	$A_2 + E + T_1 + T_2$	$[A_1 + E + T_2] + \{T_1\}$

O	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2	A_2	A_1	E	T_2	T_1
E	E	E	$[A_1 + E] + \{A_2\}$	$T_1 + T_2$	$T_1 + T_2$
T_1	T_1	T_2	$T_1 + T_2$	$[A_1 + E + T_2] + \{T_1\}$	$A_2 + E + T_1 + T_2$
T_2	T_2	T_1	$T_1 + T_2$	$A_2 + E + T_1 + T_2$	$[A_1 + E + T_2] + \{T_1\}$

I	A	T_1	T_2	G	H
A	A	T_1	T_2	G	H
T_1	T_1	$[A + H] + \{T_1\}$	$G + H$	$T_2 + G + H$	$T_1 + T_2 + G + H$
T_2	T_2	$G + H$	$[A + H] + \{T_2\}$	$T_1 + G + H$	$T_1 + T_2 + G + H$
G	G	$T_2 + G + H$	$T_1 + G + H$	$[A + G + H] + \{T_1 + T_2\}$	$T_1 + T_2 + G + 2H$
H	H	$T_1 + T_2 + G + H$	$T_1 + T_2 + G + H$	$T_1 + T_2 + G + 2H$	$[A + G + 2H] + \{T_1 + T_2 + G\}$

Appendix F
Coupling Coefficients

Coupling coefficients are denoted as 3Γ symbols: $\langle \Gamma_a \gamma_a \Gamma_b \gamma_b | \Gamma \gamma \rangle$. Their symmetry properties were given in Sect. 6.3. Octahedral coefficients have been listed by Griffith. Icosahedral coefficients are taken from the work of Fowler and Ceulemans [11].

D_3		
$A_2 \times E$	E	
	x	y
a_2 x	0	-1
a_2 y	1	0

D_3				
$E \times E$	A_1	A_2	E	
	a_1	a_2	x	y
x x	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
y y	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
x y	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
y x	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_4				
$E \times E$	A_1	A_2	B_1	B_2
	a_1	a_2	b_1	b_2
x x	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
y y	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
x y	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
y x	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

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D_5				
$E_1 \times E_1$	A_1	A_2	E_2	
	a_1	a_2	c	s
$x\ x$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$y\ y$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$x\ y$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$y\ x$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_5				
$E_2 \times E_2$	A_1	A_2	E_1	
	a_1	a_2	x	y
$c\ c$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$s\ s$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$c\ s$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$s\ c$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_5				
$E_1 \times E_2$	E_1		E_2	
	x	y	c	s
$x\ c$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$y\ s$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$x\ s$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$y\ c$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_6				
$E_1 \times E_1$	A_1	A_2	E_2	
	a_1	a_2	c	s
$x\ x$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$y\ y$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$x\ y$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$y\ x$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_6				
$E_2 \times E_2$	A_1	A_2	E_1	
	a_1	a_2	x	y
$c\ c$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$s\ s$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$c\ s$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$s\ c$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

D_6				
$E_1 \times E_2$	B_1	B_2	E_1	
	b_1	b_2	x	y
$x\ c$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$y\ s$	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$x\ s$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$y\ c$	0	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$

O		
$A_2 \times E$	E	
	θ	ϵ
$a_2\ \theta$	0	−1
$a_2\ \epsilon$	1	0

O			
$A_2 \times T_1$	T_2		
	ξ	η	ζ
$a_2\ x$	1	0	0
$a_2\ y$	0	1	0
$a_2\ z$	0	0	1

O			
$A_2 \times T_2$	T_1		
	x	y	z
$a_2\ \xi$	1	0	0
$a_2\ \eta$	0	1	0
$a_2\ \zeta$	0	0	1

O				
$E \times E$	A_1	A_2	E	
	a_1	a_2	θ	ϵ
$\theta\ \theta$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$\epsilon\ \epsilon$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	0
$\theta\ \epsilon$	0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$\epsilon\ \theta$	0	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$

O						
$E \times T_1$	T_1			T_2		
	x	y	z	ξ	η	ζ
$\theta\ x$	$-\frac{1}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	0	0
$\theta\ y$	0	$-\frac{1}{2}$	0	0	$\frac{\sqrt{3}}{2}$	0
$\theta\ z$	0	0	1	0	0	0
$\epsilon\ x$	$\frac{\sqrt{3}}{2}$	0	0	$-\frac{1}{2}$	0	0
$\epsilon\ y$	0	$-\frac{\sqrt{3}}{2}$	0	0	$-\frac{1}{2}$	0
$\epsilon\ z$	0	0	0	0	0	1

O						
$E \times T_2$	T_1			T_2		
	x	y	z	ξ	η	ζ
$\theta\ \xi$	$\frac{-\sqrt{3}}{2}$	0	0	$-\frac{1}{2}$	0	0
$\theta\ \eta$	0	$\frac{\sqrt{3}}{2}$	0	0	$-\frac{1}{2}$	0
$\theta\ \zeta$	0	0	0	0	0	1
$\epsilon\ \xi$	$-\frac{1}{2}$	0	0	$\frac{\sqrt{3}}{2}$	0	0
$\epsilon\ \eta$	0	$-\frac{1}{2}$	0	0	$-\frac{\sqrt{3}}{2}$	0
$\epsilon\ \zeta$	0	0	1	0	0	0

O				
$T_1 \times T_1$ or $T_2 \times T_2$		A_1	E	
		a_1	θ	ϵ
$x\ x$	$\xi\ \xi$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{2}}$
$y\ y$	$\eta\ \eta$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$
$z\ z$	$\zeta\ \zeta$	$\frac{1}{\sqrt{3}}$	$-\frac{2}{\sqrt{6}}$	0

O			
$T_1 \times T_2$	A_2	E	
	a_2	θ	ϵ
$x\ \xi$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{6}}$
$y\ \eta$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{6}}$
$z\ \zeta$	$\frac{1}{\sqrt{3}}$	0	$\frac{2}{\sqrt{6}}$

O							
$T_1 \times T_1$ or $T_2 \times T_2$		T_1			T_2		
		x	y	z	ξ	η	ζ
$x\ y$	$\xi\ \eta$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$
$x\ z$	$\xi\ \zeta$	0	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0
$y\ x$	$\eta\ \xi$	0	0	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$
$y\ z$	$\eta\ \zeta$	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0	0
$z\ x$	$\zeta\ \xi$	0	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0
$z\ y$	$\zeta\ \eta$	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0	0

O						
$T_1 \times T_2$	T_1			T_2		
	x	y	z	ξ	η	ζ
$x\ \eta$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$
$x\ \zeta$	0	$-\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$	0
$y\ \xi$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$
$y\ \zeta$	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0	0
$z\ \xi$	0	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0
$z\ \eta$	$-\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$	0	0

In the icosahedral tables, ϕ denotes the golden number $(1 + \sqrt{5})/2$, and $\alpha = 3\phi - 1,\ \beta = 3\phi^{-1} + 1$.

I									
$T_1 \times T_1$	A	T_1			H				
		x	y	z	θ	ϵ	ξ	η	θ
$x\ x$	$\frac{1}{\sqrt{3}}$	0	0	0	$\frac{\phi^{-1}}{2}$	$\frac{\phi^2}{2\sqrt{3}}$	0	0	0
$x\ y$	0	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$
$x\ z$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0
$y\ x$	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$
$y\ y$	$\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{\phi}{2}$	$-\frac{\phi^{-2}}{2\sqrt{3}}$	0	0	0
$y\ z$	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0
$z\ x$	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0
$z\ y$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0
$z\ z$	$\frac{1}{\sqrt{3}}$	0	0	0	$\frac{1}{2}$	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0

I									
$T_1 \times T_2$	G				H				
	a	x	y	z	θ	ϵ	ξ	η	ζ
$x\ x$	$\frac{1}{\sqrt{3}}$	0	0	0	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{2}}$	0	0	0
$x\ y$	0	0	0	$-\frac{\phi^{-1}}{\sqrt{3}}$	0	0	0	0	$\frac{\phi}{\sqrt{3}}$
$x\ z$	0	0	$-\frac{\phi}{\sqrt{3}}$	0	0	0	0	$-\frac{\phi^{-1}}{\sqrt{3}}$	0
$y\ x$	0	0	0	$-\frac{\phi}{\sqrt{3}}$	0	0	0	0	$-\frac{\phi^{-1}}{\sqrt{3}}$
$y\ y$	$\frac{1}{\sqrt{3}}$	0	0	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$	0	0	0
$y\ z$	0	$-\frac{\phi^{-1}}{\sqrt{3}}$	0	0	0	0	$\frac{\phi}{\sqrt{3}}$	0	0
$z\ x$	0	0	$-\frac{\phi^{-1}}{\sqrt{3}}$	0	0	0	0	$\frac{\phi}{\sqrt{3}}$	0
$z\ y$	0	$-\frac{\phi}{\sqrt{3}}$	0	0	0	0	$-\frac{\phi^{-1}}{\sqrt{3}}$	0	0
$z\ z$	$\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{\sqrt{2}}{\sqrt{3}}$	0	0	0	0

I												
$T_1 \times G$	T_2			G				H				
	x	y	z	a	x	y	z	θ	ϵ	ξ	η	ζ
$x\ a$	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0	0
$x\ x$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{\beta}{2\sqrt{6}}$	$-\frac{\phi}{2\sqrt{2}}$	0	0	0
$x\ y$	0	0	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$
$x\ z$	0	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$	0
$y\ a$	0	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0
$y\ x$	0	0	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$
$y\ y$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$\frac{\alpha}{2\sqrt{6}}$	$-\frac{\phi^{-1}}{2\sqrt{2}}$	0	0	0
$y\ z$	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$	0	0
$z\ a$	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$
$z\ x$	0	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$	0
$z\ y$	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$	0	0
$z\ z$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{1}{2\sqrt{6}}$	$\frac{\sqrt{5}}{2\sqrt{2}}$	0	0	0

I

$T_2 \times G$	T_1			G				H				
	x	y	z	a	x	y	z	θ	ϵ	ξ	η	ζ
$x\ a$	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0	0
$x\ x$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$\frac{\alpha}{2\sqrt{6}}$	$\frac{\phi^{-1}}{2\sqrt{2}}$	0	0	0
$x\ y$	0	0	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$
$x\ z$	0	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$	0
$y\ a$	0	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0
$y\ x$	0	0	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$
$y\ y$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{\beta}{2\sqrt{6}}$	$\frac{\phi}{2\sqrt{2}}$	0	0	0
$y\ z$	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$	0	0
$z\ a$	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$
$z\ x$	0	$-\frac{\phi^{-1}}{2}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^2}{2\sqrt{3}}$	0
$z\ y$	$-\frac{\phi}{2}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$	0	0
$z\ z$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{1}{2\sqrt{6}}$	$-\frac{\sqrt{5}}{2\sqrt{2}}$	0	0	0

I

$T_1 \times H$	T_1			T_2			G			
	x	y	z	x	y	z	a	x	y	z
$x\ \theta$	$\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0	0	$\frac{1}{\sqrt{10}}$	0	0	0	$\frac{\beta}{\sqrt{30}}$	0	0
$x\ \epsilon$	$\frac{\phi^2}{2\sqrt{5}}$	0	0	$-\frac{3}{\sqrt{10}}$	0	0	0	$\frac{\phi}{\sqrt{10}}$	0	0
$x\ \xi$	0	0	0	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0
$x\ \eta$	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	0	$-\frac{\phi^2}{\sqrt{15}}$
$x\ \zeta$	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$\frac{\phi}{\sqrt{5}}$	0	0	0	$-\frac{\phi^{-2}}{\sqrt{15}}$	0
$y\ \theta$	0	$-\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0	$\frac{1}{\sqrt{10}}$	0	0	0	$-\frac{\alpha}{\sqrt{30}}$	0
$y\ \epsilon$	0	$-\frac{\phi^{-2}}{2\sqrt{5}}$	0	0	$\frac{3}{\sqrt{10}}$	0	0	0	$\frac{\phi^{-1}}{\sqrt{10}}$	0
$y\ \xi$	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$\frac{\phi}{\sqrt{5}}$	0	0	0	$-\frac{\phi^{-2}}{\sqrt{15}}$
$y\ \eta$	0	0	0	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0
$y\ \zeta$	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	0	$-\frac{\phi^2}{\sqrt{15}}$	0	0
$z\ \theta$	0	0	$\frac{\sqrt{3}}{2\sqrt{5}}$	0	0	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	$\frac{1}{\sqrt{30}}$
$z\ \epsilon$	0	0	$-\frac{1}{2}$	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$
$z\ \xi$	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	0	$-\frac{\phi^2}{\sqrt{15}}$	0
$z\ \eta$	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	$\frac{\phi}{\sqrt{5}}$	0	0	0	$-\frac{\phi^{-2}}{\sqrt{15}}$	0	0
$z\ \zeta$	0	0	0	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0

I

$T_2 \times T_2$	A	T_2			H				
		x	y	z	θ	ϵ	x	y	z
$x\ x$	$\frac{1}{\sqrt{3}}$	0	0	0	$\frac{\phi}{2}$	$-\frac{\phi^{-2}}{2\sqrt{3}}$	0	0	0
$x\ y$	0	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$
$x\ z$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0
$y\ x$	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$
$y\ y$	$\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{\phi^{-1}}{2}$	$\frac{\phi^2}{2\sqrt{3}}$	0	0	0
$y\ z$	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0
$z\ x$	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0
$z\ y$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0
$z\ z$	$\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{1}{2}$	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0

I

$T_2 \times H$	T_1			T_2			G			
	x	y	z	x	y	z	a	x	y	z
$x\ \theta$	$\frac{1}{\sqrt{10}}$	0	0	$\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0	0	$\frac{\alpha}{\sqrt{30}}$	0	0
$x\ \epsilon$	$-\frac{3}{\sqrt{10}}$	0	0	$-\frac{\phi^{-2}}{2\sqrt{5}}$	0	0	0	$\frac{\phi^{-1}}{\sqrt{10}}$	0	0
$x\ \xi$	0	0	0	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0
$x\ \eta$	0	0	$\frac{\phi}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^{-2}}{\sqrt{15}}$
$x\ \zeta$	0	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^2}{\sqrt{15}}$	0
$y\ \theta$	0	$\frac{1}{\sqrt{10}}$	0	0	$-\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0	0	0	$-\frac{\beta}{\sqrt{30}}$	0
$y\ \epsilon$	0	$\frac{3}{\sqrt{10}}$	0	0	$\frac{\phi^2}{2\sqrt{5}}$	0	0	0	$\frac{\phi}{\sqrt{10}}$	0
$y\ \xi$	0	0	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^2}{\sqrt{15}}$
$y\ \eta$	0	0	0	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0
$y\ \zeta$	$\frac{\phi}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^{-2}}{\sqrt{15}}$	0	0
$z\ \theta$	0	0	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{2\sqrt{5}}$	0	0	0	$-\frac{1}{\sqrt{30}}$
$z\ \epsilon$	0	0	0	0	0	$-\frac{1}{2}$	0	0	0	$-\frac{1}{\sqrt{2}}$
$z\ \xi$	0	$\frac{\phi}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^{-2}}{\sqrt{15}}$	
$z\ \eta$	$-\frac{\phi^{-1}}{\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	$\frac{\phi^2}{\sqrt{15}}$	0	0
$z\ \zeta$	0	0	0	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0

I					
$T_1 \times H$			H		
	θ	ϵ	ξ	η	ζ
$x\ \theta$	0	0	$\frac{\phi^2}{2\sqrt{3}}$	0	0
$x\ \epsilon$	0	0	$-\frac{\phi^{-1}}{2}$	0	0
$x\ \xi$	$-\frac{\phi^2}{2\sqrt{3}}$	$\frac{\phi^{-1}}{2}$	0	0	0
$x\ \eta$	0	0	0	0	$\frac{1}{\sqrt{6}}$
$x\ \zeta$	0	0	0	$-\frac{1}{\sqrt{6}}$	0
$y\ \theta$	0	0	0	$-\frac{\phi^{-2}}{2\sqrt{3}}$	0
$y\ \epsilon$	0	0	0	$\frac{\phi}{2}$	0
$y\ \xi$	0	0	0	0	$-\frac{1}{\sqrt{6}}$
$y\ \eta$	$\frac{\phi^{-2}}{2\sqrt{3}}$	$-\frac{\phi}{2}$	0	0	0
$y\ \zeta$	0	0	$\frac{1}{\sqrt{6}}$	0	0
$z\ \theta$	0	0	0	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$
$z\ \epsilon$	0	0	0	0	$-\frac{1}{2}$
$z\ \xi$	0	0	0	$\frac{1}{\sqrt{6}}$	0
$z\ \eta$	0	0	$-\frac{1}{\sqrt{6}}$	0	0
$z\ \zeta$	$\frac{\sqrt{5}}{2\sqrt{3}}$	$\frac{1}{2}$	0	0	0

I					
$T_2 \times H$			H		
	θ	ϵ	ξ	η	ζ
$x\ \theta$	0	0	$\frac{\phi^{-2}}{2\sqrt{3}}$	0	0
$x\ \epsilon$	0	0	$\frac{\phi}{2}$	0	0
$x\ \xi$	$-\frac{\phi^{-2}}{2\sqrt{3}}$	$-\frac{\phi}{2}$	0	0	0
$x\ \eta$	0	0	0	0	$\frac{1}{\sqrt{6}}$
$x\ \zeta$	0	0	0	$-\frac{1}{\sqrt{6}}$	0
$y\ \theta$	0	0	0	$-\frac{\phi^2}{2\sqrt{3}}$	0
$y\ \epsilon$	0	0	0	$-\frac{\phi^{-1}}{2}$	0
$y\ \xi$	0	0	0	0	$-\frac{1}{\sqrt{6}}$
$y\ \eta$	$\frac{\phi^2}{2\sqrt{3}}$	$\frac{\phi^{-1}}{2}$	0	0	0
$y\ \zeta$	0	0	$\frac{1}{\sqrt{6}}$	0	0
$z\ \theta$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$
$z\ \epsilon$	0	0	0	0	$-\frac{1}{2}$
$z\ \xi$	0	0	0	$\frac{1}{\sqrt{6}}$	0
$z\ \eta$	0	0	$-\frac{1}{\sqrt{6}}$	0	0
$z\ \zeta$	$-\frac{\sqrt{5}}{2\sqrt{3}}$	$\frac{1}{2}$	0	0	0

I							
$G \times G$	A	T_1			T_2		
		x	y	z	x	y	z
$a\ a$	$\frac{1}{2}$	0	0	0	0	0	0
$a\ x$	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0
$a\ y$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0
$a\ z$	0	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$
$x\ a$	0	$-\frac{1}{2}$	0	0	$-\frac{1}{2}$	0	0
$x\ x$	$\frac{1}{2}$	0	0	0	0	0	0
$x\ y$	0	0	0	$\frac{1}{2}$	0	0	$-\frac{1}{2}$
$x\ z$	0	0	$-\frac{1}{2}$	0	0	$\frac{1}{2}$	0
$y\ a$	0	0	$-\frac{1}{2}$	0	0	$-\frac{1}{2}$	0
$y\ x$	0	0	0	$-\frac{1}{2}$	0	0	$\frac{1}{2}$
$y\ y$	$\frac{1}{2}$	0	0	0	0	0	0
$y\ z$	0	$\frac{1}{2}$	0	0	$-\frac{1}{2}$	0	0
$z\ a$	0	0	0	$-\frac{1}{2}$	0	0	$-\frac{1}{2}$
$z\ x$	0	0	$\frac{1}{2}$	0	0	$-\frac{1}{2}$	0
$z\ y$	0	$-\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0
$z\ z$	$\frac{1}{2}$	0	0	0	0	0	0

I									
$G \times G$	G				H				
	a	x	y	z	θ	ϵ	ξ	η	ζ
$a\ a$	$\frac{1}{2\sqrt{3}}$	0	0	0	0	0	0	0	0
$a\ x$	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0	0
$a\ y$	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0
$a\ z$	0	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$
$x\ a$	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0	0
$x\ x$	$-\frac{1}{2\sqrt{3}}$	0	0	0	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$	0	0	0
$x\ y$	0	0	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$
$x\ z$	0	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$	0
$y\ a$	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$	0
$y\ x$	0	0	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$
$y\ y$	$-\frac{1}{2\sqrt{3}}$	0	0	0	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{2}}$	0	0	0
$y\ z$	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$	0	0
$z\ a$	0	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	0	$\frac{\sqrt{5}}{2\sqrt{3}}$
$z\ x$	0	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$	0
$z\ y$	0	$-\frac{\sqrt{5}}{2\sqrt{3}}$	0	0	0	0	$-\frac{1}{2\sqrt{3}}$	0	0
$z\ z$	$-\frac{1}{2\sqrt{3}}$	0	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0	0	0

I							
$H \times H$	A	T_1			T_2		
		x	y	z	x	y	z
$\theta\ \theta$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0
$\theta\ \epsilon$	0	0	0	0	0	0	0
$\theta\ \xi$	0	$\frac{\phi^2}{2\sqrt{5}}$	0	0	$\frac{\phi^{-2}}{2\sqrt{5}}$	0	0
$\theta\ \eta$	0	0	$-\frac{\phi^{-2}}{2\sqrt{5}}$	0	0	$-\frac{\phi^2}{2\sqrt{5}}$	0
$\theta\ \zeta$	0	0	0	$-\frac{1}{2}$	0	0	$\frac{1}{2}$
$\epsilon\ \theta$	0	0	0	0	0	0	0
$\epsilon\ \epsilon$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0
$\epsilon\ \xi$	0	$-\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0	0	$\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0
$\epsilon\ \eta$	0	0	$\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0	$-\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0
$\epsilon\ \zeta$	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{5}}$	0	0	$-\frac{\sqrt{3}}{2\sqrt{5}}$
$\xi\ \theta$	0	$-\frac{\phi^2}{2\sqrt{5}}$	0	0	$-\frac{\phi^{-2}}{2\sqrt{5}}$	0	0
$\xi\ \epsilon$	0	$\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0	0	$-\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0
$\xi\ \xi$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0
$\xi\ \eta$	0	0	0	$\frac{1}{\sqrt{10}}$	0	0	$\frac{1}{\sqrt{10}}$
$\xi\ \zeta$	0	0	$-\frac{1}{\sqrt{10}}$	0	0	$-\frac{1}{\sqrt{10}}$	0
$\eta\ \theta$	0	0	$\frac{\phi^{-2}}{2\sqrt{5}}$	0	0	$\frac{\phi^2}{2\sqrt{5}}$	0
$\eta\ \epsilon$	0	0	$-\frac{\phi\sqrt{3}}{2\sqrt{5}}$	0	0	$\frac{\phi^{-1}\sqrt{3}}{2\sqrt{5}}$	0
$\eta\ \xi$	0	0	0	$-\frac{1}{\sqrt{10}}$	0	0	$-\frac{1}{\sqrt{10}}$
$\eta\ \eta$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0
$\eta\ \zeta$	0	$\frac{1}{\sqrt{10}}$	0	0	$\frac{1}{\sqrt{10}}$	0	0
$\zeta\ \theta$	0	0	0	$\frac{1}{2}$	0	0	$-\frac{1}{2}$
$\zeta\ \epsilon$	0	0	0	$\frac{\sqrt{3}}{2\sqrt{5}}$	0	0	$\frac{\sqrt{3}}{2\sqrt{5}}$
$\zeta\ \xi$	0	0	$\frac{1}{\sqrt{10}}$	0	0	$\frac{1}{\sqrt{10}}$	0
$\zeta\ \eta$	0	$-\frac{1}{\sqrt{10}}$	0	0	$-\frac{1}{\sqrt{10}}$	0	0
$\zeta\ \zeta$	$\frac{1}{\sqrt{5}}$	0	0	0	0	0	0

I								
$H \times H$	$[G]$				$\{G\}$			
	a	x	y	z	a	x	y	z
$\theta\ \theta$	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	0	0	0	0
$\theta\ \epsilon$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0
$\theta\ \xi$	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	$\frac{\sqrt{3}}{2\sqrt{5}}$	0	0
$\theta\ \eta$	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{5}}$	0
$\theta\ \zeta$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0
$\epsilon\ \theta$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0	0
$\epsilon\ \epsilon$	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0	0	0	0	0
$\epsilon\ \xi$	0	$\frac{1}{2}$	0	0	0	$\frac{1}{2\sqrt{5}}$	0	0
$\epsilon\ \eta$	0	0	$-\frac{1}{2}$	0	0	0	$\frac{1}{2\sqrt{5}}$	0
$\epsilon\ \zeta$	0	0	0	0	0	0	0	$-\frac{1}{\sqrt{5}}$
$\xi\ \theta$	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{5}}$	0	0
$\xi\ \epsilon$	0	$\frac{1}{2}$	0	0	0	$-\frac{1}{2\sqrt{5}}$	0	0
$\xi\ \xi$	$-\frac{\sqrt{2}}{\sqrt{15}}$	0	0	0	0	0	0	0
$\xi\ \eta$	0	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$
$\xi\ \zeta$	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0
$\eta\ \theta$	0	0	$-\frac{1}{2\sqrt{3}}$	0	0	0	$\frac{\sqrt{3}}{2\sqrt{5}}$	0
$\eta\ \epsilon$	0	0	$-\frac{1}{2}$	0	0	0	$-\frac{1}{2\sqrt{5}}$	0
$\eta\ \xi$	0	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$
$\eta\ \eta$	$-\frac{\sqrt{2}}{\sqrt{15}}$	0	0	0	0	0	0	0
$\eta\ \zeta$	0	$\frac{1}{\sqrt{6}}$	0	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0	0
$\zeta\ \theta$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	0
$\zeta\ \epsilon$	0	0	0	0	0	0	0	$\frac{1}{\sqrt{5}}$
$\zeta\ \xi$	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0
$\zeta\ \eta$	0	$\frac{1}{\sqrt{6}}$	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0
$\zeta\ \zeta$	$-\frac{\sqrt{2}}{\sqrt{15}}$	0	0	0	0	0	0	0

I										
$H \times H$	H_a					H_b				
	θ	ϵ	ξ	η	ζ	θ	ϵ	ξ	η	ζ
$\theta\ \theta$	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	0	0	$\frac{1}{2\sqrt{2}}$	0	0	0
$\theta\ \epsilon$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	$\frac{1}{2\sqrt{2}}$	0	0	0	0
$\theta\ \xi$	0	0	$-\frac{1}{2\sqrt{6}}$	0	0	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0
$\theta\ \eta$	0	0	0	$-\frac{1}{2\sqrt{6}}$	0	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0
$\theta\ \zeta$	0	0	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	0
$\epsilon\ \theta$	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	$\frac{1}{2\sqrt{2}}$	0	0	0	0
$\epsilon\ \epsilon$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0	0	0	0	0	$-\frac{1}{2\sqrt{2}}$	0	0	0
$\epsilon\ \xi$	0	0	$\frac{1}{2\sqrt{2}}$	0	0	0	0	$\frac{1}{2\sqrt{2}}$	0	0
$\epsilon\ \eta$	0	0	0	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	$\frac{1}{2\sqrt{2}}$	0
$\epsilon\ \zeta$	0	0	0	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$
$\xi\ \theta$	0	0	$-\frac{1}{2\sqrt{6}}$	0	0	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	0	0
$\xi\ \epsilon$	0	0	$\frac{1}{2\sqrt{2}}$	0	0	0	0	$\frac{1}{2\sqrt{2}}$	0	0
$\xi\ \xi$	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{2}}$	0	0	0	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	0
$\xi\ \eta$	0	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0
$\xi\ \zeta$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0	0
$\eta\ \theta$	0	0	0	$-\frac{1}{2\sqrt{6}}$	0	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	0
$\eta\ \epsilon$	0	0	0	$-\frac{1}{2\sqrt{2}}$	0	0	0	0	$\frac{\sqrt{1}}{2\sqrt{2}}$	0
$\eta\ \xi$	0	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0
$\eta\ \eta$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{2}}$	0	0	0	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	0	0
$\eta\ \zeta$	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0	0	0
$\zeta\ \theta$	0	0	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	0
$\zeta\ \epsilon$	0	0	0	0	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$
$\zeta\ \xi$	0	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0	0
$\zeta\ \eta$	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	0	0	0
$\zeta\ \zeta$	$\frac{1}{\sqrt{6}}$	0	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0

Appendix G
Spinor Representations

Contents

Extensive character tables for double groups were provided by Herzberg. The $\aleph$ symbol in the present table corresponds to the Bethe rotation through an angle of 2π. Spin-orbit coupling coefficients for the icosahedral double group have been listed by Fowler and Ceulemans [12]. The notation ρ_1, ρ_2 for conjugate components follows Griffith. The single-valued irreps in Appendix A also represent the double groups. The rotation through 2π leaves these irreps invariant. Their characters under $\hat{R}$ and $\aleph\hat{R}$ are thus the same.

G.1 Character Tables

D_2^*	$\hat{E}$	$\hat{\aleph}$	$2\hat{C}_2^z$	$2\hat{C}_2^y$	$2\hat{C}_2^x$
$E_{1/2}(\Gamma_5)$	2	-2	0	0	0

D_3^*		$\hat{E}$	$\hat{\aleph}$	$2\hat{C}_3$	$2\hat{\aleph}\hat{C}_3$	$3\hat{C}_2$	$3\hat{\aleph}\hat{C}_2$
$E_{1/2}(\Gamma_4)$		2	-2	1	-1	0	0
$E_{3/2}$	ρ_1	1	-1	-1	1	i	$-i$
	ρ_2	1	-1	-1	1	$-i$	i

A.J. Ceulemans, *Group Theory Applied to Chemistry*, Theoretical Chemistry and Computational Modelling, DOI 10.1007/978-94-007-6863-5,

D_4^*	$\hat{E}$	$\hat{\aleph}$	$2\hat{C}_4$	$2\hat{\aleph}\hat{C}_4$	$2\hat{C}_2\ (=\hat{C}_4^2)$	$4\hat{C}_2'$	$4\hat{C}_2''$
$E_{1/2}(\Gamma_6)$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0
$E_{3/2}(\Gamma_7)$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0

D_5^*		$\hat{E}$	$\hat{\aleph}$	$2\hat{C}_5$	$2\hat{\aleph}\hat{C}_5$	$2\hat{C}_5^2$	$2\hat{\aleph}\hat{C}_5^2$	$5\hat{C}_2'$	$5\hat{\aleph}\hat{C}_2'$
$E_{1/2}$		2	-2	ϕ	$-\phi$	ϕ^{-1}	$-\phi^{-1}$	0	0
$E_{3/2}$		2	-2	$-\phi^{-1}$	ϕ^{-1}	$-\phi$	ϕ	0	0
$E_{5/2}$	ρ_1	1	-1	-1	1	1	-1	i	$-i$
	ρ_2	1	-1	-1	1	1	-1	$-i$	i

D_6^*	$\hat{E}$	$\hat{\aleph}$	$2\hat{C}_6$	$2\hat{\aleph}\hat{C}_6$	$2\hat{C}_3$	$2\hat{\aleph}\hat{C}_3$	$2\hat{C}_2$	$6\hat{C}_2'$	$6\hat{C}_2''$
$E_{1/2}(\Gamma_7)$	2	-2	$\sqrt{3}$	$-\sqrt{3}$	1	-1	0	0	0
$E_{5/2}(\Gamma_8)$	2	-2	$-\sqrt{3}$	$\sqrt{3}$	1	-1	0	0	0
$E_{3/2}(\Gamma_9)$	2	-2	0	0	-2	2	0	0	0

T^*		$\hat{E}$	$\hat{\aleph}$	$4\hat{C}_3$	$4\hat{\aleph}\hat{C}_3$	$4\hat{C}_3^2$	$4\hat{\aleph}\hat{C}_3^2$	$6\hat{C}_2$	$\epsilon = \exp(2\pi i/3)$
$E_{1/2}$		2	-2	1	-1	-1	1	0	
$G_{3/2}$	E''	2	-2	ϵ	$-\epsilon$	$-\bar{\epsilon}$	$\bar{\epsilon}$	0	
	E'''	2	-2	$\bar{\epsilon}$	$-\bar{\epsilon}$	$-\epsilon$	ϵ	0	

T_d^*	$\hat{E}$	$\hat{\aleph}$	$8\hat{C}_3$	$8\hat{\aleph}\hat{C}_3$	$6\hat{C}_2$	$6\hat{S}_4$	$6\hat{\aleph}\hat{S}_4$	$12\hat{\sigma}_d$
O^*	$\hat{E}$	$\hat{\aleph}$	$8\hat{C}_3$	$8\hat{\aleph}\hat{C}_3$	$6\hat{C}_2$	$6\hat{C}_4$	$6\hat{\aleph}\hat{C}_4$	$12\hat{C}_2'$
$E_{1/2}(\Gamma_6)$	2	-2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0
$E_{5/2}(\Gamma_7)$	2	-2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0
$G_{3/2}(\Gamma_8)$	4	-4	-1	1	0	0	0	0

I^*	$\hat{E}$	$\hat{\aleph}$	$12\hat{C}_5$	$12\hat{\aleph}\hat{C}_5$	$12\hat{C}_5^2$	$12\hat{\aleph}\hat{C}_5^2$	$20\hat{C}_3$	$20\hat{\aleph}\hat{C}_3$	$30\hat{C}_2$
$E_{1/2}(\Gamma_6)$	2	-2	ϕ	$-\phi$	ϕ^{-1}	$-\phi^{-1}$	1	-1	0
$E_{7/2}(\Gamma_7)$	2	-2	$-\phi^{-1}$	ϕ^{-1}	$-\phi$	ϕ	1	-1	0
$G_{3/2}(\Gamma_8)$	4	-4	1	-1	-1	1	-1	1	0
$I_{5/2}(\Gamma_9)$	6	-6	-1	1	1	-1	0	0	0

G.2 Subduction

$SO(3)$ j	I	O
1/2	$E_{1/2}$	$E_{1/2}$
3/2	$G_{3/2}$	$G_{3/2}$
5/2	$I_{5/2}$	$E_{5/2}+G_{3/2}$
7/2	$E_{7/2}+I_{5/2}$	$E_{1/2}+E_{5/2}+G_{3/2}$
9/2	$G_{3/2}+I_{5/2}$	$E_{1/2}+2G_{3/2}$
11/2	$E_{1/2}+G_{3/2}+I_{5/2}$	$E_{1/2}+E_{5/2}+2G_{3/2}$
13/2	$E_{1/2}+E_{7/2}+G_{3/2}+I_{5/2}$	$E_{1/2}+2E_{5/2}+2G_{3/2}$
15/2	$G_{3/2}+2I_{5/2}$	$E_{1/2}+E_{5/2}+3G_{3/2}$
17/2	$E_{7/2}+G_{3/2}+2I_{5/2}$	$2E_{1/2}+E_{5/2}+3G_{3/2}$
19/2	$E_{1/2}+E_{7/2}+G_{3/2}+2I_{5/2}$	$2E_{1/2}+2E_{5/2}+3G_{3/2}$

G.3 Canonical-Basis Relationships

D_3^*	$\mathbb{D}(C_3^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_{1/2}\alpha\rangle, \lvert E_{1/2}\beta\rangle$	$\begin{pmatrix} \frac{1-i\sqrt{3}}{2} & 0 \\ 0 & \frac{1+i\sqrt{3}}{2} \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$
$\lvert E_{3/2}\rho_1\rangle$	(-1)	(i)
$\lvert E_{3/2}\rho_2\rangle$	(-1)	$(-i)$

D_4^*	$\mathbb{D}(C_4^z)$	$\mathbb{D}(C_2^x)$
$\lvert E_{1/2}\alpha\rangle, \lvert E_{1/2}\beta\rangle$	$\begin{pmatrix} \frac{1-i}{\sqrt{2}} & 0 \\ 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$
$\lvert E_{3/2}\alpha'\rangle, \lvert E_{3/2}\beta'\rangle$	$\begin{pmatrix} \frac{-1+i}{\sqrt{2}} & 0 \\ 0 & \frac{-1-i}{\sqrt{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$

The components of the fourfold-degenerate $G_{3/2}$ irrep in O^* and I^* are labeled as κ, λ, μ, and ν. For a quartet spin, these labels correspond to $M_S = +3/2, +1/2, -1/2$, and $-3/2$, respectively.

O^*	$\mathbb{D}(C_4^z)$	$\mathbb{D}(C_3^{xyz})$
$\lvert E_{1/2}\alpha\rangle, \lvert E_{1/2}\beta\rangle$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1-i & 0 \\ 0 & 1+i \end{pmatrix}$	$\begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix}$
$\lvert E_{5/2}\alpha'\rangle, \lvert E_{5/2}\beta'\rangle$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1+i & 0 \\ 0 & -1-i \end{pmatrix}$	$\begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix}$

O^*	$\lvert G_{3/2}\kappa\rangle, \lvert G_{3/2}\lambda\rangle \lvert G_{3/2}\mu\rangle, \lvert G_{3/2}\nu\rangle$
	$\mathbb{D}(C_4^z)$
	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1-i & 0 & 0 & 0 \\ 0 & 1-i & 0 & 0 \\ 0 & 0 & 1+i & 0 \\ 0 & 0 & 0 & -1+i \end{pmatrix}$
	$\mathbb{D}(C_3^{xyz})$
	$\frac{1}{4}\begin{pmatrix} -1-i & \sqrt{3}(-1+i) & \sqrt{3}(1+i) & 1-i \\ \sqrt{3}(-1-i) & -1+i & -1-i & \sqrt{3}(-1+i) \\ \sqrt{3}(-1-i) & 1-i & -1-i & \sqrt{3}(1-i) \\ -1-i & \sqrt{3}(1-i) & \sqrt{3}(1+i) & -1+i \end{pmatrix}$

I^*	$\mathbb{D}(C_5)$	$\mathbb{D}(C_3^{x,y,z})$
$\lvert E_{1/2}\alpha\rangle, \lvert E_{1/2}\beta\rangle$	$\frac{1}{2}\begin{pmatrix} \phi-i & -i\phi^{-1} \\ -i\phi^{-1} & \phi+i \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1-i & -1-i \\ 1-i & 1+i \end{pmatrix}$
$\lvert E_{7/2}\alpha'\rangle, \lvert E_{7/2}\beta'\rangle$	$\frac{1}{2}\begin{pmatrix} -\phi^{-1}-i & i\phi \\ i\phi & -\phi^{-1}+i \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1-i & -1-i \\ 1-i & 1+i \end{pmatrix}$

I^*	$\lvert G_{3/2}\kappa\rangle, \lvert G_{3/2}\lambda\rangle \lvert G_{3/2}\mu\rangle, \lvert G_{3/2}\nu\rangle$
	$\mathbb{D}(C_5)$
	$\frac{1}{8}\begin{pmatrix} -\phi^{-1}-i\phi^4 & -\sqrt{3}(2+i) & -\sqrt{3}(\phi^{-1}-i\phi^{-2}) & i\phi^{-3} \\ -\sqrt{3}(2+i) & 3+\phi+i(3-\phi^{-4}) & -i(4+\phi^{-3}) & -\sqrt{3}(\phi^{-1}+i\phi^{-2}) \\ -\sqrt{3}(\phi^{-1}-i\phi^{-2}) & -i(4+\phi^{-3}) & 3+\phi+i(3-\phi^{-4}) & \sqrt{3}(2-i) \\ i\phi^{-3} & -\sqrt{3}(\phi^{-1}+i\phi^{-2}) & \sqrt{3}(2-i) & -\phi^{-1}+i\phi^4 \end{pmatrix}$
	$\mathbb{D}(C_3^{x,y,z})$
	$\frac{1}{4}\begin{pmatrix} -1-i & \sqrt{3}(-1+i) & \sqrt{3}(1+i) & 1-i \\ \sqrt{3}(-1-i) & -1+i & -1-i & \sqrt{3}(-1+i) \\ \sqrt{3}(-1-i) & 1-i & -1-i & \sqrt{3}(1-i) \\ -1-i & \sqrt{3}(1-i) & \sqrt{3}(1+i) & -1+i \end{pmatrix}$

$I^*I_{5/2} : |5/2\rangle, |3/2\rangle|1/2\rangle, |-1/2\rangle, |-3/2\rangle, |-5/2\rangle$

$\mathbb{D}(C_5)$

$$\frac{1}{32}\begin{pmatrix} -7-i-\phi(10+5i) & -\sqrt{5}\phi(4-3i) & \sqrt{10}(\phi^{-3}+i\phi^{2}) & \sqrt{10}\phi^{-2}(2+i) & \sqrt{5}(\phi^{-3}-i\phi^{-4}) & -i\phi^{-5} \\ -\sqrt{5}\phi(4-3i) & -5-3i+6\phi^{-1}-7i\phi & -\sqrt{2}(2+i)(5\phi-2) & -\sqrt{2}(3+2\phi+i-3i\phi) & i(-8+7\phi) & \sqrt{5}(\phi^{-3}+i\phi^{-4}) \\ \sqrt{10}(\phi^{-3}+i\phi^{2}) & -\sqrt{2}(2+i)(5\phi-2) & 2\phi^{3}-2i\phi^{2} & -2i(8+\phi) & -\sqrt{2}(3+2\phi-i+3i\phi) & -\sqrt{10}\phi^{-2}(2-i) \\ \sqrt{10}\phi^{-2}(2+i) & -\sqrt{2}(3+2\phi+i-3i\phi) & -2i(8+\phi) & 2\phi^{3}+2i\phi^{2} & \sqrt{2}(2-i)(5\phi-2) & \sqrt{10}(\phi^{-3}-i\phi^{2}) \\ \sqrt{5}(\phi^{-3}-i\phi^{-4}) & i(-8+7\phi) & -\sqrt{2}(3+2\phi-i+3i\phi) & \sqrt{2}(2-i)(5\phi-2) & -5+3i+6\phi^{-1}+7i\phi & \sqrt{5}\phi(4+3i) \\ -i\phi^{-5} & \sqrt{5}(\phi^{-3}+i\phi^{-4}) & -\sqrt{10}\phi^{-2}(2-i) & \sqrt{10}(\phi^{-3}-i\phi^{2}) & \sqrt{5}\phi(4+3i) & -7+i-\phi(10-5i) \end{pmatrix}$$

$\mathbb{D}(C_3^{x,y,z})$

$$\frac{1}{8}\begin{pmatrix} -1+i & \sqrt{5}(1+i) & \sqrt{10}(1-i) & -\sqrt{10}(1+i) & -\sqrt{5}(1-i) & 1+i \\ -\sqrt{5}(1-i) & 3(1+i) & \sqrt{2}(1-i) & \sqrt{2}(1+i) & 3(1-i) & -\sqrt{5}(1+i) \\ -\sqrt{10}(1-i) & \sqrt{2}(1+i) & 2(-1+i) & 2(1+i) & -\sqrt{2}(1-i) & \sqrt{10}(1+i) \\ -\sqrt{10}(1-i) & -\sqrt{2}(1+i) & 2(-1+i) & -2(1+i) & -\sqrt{2}(1-i) & -\sqrt{10}(1+i) \\ -\sqrt{5}(1-i) & -3(1+i) & \sqrt{2}(1-i) & -\sqrt{2}(1+i) & 3(1-i) & \sqrt{5}(1+i) \\ -1+i & -\sqrt{5}(1+i) & \sqrt{10}(1-i) & \sqrt{10}(1+i) & -\sqrt{5}(1-i) & -1-i \end{pmatrix}$$

G.4 Direct-Product Tables

D_3^*	$E_{1/2}$	ρ_1	ρ_2
A_1	$E_{1/2}$	ρ_1	ρ_2
A_2	$E_{1/2}$	ρ_2	ρ_1
E	$E_{1/2}+E_{3/2}$	$E_{1/2}$	$E_{1/2}$
$E_{1/2}$	$[A_2+E]+\{A_1\}$	E	E
ρ_1	E	A_2	A_1
ρ_2	E	A_1	A_2

D_4^*	$E_{1/2}$	$E_{3/2}$
A_1	$E_{1/2}$	$E_{3/2}$
A_2	$E_{1/2}$	$E_{3/2}$
B_1	$E_{3/2}$	$E_{1/2}$
B_2	$E_{3/2}$	$E_{1/2}$
E	$E_{1/2}+E_{3/2}$	$E_{1/2}+E_{3/2}$
$E_{1/2}$	$[A_2+E]+\{A_1\}$	B_1+B_2+E
$E_{3/2}$	B_1+B_2+E	$[A_2+E]+\{A_1\}$

D_5^*	$E_{1/2}$	$E_{3/2}$	ρ_1	ρ_2
A_1	$E_{1/2}$	$E_{3/2}$	ρ_1	ρ_2
A_2	$E_{1/2}$	$E_{3/2}$	ρ_2	ρ_1
E_1	$E_{1/2}+E_{3/2}$	$E_{1/2}+E_{5/2}$	$E_{3/2}$	$E_{3/2}$
E_2	$E_{3/2}+E_{5/2}$	$E_{1/2}+E_{3/2}$	$E_{1/2}$	$E_{1/2}$
$E_{1/2}$	$[A_2+E_1]+\{A_1\}$	E_1+E_2	E_2	E_2
$E_{3/2}$	E_1+E_2	$[A_2+E_2]+\{A_1\}$	E_1	E_1
ρ_1	E_2	E_1	A_2	A_1
ρ_2	E_2	E_1	A_1	A_2

D_6^*	$E_{1/2}(\Gamma_7)$	$E_{5/2}(\Gamma_8)$	$E_{3/2}(\Gamma_9)$
A_1	$E_{1/2}$	$E_{5/2}$	$E_{3/2}$
A_2	$E_{1/2}$	$E_{5/2}$	$E_{3/2}$
B_1	$E_{5/2}$	$E_{1/2}$	$E_{3/2}$
B_2	$E_{5/2}$	$E_{1/2}$	$E_{3/2}$
E_1	$E_{1/2}+E_{3/2}$	$E_{5/2}+E_{3/2}$	$E_{1/2}+E_{5/2}$
E_2	$E_{5/2}+E_{3/2}$	$E_{1/2}+E_{3/2}$	$E_{1/2}+E_{5/2}$
$E_{1/2}$	$[A_2+E_1]+\{A_1\}$	$B_1+B_2+E_2$	E_1+E_2
$E_{5/2}$	$B_1+B_2+E_2$	$[A_2+E_1]+\{A_1\}$	E_1+E_2
$E_{3/2}$	E_1+E_2	E_1+E_2	$[A_2+B_1+B_2]+\{A_1\}$

O^*	$E_{1/2}$	$E_{5/2}$	$G_{3/2}$
A_1	$E_{1/2}$	$E_{5/2}$	$G_{3/2}$
A_2	$E_{5/2}$	$E_{1/2}$	$G_{3/2}$
E	$G_{3/2}$	$G_{3/2}$	$E_{1/2}+E_{5/2}+G_{3/2}$
T_1	$E_{1/2}+G_{3/2}$	$E_{5/2}+G_{3/2}$	$E_{1/2}+E_{5/2}+2G_{3/2}$
T_2	$E_{5/2}+G_{3/2}$	$E_{1/2}+G_{3/2}$	$E_{1/2}+E_{5/2}+2G_{3/2}$
$E_{1/2}$	$[T_1]+\{A_1\}$	A_2+T_2	$E+T_1+T_2$
$E_{5/2}$	A_2+T_2	$[T_1]+\{A_1\}$	$E+T_1+T_2$
$G_{3/2}$	$E+T_1+T_2$	$E+T_1+T_2$	$[A_2+2T_1+T_2]+\{A_1+E+T_2\}$

I^*	$E_{1/2}$	$E_{7/2}$	$G_{3/2}$	$I_{5/2}$
A	$E_{1/2}$	$E_{7/2}$	$G_{3/2}$	$I_{5/2}$
T_1	$E_{1/2}+G_{3/2}$	$I_{5/2}$	$E_{1/2}+G_{3/2}+I_{5/2}$	$E_{7/2}+G_{3/2}+2I_{5/2}$
T_2	$I_{5/2}$	$E_{7/2}+G_{3/2}$	$E_{7/2}+G_{3/2}+I_{5/2}$	$E_{1/2}+G_{3/2}+2I_{5/2}$
G	$E_{7/2}+I_{5/2}$	$E_{1/2}+I_{5/2}$	$G_{3/2}+2I_{5/2}$	$E_{1/2}+E_{7/2}+2G_{3/2}+2I_{5/2}$
H	$G_{3/2}+I_{5/2}$	$G_{3/2}+I_{5/2}$	$E_{1/2}+E_{7/2}+G_{3/2}+2I_{5/2}$	$E_{1/2}+E_{7/2}+2G_{3/2}+3I_{5/2}$
$E_{1/2}$	$[T_1]+\{A\}$	G	T_1+H	T_2+G+H
$E_{7/2}$	G	$[T_2]+\{A\}$	T_2+H	T_1+G+H
$G_{3/2}$	T_1+H	T_2+H	$[T_1+T_2+G]+\{A+H\}$	$T_1+T_2+2G+2H$
$I_{5/2}$	T_2+G+H	T_1+G+H	$T_1+T_2+2G+2H$	$[2T_1+2T_2+G+H]+\{A+G+2H\}$

G.5 Coupling Coefficients

O^*				
$A_2\times G_{3/2}$	$G_{3/2}$			
	κ	λ	μ	ν
$a_2\ \kappa$	0	0	1	0
$a_2\ \lambda$	0	0	0	−1
$a_2\ \mu$	−1	0	0	0
$a_2\ \nu$	0	1	0	0

O^*				
$E\times E_{1/2}$	$G_{3/2}$			
	κ	λ	μ	ν
$\theta\ \alpha$	0	−1	0	0
$\theta\ \beta$	0	0	1	0
$\epsilon\ \alpha$	0	0	0	−1
$\epsilon\ \beta$	1	0	0	0

O^*				
$E \times E_{5/2}$	$G_{3/2}$			
	κ	λ	μ	ν
$\theta\ \alpha'$	0	0	0	−1
$\theta\ \beta'$	1	0	0	0
$\epsilon\ \alpha'$	0	1	0	0
$\epsilon\ \beta'$	0	0	−1	0

O^*								
$E \times G_{3/2}$	$E_{1/2}$		$E_{5/2}$		$G_{3/2}$			
	α	β	α'	β'	κ	λ	μ	ν
$\theta\ \kappa$	0	0	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	0	0
$\theta\ \lambda$	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0	0
$\theta\ \mu$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{1}{\sqrt{2}}$	0
$\theta\ \nu$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$
$\epsilon\ \kappa$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0
$\epsilon\ \lambda$	0	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$
$\epsilon\ \mu$	0	0	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	0	0
$\epsilon\ \nu$	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{1}{\sqrt{2}}$	0	0

Canonical complex T_1 and T_2 basis functions:

$$T_1: \quad |1\rangle = \frac{1}{\sqrt{2}}\big[-|T_{1x}\rangle - i|T_{1y}\rangle\big]$$

$$|0\rangle = |T_{1z}\rangle$$

$$|-1\rangle = \frac{1}{\sqrt{2}}\big[|T_{1x}\rangle - i|T_{1y}\rangle\big]$$

$$T_2: \quad |1\rangle = \frac{1}{\sqrt{2}}\big[-|T_{2x}\rangle - i|T_{2y}\rangle\big]$$

$$|0\rangle = |T_{2z}\rangle$$

$$|-1\rangle = \frac{1}{\sqrt{2}}\big[|T_{2x}\rangle - i|T_{2y}\rangle\big]$$

O^* $T_1 \times E_{1/2}$	$E_{1/2}$ α	β	$G_{3/2}$ κ	λ	μ	ν
$1\ \alpha$	0	0	1	0	0	0
$0\ \alpha$	$\frac{1}{\sqrt{3}}$	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0
$-1\ \alpha$	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0
$1\ \beta$	$-\frac{\sqrt{2}}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	0
$0\ \beta$	0	$-\frac{1}{\sqrt{3}}$	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0
$-1\ \beta$	0	0	0	0	0	1

O^* $T_2 \times E_{1/2}$	$E_{5/2}$ α'	β'	$G_{3/2}$ κ	λ	μ	ν
$1\ \alpha'$	0	0	0	0	1	0
$0\ \alpha'$	$\frac{1}{\sqrt{3}}$	0	0	0	0	$-\frac{\sqrt{2}}{\sqrt{3}}$
$-1\ \alpha'$	0	$\frac{\sqrt{2}}{\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$	0	0	0
$1\ \beta'$	$-\frac{\sqrt{2}}{\sqrt{3}}$	0	0	0	0	$-\frac{1}{\sqrt{3}}$
$0\ \beta'$	0	$-\frac{1}{\sqrt{3}}$	$-\frac{\sqrt{2}}{\sqrt{3}}$	0	0	0
$-1\ \beta'$	0	0	0	1	0	0

O^*	$T_1 \times G_{3/2}$											
	$E_{1/2}$		$E_{5/2}$		$G_{3/2}$				$G_{3/2}$			
	α	β	α'	β'	κ	λ	μ	ν	κ	λ	μ	ν
$1\ \kappa$	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	0	0	0	0	$\frac{\sqrt{5}}{\sqrt{6}}$
$0\ \kappa$	0	0	0	$-\frac{1}{\sqrt{3}}$	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0	$-\frac{1}{\sqrt{15}}$	0	0	0
$-1\ \kappa$	$\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	$\frac{1}{\sqrt{10}}$	0	0
$1\ \lambda$	0	0	0	$-\frac{1}{\sqrt{2}}$	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	$-\frac{1}{\sqrt{10}}$	0	0	0
$0\ \lambda$	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$\frac{1}{\sqrt{15}}$	0	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0
$-1\ \lambda$	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	$\frac{2\sqrt{2}}{\sqrt{15}}$	0	0	0	$-\frac{\sqrt{3}}{\sqrt{10}}$	0
$1\ \mu$	$\frac{1}{\sqrt{6}}$	0	0	0	0	$-\frac{2\sqrt{2}}{\sqrt{15}}$	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0
$0\ \mu$	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$-\frac{1}{\sqrt{15}}$	0	0	0	$-\frac{\sqrt{3}}{\sqrt{5}}$	0
$-1\ \mu$	0	0	$-\frac{1}{\sqrt{2}}$	0	0	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	$\frac{1}{\sqrt{10}}$
$1\ \nu$	0	$\frac{1}{\sqrt{2}}$	0	0	0	0	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	$-\frac{1}{\sqrt{10}}$	0
$0\ \nu$	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	0	$-\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0	$\frac{1}{\sqrt{15}}$
$-1\ \nu$	0	0	0	$\frac{1}{\sqrt{6}}$	0	0	0	0	$-\frac{\sqrt{5}}{\sqrt{6}}$	0	0	0

I^*	$T_1 \times E_{1/2}$					
	$E_{1/2}$		$G_{3/2}$			
	α	β	κ	λ	μ	ν
$1\ \alpha$	0	0	1	0	0	0
$0\ \alpha$	$\frac{1}{\sqrt{3}}$	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0
$-1\ \alpha$	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0
$1\ \beta$	$-\frac{\sqrt{2}}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	0
$0\ \beta$	0	$-\frac{1}{\sqrt{3}}$	0	0	$\frac{\sqrt{2}}{\sqrt{3}}$	0
$-1\ \beta$	0	0	0	0	0	1

I^*	$T_2 \times E_{1/2}$					
	$I_{5/2}$					
	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
$1\ \alpha'$	0	$-\frac{1}{4}$	0	$\frac{\sqrt{5}}{2\sqrt{2}}$	0	$-\frac{\sqrt{5}}{4}$
$0\ \alpha'$	$\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2}$	0	$\frac{\sqrt{5}}{2\sqrt{2}}$	0
$-1\ \alpha'$	0	$\frac{\sqrt{5}}{4}$	0	$-\frac{1}{2\sqrt{2}}$	0	$-\frac{3}{4}$
$1\ \beta'$	$\frac{3}{4}$	0	$\frac{1}{2\sqrt{2}}$	0	$-\frac{\sqrt{5}}{4}$	0
$0\ \beta'$	0	$-\frac{\sqrt{5}}{2\sqrt{2}}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2\sqrt{2}}$
$-1\ \beta'$	$\frac{\sqrt{5}}{4}$	0	$-\frac{\sqrt{5}}{2\sqrt{2}}$	0	$\frac{1}{4}$	0

I^*	$T_1 \times G_{3/2}$											
	$E_{1/2}$		$G_{3/2}$				$I_{5/2}$					
	α	β	κ	λ	μ	ν	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
$1\ \kappa$	0	0	0	0	0	0	1	0	0	0	0	0
$0\ \kappa$	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	0
$-1\ \kappa$	$-\frac{1}{\sqrt{2}}$	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	0	$\frac{1}{\sqrt{10}}$	0	0	0
$1\ \lambda$	0	0	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0	0
$0\ \lambda$	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{15}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0
$-1\ \lambda$	0	$-\frac{1}{\sqrt{6}}$	0	0	$\frac{2\sqrt{2}}{\sqrt{15}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0
$1\ \mu$	$-\frac{1}{\sqrt{6}}$	0	0	$-\frac{2\sqrt{2}}{\sqrt{15}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{10}}$	0	0	0
$0\ \mu$	0	$\frac{1}{\sqrt{3}}$	0	0	$-\frac{1}{\sqrt{15}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0	0
$-1\ \mu$	0	0	0	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	0	$\frac{\sqrt{3}}{\sqrt{5}}$	0
$1\ \nu$	0	$-\frac{1}{\sqrt{2}}$	0	0	$-\frac{\sqrt{2}}{\sqrt{5}}$	0	0	0	0	$\frac{1}{\sqrt{10}}$	0	0
$0\ \nu$	0	0	0	0	0	$-\frac{\sqrt{3}}{\sqrt{5}}$	0	0	0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	0
$-1\ \nu$	0	0	0	0	0	0	0	0	0	0	0	1

Solutions to Problems

1.1 The diagram for the product $\hat{C}_2^z\,\hat{\imath}$ is the same as in Fig. 1.1, except for the intermediate point P_2, which should be denoted by a circle instead of a cross, since it is now below the gray disc. However, the end point P_3 remains the same, irrespective of the order of the operators. This implies that their commutator vanishes.

1.2 Represent the rotation of the coordinates by the rotational matrix $\mathbb{D}$ as given by

$$\begin{pmatrix} \mathrm{x}_2 \\ \mathrm{y}_2 \end{pmatrix} = \mathbb{D} \begin{pmatrix} \mathrm{x}_1 \\ \mathrm{y}_1 \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \mathrm{x}_1 \\ \mathrm{y}_1 \end{pmatrix}$$

$$\begin{pmatrix} \mathrm{x}_2 & \mathrm{y}_2 \end{pmatrix} = \begin{pmatrix} \mathrm{x}_1 & \mathrm{y}_1 \end{pmatrix} \mathbb{D}^T = \begin{pmatrix} \mathrm{x}_1 & \mathrm{y}_1 \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}$$

Express the sum $\mathrm{x}_2^2 + \mathrm{y}_2^2$ as the scalar product of the coordinate row with the coordinate column and verify that this scalar product remains invariant under the matrix transformation.

1.3 In general, the radius does not change if $\mathbb{D}$ is orthogonal, i.e., if

$$\mathbb{D}^T \times \mathbb{D} = \mathbb{I}$$

1.4 Apply the general rule that a displacement of the function corresponds to an opposite coordinate displacement. As a result of the transformation, the function acquires an additional phase factor:

$$\mathcal{T}_a\, e^{ikx} = e^{ik(x-a)} = e^{-ika} e^{ikx}$$

1.5 The action of a rotation about the z-axis can be expressed by a differential operator as

$$\hat{O}(\alpha) = \cos\alpha \left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} \right) + \sin\alpha \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right)$$

The unit element corresponds to $\alpha = 0$, and hence,

$$\hat{E} = \hat{O}(0) = \left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} \right)$$

A.J. Ceulemans, *Group Theory Applied to Chemistry*, Theoretical Chemistry and Computational Modelling, DOI 10.1007/978-94-007-6863-5,

The angular momentum operator is given by

$$\begin{aligned}\mathcal{L}_z &= xp_y - yp_x \\ &= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \\ &= -\frac{\hbar}{i}\lim_{\alpha\to 0}\frac{\hat{O}(\alpha) - \hat{E}}{\alpha}\end{aligned}$$

The angular momentum operator thus is proportional to an infinitesimal rotation in the neighborhood of the unit element.

2.1 The condition that $\mathbb{C}$ be unitary gives rise to six equations:

$$\begin{aligned}1 &= |a|^2 + |b|^2 \\ 1 &= |a|^2 + |c|^2 \\ 1 &= |b|^2 + |d|^2 \\ 1 &= |c|^2 + |d|^2 \\ 0 &= |ac|e^{i(\alpha-\gamma)} + |bd|e^{i(\beta-\delta)} \\ 0 &= |ab|e^{i(\alpha-\beta)} + |cd|e^{i(\gamma-\delta)}\end{aligned}$$

From these equations it is clear that $|a| = |d|$ and $|b| = |c|$. The phase relationships may be reduced to

$$e^{i(\beta+\gamma)} = -e^{i(\alpha+\delta)}$$

With the help of these results the four matrix entries can be rewritten as

$$\begin{aligned}|a|e^{i\alpha} &= |a|e^{i(\alpha+\delta)/2}e^{i(\alpha-\delta)/2} \\ |d|e^{i\delta} &= |a|e^{i(\alpha+\delta)/2}e^{-i(\alpha-\delta)/2} \\ |b|e^{i\beta} &= |b|e^{i(\alpha+\delta)/2}e^{i[\beta-\frac{\alpha+\delta}{2}]} \\ |c|e^{i\gamma} &= -|b|e^{i(\alpha+\delta)/2}e^{i[-\beta+\frac{\alpha+\delta}{2}]}\end{aligned}$$

The general $U(2)$ matrix may thus be rewritten as

$$\mathbb{U} = e^{i(\alpha+\delta)/2}\begin{pmatrix} |a|e^{i(\alpha-\delta)/2} & |b|e^{i[\beta-\frac{\alpha+\delta}{2}]} \\ -|b|e^{i[-\beta+\frac{\alpha+\delta}{2}]} & |a|e^{-i(\alpha-\delta)/2}\end{pmatrix}$$

with $|a|^2 + |b|^2 = 1$. Note that a general phase factor has been taken out. The remaining matrix has determinant $+1$ and is called a special unitary matrix (see further in Chap. 7).

2.2 The relevant integrals are given by

$$\int_0^{2\pi} e^{-ik\phi}e^{ik\phi}d\phi = [\phi]_0^{2\pi} = 2\pi$$

$$\int_0^{2\pi} e^{\pm 2ik\phi}d\phi = \frac{1}{\pm 2ik}\left[e^{\pm 2ik\phi}\right]_0^{2\pi} = 0$$

The normalized cyclic waves are thus given by

$$|\pm k\rangle = \frac{1}{\sqrt{2\pi}} e^{\pm ik\phi}$$

and these waves are orthogonal: $\langle -k|k\rangle = 0$.

2.3 The combination of transposition and complex conjugation is called the *adjoint* operation, indicated by a dagger. A Hermitian matrix is thus self-adjoint. An eigenfunction of this matrix, operating in a function space, may be expressed as a linear combination

$$|\psi_m\rangle = \sum_k c_k |f_k\rangle$$

We may arrange the expansion coefficients as a column vector **c**. This is called the eigenvector. Its adjoint, $\mathbf{c}^\dagger$, is then the complex-conjugate row vector. The corresponding eigenvalue is denoted as E_m. Now start by writing the eigenvalue equation and multiply left and right with the adjoint eigenvector:

$$\mathbb{H}\mathbf{c} = E_m \mathbf{c}$$
$$\mathbf{c}^\dagger \mathbb{H}\mathbf{c} = E_m \mathbf{c}^\dagger \mathbf{c}$$

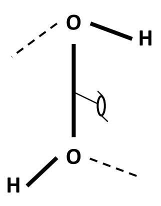
Now take the adjoint and use the self-adjoint property of $\mathbb{H}$:

$$\mathbf{c}^\dagger \mathbb{H}^\dagger \mathbf{c} = \bar{E}_m \mathbf{c}^\dagger \mathbf{c}$$
$$\mathbf{c}^\dagger \mathbb{H}\mathbf{c} = \bar{E}_m \mathbf{c}^\dagger \mathbf{c}$$

A comparison of both results shows that the eigenvalue must be equal to its complex conjugate and hence be real. If $\mathbb{H}$ is skew-symmetric, a similar argument shows that the eigenvalue must be imaginary.

3.1 The table is a valid multiplication table of a group that is isomorphic to D_2. The element C is the unit element. There are six ways to assign the three twofold axes to the letters A, B, D.

3.2 Any nonlinear triatomic molecule with three different atoms has only C_s symmetry, e.g., a water molecule with one hydrogen replaced by deuterium. C_2 symmetry requires a nonplanar tetra-atomic molecule, such as H_2O_2. In the free state the dihedral angle of this molecule is almost a right angle (see the figure). To realize C_i symmetry, one needs at least six atoms. Since three atoms are always coplanar, the smallest molecule with no symmetry at all has at least four atoms.



3.3 There are only three regular tesselations of the plane: triangles, squares, and hexagons.

3.4 The rotation generates points that are lying on a circle, perpendicular to the rotation. If the rotational angle is not a rational fraction of a full angle, every time the rotation is repeated, a new point will be generated. To obtain an integer order, the additional requirement is to be added that the original point is retrieved after one full turn.

3.5 Consider a subgroup $H \subset G$ such that $|G|/|H| = 2$. Then the coset expansion of G will be limited to only two cosets:

$$G = H + \hat{g}H$$

Here $\hat{g}$ is a coset generator outside H. The subgroup is normal if the right and left cosets coincide, Since there is only one coset outside H, it is required that

$$\hat{g}H = H\hat{g}$$

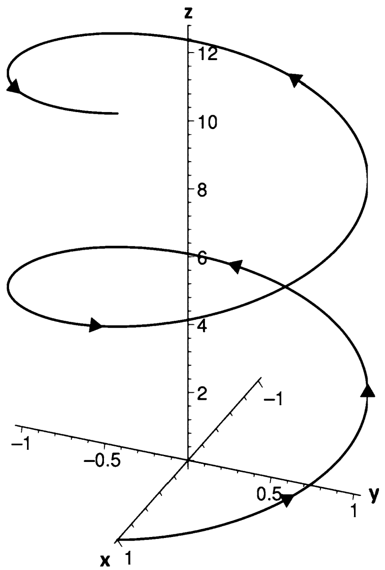
Suppose that this equation does not hold. Then this can only mean that there are elements in H such that

$$\hat{h}_x \hat{g} = \hat{h}_y$$

But then the coset generator must be an element of H, which contradicts the staring assumption.

3.6 Soccer ball: I_h. Tennis ball: D_{2d}. Basketball: D_{2h}. Trefoil knot: D_3.

3.7 The figure (from Wikipedia) shows the helix function for $n = 1$. One full turn is realized for $t/a = 2\pi \approx 6.283$. This is a right-handed helix.



The enantiomeric function reads:

$$x(t) = a\cos\left(\frac{nt}{a}\right)$$
$$y(t) = a\sin\left(-\frac{nt}{a}\right)$$
$$z(t) = t$$

Note that a uniform sign change of t would leave the right-handed helix unchanged. For the discrete helix, the screw symmetry consists of a translation in the z-direction over a distance $2\pi a/m$ in combination with a rotation around the z-axis over an angle $2\pi n/m$. If m is irrational, the helix will not be periodic, and the screw symmetry is lost.

4.1 The site symmetry of a cube is T_h. The cube is an invariant of its site group and transforms as a_g in T_h. The set of five cubes thus spans the induced representation: $aT_h \uparrow I_h$. Applying the Frobenius theorem to the subduction (see Sect. C.1), one obtains

$$aT_h \uparrow I_h = A_g + G_g \tag{1}$$

4.2 The irreps can be obtained from the induction table in Sect. C.2, as $\Gamma_\pi C_{3v} \uparrow T_d$:

$$\Gamma_\pi C_{3v} \uparrow T_d = E + T_1 + T_2 \tag{2}$$

The SALCs shown span the tetrahedral E irrep, the one on the left is the E_θ component, and the one on the right is the E_ϵ component. Note that they transform into each other by rotating all π-orbitals over 90° in the same sense [13].

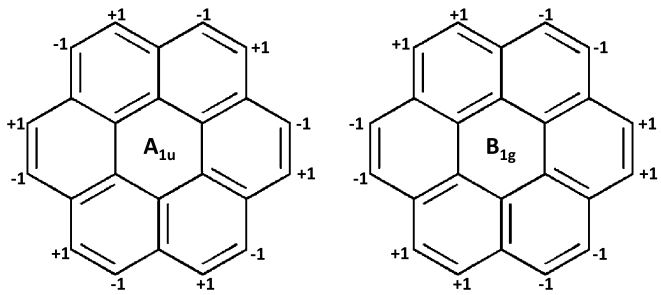
4.3 The 24 carbon atoms of coronene form three orbits: two orbits of six atoms, corresponding to the internal hexagon and to the six atoms on the outer ring that have bonds to the inner ring, and one orbit of the twelve remaining atoms. The elements of the 6-orbit occupy sites of C'_{2v} symmetry, based on $\hat{C}'_2, \hat{\sigma}_h, \hat{\sigma}_v$ in D_{6h}. The p_z orbitals on these sites transform as b_1, and hence the induced irreps are as in the case of benzene:

$$b_1C_{2v} \uparrow D_{6h} = B_{2g} + A_{2u} + E_{1g} + E_{2u} \tag{3}$$

The remaining 12-orbit connects carbon atoms with only C_s site symmetry, the p_z orbitals on these sites transforming as a''. The induced irreps read:

$$a''C_s \uparrow D_{6h} = B_{1g} + B_{2g} + A_{1u} + A_{2u} + 2E_{1g} + 2E_{2u} \tag{4}$$

The A_{1u} and B_{1g} irreps only appear in the 12-orbit, so we can infer that the molecular orbitals with this symmetry will entirely be localized on the 12-orbit. The SALCs can easily be constructed, as they should be antisymmetric with respect to the $\hat{\sigma}_v$ planes in order not to hybridize with the SALCs based on the 6-orbits.



4.4 The tangential π-orbitals transform as Γ_π in the C_{5v} site group of I_h. According to Sect. C.2, one has:

$$\Gamma_\pi \; C_{5v} \uparrow I_h = T_{1g} + T_{1u} + G_g + G_u + H_g + H_u$$

4.5 When the projector that generated the component is characterized as $\hat{P}_{kl}^{\Gamma_i}$, the other components may be found by varying the k index.

4.6 Act with an operator $\hat{S}$ on the projector and carry out the substitution $\hat{R} = \hat{S}^{-1}\hat{T}$:

$$\begin{aligned}\hat{S}\hat{P}_{11}^{\Gamma_0} &= \hat{S}\frac{1}{|G|}\sum_R \hat{R} \\ &= \frac{1}{|G|}\sum_R \hat{S}\hat{R} = \frac{1}{|G|}\sum_T \hat{T} = \hat{P}_{11}^{\Gamma_0}\end{aligned}$$

4.7 Applying the inverse transformation to the SALCs of the hydrogens in ammonia yields

$$\left(|sp_A^2\rangle \quad |sp_B^2\rangle \quad |sp_C^2\rangle \right) = \left(|2s\rangle \quad |2p_x\rangle \quad |2p_y\rangle \right) \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

4.8 This mode transforms as E_y. It can be written as a linear combination of a radial and a tangent mode:

$$Q = \frac{-1}{\sqrt{2}} Q_y^{\text{rad}} + \frac{1}{\sqrt{2}} Q_y^{\tan}$$

with

$$\begin{aligned} Q_y^{\text{rad}} &= \frac{1}{\sqrt{2}}(\Delta R_B - \Delta R_C) \\ Q_y^{\tan} &= \frac{1}{\sqrt{6}} R(2\Delta\phi_A - \Delta\phi_B - \Delta\phi_C) \end{aligned}$$

This mode preserves the center of mass and is a genuine normal mode.

4.9 Since all irreps are one-dimensional, the characters can only consist of a phase factor:

$$\mathbb{D}(C_5) = e^{i\lambda}\mathbb{I} \tag{5}$$

The fifth power of the generator will yield the unit element, and hence,

$$e^{5i\lambda} = 1 \tag{6}$$

This is the Euler equation. Its solutions are the characters in the table of C_5, as given in Appendix A.

4.10 The product of inversion with a $\hat{C}_2$ axis must yield a reflection plane, perpendicular to this axis. As an example, a product of type $\hat{\imath} \cdot \hat{C}_2'$ must yield a reflection plane of $\hat{\sigma}_d$ type, as this is perpendicular to the primed twofold axis. For the one-dimensional irreps of D_{6h}, one thus should have

$$\chi(\imath)\chi\left(C_2'\right) = \chi(\sigma_d) \tag{7}$$

This is indeed verified to be the case.

4.11 The a_2'' distortion is antisymmetric with respect to $3\hat{C}_2, \hat{\sigma}_h$, and $2\hat{S}_3$. As a result, when the mode is launched, all these symmetry elements will be destroyed, and the symmetry reduces to the subgroup C_{3v}. In general, the result of a distortion will always be the maximal subgroup for which the distortion is totally symmetric [14].

4.12 The group of this fullerene is D_{6d}. The 24 atoms separate into two orbits: a 12-orbit containing the top and bottom hexagons and another 12-orbit containing the crown of the 12 atoms, numbered from 7 to 18. In both cases the site group is only C_s, and hence both orbits will span the same irreps:

$$a'C_s \uparrow D_{6d} = A_1 + B_2 + E_1 + E_2 + E_3 + E_4 + E_5$$

Quite remarkably, the Hückel spectrum for this fullerene has a nonbonding level of E_4 symmetry.

5.1 Let $\mathbf{r}_i$ and $\mathbf{r}_j$ denote the position vectors of electrons i and j. The electron repulsion operator contains the distance between both electrons as $|\mathbf{r}_i - \mathbf{r}_j|$. The matrix $\mathbb{D}(R)$ expresses the transformation of the Cartesian coordinates under a rotation. This matrix will also rotate the coordinate *differences*:

$$\hat{R}\begin{pmatrix} \mathrm{x}_i - \mathrm{x}_j \\ \mathrm{y}_i - \mathrm{y}_j \\ \mathrm{z}_i - \mathrm{z}_j \end{pmatrix} = \mathbb{D}(R)\begin{pmatrix} \mathrm{x}_i - \mathrm{x}_j \\ \mathrm{y}_i - \mathrm{y}_j \\ \mathrm{z}_i - \mathrm{z}_j \end{pmatrix} \tag{8}$$

Exactly as in the derivation for Problem 1.2, the square of the distance between the two electrons is then found to be invariant under any orthogonal transformation of the coordinates.

5.2 For the G irrep, it is noted from Sect. C.1 that a tetrahedral splitting field will branch G into $A + T$. It thus acts as a splitting field to isolate the unique Ga component. Symmetry adaptation to $\hat{C}_2^z$ will yield two totally symmetric components, one of which will be the Ga already obtained; the remaining one is then Gz. The corresponding Gx and Gy may then be found by cyclic permutation under the $\hat{C}_3^{xyz}$ axis.

For the H irrep, one may make use of the $\hat{C}_3^{xyz}$ axis again. It resolves H into $A_1 + 2E$. This unique A_1 component will be the sum $H\xi + H\eta + H\zeta$. We can project the $H\zeta$ component out of this sum by using the $\hat{C}_2^z$ axis. Although the H level subduces three totally symmetric irreps in C_2, there will be no contamination with $H\theta$ and $H\epsilon$ since these were already removed in the first step by projecting out the trigonal A_1.

5.3 The total number of nuclear permutations and permutation-inversions for CH_3BF_2 is 24. This is the product of six permutations of the protons, two permutations of the fluorine nuclei, and the binary group of the spatial inversion. However, as the fluxionality of this molecule is limited to free rotations of the methyl group, the operations should be limited to those permutations or permutation-inversions that lead to structures that can be rotated back to the original frame *or to a rotamer of this frame*. Only half of the operations will comply with this requirement. As an example, the odd permutations of the protons are not allowed since the resulting structure cannot be turned into the original one by outer rotations or by rotations of the methyl group around the C-B bond. The results are given in [15]. The corresponding symmetry group is isomorphic with D_{3h}.

5.4 Ferrocene is a molecule with two identical coaxial rotors. Its nuclear permutation-inversion group consists of 100 elements. It has a halving rotational subgroup of 50 proper permutations: for each of the cyclo-pentadienyl rings, there are 5 cyclic permutation operations, yielding a total of $5^2 = 25$ operations, and this number must be doubled to account for the permutation of the upper and lower rings. In addition, there is a coset of improper permutation-inversions containing the other 50 elements. This coset also contains two kinds of elements. In the table we summarize the structure of the group. The carbon atoms are numbered $1, \ldots, 5$ in the upper ring and $6, \ldots, 10$ in the lower ring.

Nuclear permutation-inversion group for ferrocene (u and l refer to upper and lower rotor)

	$\hat{R}$	#
$C_5^u \times C_5^l$	(12345)	25
(ul)	(16) (2, 10) (39) (48) (57)	25
$5\hat{\sigma}_v^u \times 5\hat{\sigma}_v^l$	(25) (34) (7, 10) (89)*	25
$(ul)^*$	(16) (27) (38) (49) (5, 10)*	25

6.1 The $(t_{1u})^2$ configuration gives rise to 15 states. The direct product decomposes as follows (see Appendix D):

$$T_{1u} \times T_{1u} = [A_{1g} + E_g + T_{2g}] + \{T_{1g}\}$$

The symmetrized part will give rise to six singlet functions, while there are nine triplet substates, forming a $^3T_{1g}$ multiplet. Since the 3-electron Ψ state is a quartet, the singlet states cannot contribute, and we need to couple the triplet to a $^2T_{1u}$ state, resulting from a $(t_{1u})^1$ configuration. The orbital part of the triplet is obtained from the $T_1 \times T_1 = T_1$ coupling table in Appendix F:

$$|T_{1g}x\rangle = \frac{1}{\sqrt{2}}\big[-y(1)z(2) + z(1)y(2)\big]$$

$$|T_{1g}y\rangle = \frac{1}{\sqrt{2}}\big[x(1)z(2) - z(1)x(2)\big]$$

$$|T_{1g}z\rangle = \frac{1}{\sqrt{2}}\big[-x(1)y(2) + y(1)x(2)\big]$$

The coupling with the third electron can yield A_{1u}, E_u, T_{1u}, and T_{2u} states. Our results is based on the A_{1u} product. This yields

$$A_{1u} = \frac{1}{\sqrt{3}}\big[|T_{1g}x\rangle|x(3)\rangle + |T_{1g}y\rangle|y(3)\rangle + |T_{1g}z\rangle|z(3)\rangle\big]$$
$$= -\frac{1}{\sqrt{6}}\begin{vmatrix} x(1) & y(1) & z(1) \\ x(2) & y(2) & z(2) \\ x(3) & y(3) & z(3) \end{vmatrix}$$

This should be multiplied by the product of the three α-spins, $\alpha_1\alpha_2\alpha_3$, to obtain the $^4A_{1u}$ ground state of the $(t_{1u})^3$ configuration.

6.2 The JT problem is determined by the symmetrized direct product of T_{1u}. As we have seen in the previous problem, this product contains $A_{1g} + E_g + T_{2g}$. Since A_{1g} modes do not break the symmetry, the JT problem is of type $T_1 \times (e+t_2)$. In the linear problem only two force elements are required. The distortion matrix is thus as follows:

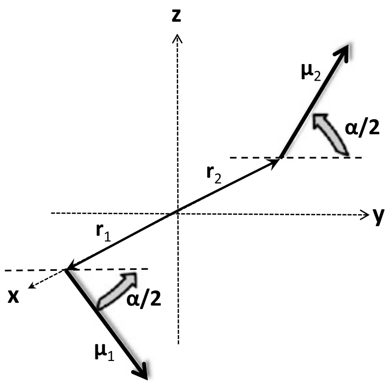
$$\mathcal{H}' = \frac{F_E}{\sqrt{6}}\begin{pmatrix} Q_\theta & 0 & 0 \\ 0 & Q_\theta & 0 \\ 0 & 0 & -2Q_\theta \end{pmatrix} + \frac{F_T}{\sqrt{2}}\begin{pmatrix} 0 & -Q_\zeta & -Q_\eta \\ -Q_\zeta & 0 & -Q_\xi \\ -Q_\eta & 0_\xi & 0 \end{pmatrix}$$

6.3 The magnetic dipole operator transforms as T_{1g}, while the direct square of e_g irreps yields $A_{1g} + A_{2g} + E_g$. Since the operator irrep is not contained in the product space, the selection rules will not allow a dipole matrix element between e_g orbitals.

6.4 We first draw a simple diagram representing the R-conformation. The point group is C_2. The twofold-axis is oriented along the y-direction, and the centers of the two chromophores are placed on the positive and negative x-axes. The dipole moments are then oriented as

$$\boldsymbol{\mu}_1 = \mu\left(0, \cos\frac{\alpha}{2}, -\sin\frac{\alpha}{2}\right)$$

$$\boldsymbol{\mu}_2 = \mu\left(0, \cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}\right)$$



The exciton states on both chromophores are interchanged by the twofold axis and can be recombined to yield a symmetric and an antisymmetric combination, denoted as A and B, respectively. One has:

$$|\Psi_A\rangle = \frac{1}{\sqrt{2}}\big(|\Psi_1\rangle + |\Psi_2\rangle\big)$$
$$|\Psi_B\rangle = \frac{1}{\sqrt{2}}\big(|\Psi_1\rangle - |\Psi_2\rangle\big)$$

The corresponding transition dipoles are oriented along the positive y- and negative z-direction, respectively:

$$\boldsymbol{\mu}_A = \sqrt{2}\mu\left(0, \cos\frac{\alpha}{2}, 0\right)$$
$$\boldsymbol{\mu}_B = \sqrt{2}\mu\left(0, 0, -\sin\frac{\alpha}{2}\right)$$

The dipole-dipole interaction is given by

$$V_{12} = \frac{1}{4\pi\epsilon_0}\frac{\cos\alpha}{R_{12}^3} \tag{9}$$

For $\alpha < \pi/2$, the dipole orientation is repulsive. As a result, the in-phase coupled exciton state $|\Psi_A\rangle$ will be at higher energy than the out-of-phase $|\Psi_B\rangle$ state. Finally, we also calculate the magnetic transition dipoles, using the expressions from Sect. 6.8:

$$\mathbf{m}_A = \frac{i\pi\nu}{\sqrt{2}}(\mathbf{r}_1 \times \boldsymbol{\mu}_1 + \mathbf{r}_2 \times \boldsymbol{\mu}_2) = \frac{i\pi\nu\mu}{\sqrt{2}}R_{12}\sin\frac{\alpha}{2}(0, 1, 0)$$
$$\mathbf{m}_B = \frac{i\pi\nu}{\sqrt{2}}(\mathbf{r}_1 \times \boldsymbol{\mu}_1 - \mathbf{r}_2 \times \boldsymbol{\mu}_2) = \frac{i\pi\nu\mu}{\sqrt{2}}R_{12}\cos\frac{\alpha}{2}(0, 0, 1)$$

These results are now combined in the Rosenfeld equation to yield the rotatory strength of both exciton states:

$$\mathcal{R}_A = \frac{\pi\nu\mu^2}{2}R_{12}\sin\alpha$$

$$\mathcal{R}_B = -\frac{\pi \nu \mu^2}{2} R_{12} \sin\alpha$$

This result predicts a normal CD sign, with a lower negative branch (B-state) and an upper positive branch (A-state) [16]. This is a typical right-handed helix, corresponding to a rotation of the dipoles in the right-handed sense when going from chromophore 1 to chromophore 2 along the inter-chromophore axis. In the S-conformation the sign of α will change, and the CD spectrum will be inverted.

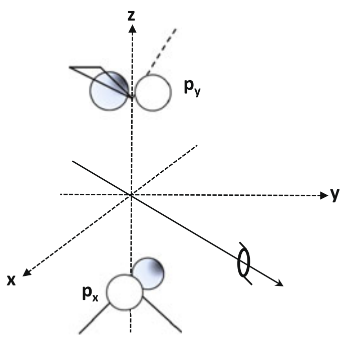
6.5 The direct square of the e-irrep in D_{2d} yields four coupled states:

$$e \times e = A_1 + A_2 + B_1 + B_2 \tag{10}$$

The corresponding coupling coefficients are given in the table below. This table is almost the same as the table for D_4 in Appendix F, but note that B_1 and B_2 are interchanged. Such details are important, and therefore we draw again a simple picture of the molecule in a Cartesian system. Both in D_4 and in D_{2d}, the B_1 and B_2 irreps are distinguished by their symmetry with respect to the $\hat{C}_2'$ axes.

D_{2d}				
$E \times E$	A_1 / a_1	A_2 / a_2	B_1 / b_1	B_2 / b_2
$x\ x$	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$
$y\ y$	$\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$
$x\ y$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0
$y\ x$	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0

In the orientation of twisted ethylene, as indicated in the figure below, the directions of these axes are along the bisectors of x and y. In contrast, in the standard orientation for D_4 they are *along* the x and y axes, while the bisector directions coincide with the $\hat{C}_2''$ axes, and hence the interchange between B_1 and B_2.



Note that the two-electron states are symmetrized, except the A_2 combination. The symmetrized states will combine with singlet spin states, while the A_2 state will be a triplet. One thus has:

$$
\begin{aligned}
{}^1A_1 &= \frac{1}{\sqrt{2}}\big(x(1)x(2) + y(1)y(2)\big)\frac{1}{\sqrt{2}}\big(\alpha(1)\beta(2) - \beta(1)\alpha(2)\big) \\
&= \frac{1}{\sqrt{2}}\big(\big|(x\alpha)(x\beta)\big| + \big|(y\alpha)(y\beta)\big|\big) \\
{}^1B_1 &= \frac{1}{\sqrt{2}}\big(\big|(x\alpha)(y\beta)\big| + \big|(y\alpha)(x\beta)\big|\big) \\
{}^1B_2 &= \frac{1}{\sqrt{2}}\big(-\big|(x\alpha)(x\beta)\big| + \big|(y\alpha)(y\beta)\big|\big) \\
{}^3A_2 &= \big|(x\alpha)(y\alpha)\big|
\end{aligned}
$$

The ${}^1A_1$ and ${}^1B_2$ states are the *zwitterionic states*, while the ${}^1B_1$ and ${}^3A_2$ states are called the *diradical* states. It is clear from the expressions that in both cases the two radical carbon sites are neutral. The zwitterionic states are easily polarizable though.

6.6 The carbon atoms form two orbits. The p_z orbital on the central atom is in the center of the symmetry group and transforms as a_2''. The three methylene orbitals are in C_{2v} sites, transforming as the b_2 irrep of the site group, i.e., they are antisymmetric with respect to $\hat{\sigma}_h$ and symmetric with respect to $\hat{\sigma}_v$. The induced representation is

$$b_2 C_{2v} \uparrow D_{3h} = a_2'' + e'' \tag{11}$$

The SALCs are entirely similar to the hydrogen SALCs in the case of ammonia; this implies, for instance, that the component labeled x is symmetric under the vertical symmetry plane through atom A. It will be antisymmetric for the twofold-axis going through atom A since the relevant orbital is of p_z type:

$$
\begin{aligned}
|\Psi_a\rangle &= \frac{1}{\sqrt{3}}\big(|p_A\rangle + |p_B\rangle + |p_C\rangle\big) \\
|\Psi_x\rangle &= \frac{1}{\sqrt{6}}\big(2|p_A\rangle - |p_B\rangle - |p_C\rangle\big) \\
|\Psi_y\rangle &= \frac{1}{\sqrt{2}}\big(|p_B\rangle - |p_C\rangle\big)
\end{aligned}
$$

The a_2'' orbitals interact to yield bonding and antibonding combinations at $E = \alpha \pm \sqrt{3}\beta$. Since the graph is bipartite, the remaining e'' orbitals are necessarily nonbonding and will be occupied by two electrons. The direct square of this irrep yields symmetrized A_1' and E' states and an antisymmetrized A_2' state. The expressions for these states are obtained from the coupling coefficients for D_3 in Appendix F:

$$
\begin{aligned}
{}^1A_1' &= \frac{1}{\sqrt{2}}\big(x(1)x(2) + y(1)y(2)\big)\frac{1}{\sqrt{2}}\big(\alpha(1)\beta(2) - \beta(1)\alpha(2)\big) \\
&= \frac{1}{\sqrt{2}}\big(\left|(x\alpha)(x\beta)\right| + \left|(y\alpha)(y\beta)\right|\big) \\
{}^1E_x' &= \frac{1}{\sqrt{2}}\big(\left|(x\alpha)(y\beta)\right| + \left|(y\alpha)(x\beta)\right|\big) \\
{}^1E_y' &= \frac{1}{\sqrt{2}}\big(-\left|(x\alpha)(x\beta)\right| + \left|(y\alpha)(y\beta)\right|\big) \\
{}^3A_2 &= \left|(x\alpha)(y\alpha)\right|
\end{aligned}
$$

Note that the distinction between zwitterionic and diradical states does not hold in this case. Formally, TMM can be described as a valence isomer between three configurations in which one of the peripheral atoms has a double bond to the central atom and the other two sites carry an unpaired electron.

7.1 In a cube the d-shell also splits in $e_g + t_{2g}$, but the ordering is reversed. Explicit calculation of the potential shows that the splitting is reduced by a factor $8/9$:

$$\Delta_{\text{cube}} = -\frac{8}{9}\Delta_{\text{octahhedron}}$$

7.2 Perform the matrix multiplication and verify that the product matrix is of Cayley–Klein form. The multiplication is not commutative:

$$\begin{pmatrix} a_1 & b_1 \\ -\bar{b}_1 & \bar{a}_1 \end{pmatrix} \times \begin{pmatrix} a_2 & b_2 \\ -\bar{b}_2 & \bar{a}_2 \end{pmatrix} = \begin{pmatrix} a_1a_2 - b_1\bar{b}_2 & a_1b_2 + \bar{a}_2b_1 \\ -\bar{a}_1\bar{b}_2 - a_2\bar{b}_1 & \bar{a}_1\bar{a}_2 - \bar{b}_1b_2 \end{pmatrix} \tag{12}$$

7.3 The double group D_3^* contains 12 elements. In Table 7.5 we have listed the six representation matrices for the elements on the positive hemisphere. The $\hat{C}_2^A$ axis is along the x-direction, $\hat{C}_2^B$ is at $-60°$ and $\hat{C}_2^C$ is at $+60°$. The derivation of the multiplication table and the underlying class structure (see Table 7.6) is based on a straightforward matrix multiplication.

Multiplication table for the double group D_3^*

D_3^*	$\hat{E}$	$\hat{C}_3$	$\hat{C}_3^2$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^C$
$\hat{E}$	$\hat{E}$	$\hat{C}_3$	$\hat{C}_3^2$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^C$
$\hat{C}_3$	$\hat{C}_3$	$\hat{C}_3^2$	$\aleph$	$\aleph\hat{C}_3^2$	$\hat{E}$	$\aleph\hat{C}_3$	$\hat{C}_2^C$	$\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\hat{C}_2^B$
$\hat{C}_3^2$	$\hat{C}_3^2$	$\aleph$	$\aleph\hat{C}_3$	$\hat{E}$	$\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph\hat{C}_2^B$	$\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\hat{C}_2^A$
$\aleph\hat{C}_3$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\hat{E}$	$\hat{C}_3^2$	$\aleph$	$\hat{C}_3$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\hat{C}_2^B$	$\hat{C}_2^C$	$\hat{C}_2^A$	$\aleph\hat{C}_2^B$
$\aleph\hat{C}_3^2$	$\aleph\hat{C}_3^2$	$\hat{E}$	$\hat{C}_3$	$\aleph$	$\aleph\hat{C}_3$	$\hat{C}_3^2$	$\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\hat{C}_2^C$	$\aleph\hat{C}_2^A$
$\aleph$	$\aleph$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\hat{C}_3$	$\hat{C}_3^2$	$\hat{E}$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\hat{C}_2^C$
$\hat{C}_2^A$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^B$	$\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\aleph$	$\aleph\hat{C}_3$	$\hat{C}_3^2$	$\hat{E}$	$\hat{C}_3$	$\aleph\hat{C}_3^2$
$\hat{C}_2^B$	$\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\hat{C}_2^C$	$\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\hat{C}_3^2$	$\aleph$	$\hat{C}_3$	$\aleph\hat{C}_3^2$	$\hat{E}$	$\aleph\hat{C}_3$
$\hat{C}_2^C$	$\hat{C}_2^C$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph$	$\hat{C}_3$	$\hat{C}_3^2$	$\hat{E}$
$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\hat{C}_2^C$	$\hat{C}_2^B$	$\aleph\hat{C}_2^C$	$\hat{C}_2^A$	$\hat{E}$	$\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph$	$\aleph\hat{C}_3$	$\hat{C}_3^2$
$\aleph\hat{C}_2^B$	$\aleph\hat{C}_2^B$	$\hat{C}_2^C$	$\hat{C}_2^A$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\hat{C}_2^B$	$\aleph\hat{C}_3^2$	$\hat{E}$	$\aleph\hat{C}_3$	$\hat{C}_3^2$	$\aleph$	$\hat{C}_3$
$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^C$	$\aleph\hat{C}_2^A$	$\aleph\hat{C}_2^B$	$\hat{C}_2^A$	$\hat{C}_2^B$	$\hat{C}_2^C$	$\hat{C}_3$	$\hat{C}_3^2$	$\hat{E}$	$\aleph\hat{C}_3$	$\aleph\hat{C}_3^2$	$\aleph$

7.4 The action of the spin operators on the components of a spin-triplet can be found by acting on the coupled states, as summarized in Table 7.2. As an example, where we have added the electron labels 1 and 2 for clarity:

$$
\begin{aligned}
S_x|+1\rangle &= S_x\big[|\alpha_1\rangle|\alpha_2\rangle\big] = \big[S_x|\alpha_1\rangle\big]|\alpha_2\rangle + |\alpha_1\rangle\big[S_x|\alpha_2\rangle\big] \\
&= \frac{\hbar}{2}\big[|\beta_1\rangle|\alpha_2\rangle + |\alpha_1\rangle|\beta_2\rangle\big] = \frac{\hbar}{\sqrt{2}}|0\rangle \\
S_y|-1\rangle &= -\frac{i\hbar}{\sqrt{2}}|0\rangle
\end{aligned}
$$

These results can be generalized as follows:

$$
\begin{aligned}
S_z|M_S\rangle &= \hbar M_S|M_S\rangle \\
(S_x \pm iS_y)|M_S\rangle &= \hbar\big[(S \mp M_S)(S \pm M_s + 1)\big]^{\frac{1}{2}}|M_s \pm 1\rangle
\end{aligned}
$$

The action of the spin Hamiltonian in the fictitious spin basis gives then rise to the following Hamiltonian matrix (in units of μ_B):

$\mathcal{H}_{Ze}$	$\|0\rangle$	$\|+1\rangle$	$\|-1\rangle$
$\langle 0\|$	0	$g_\perp\frac{1}{\sqrt{2}}(B_x + iB_y)$	$g_\perp\frac{1}{\sqrt{2}}(B_x - iB_y)$
$\langle +1\|$	$g_\perp\frac{1}{\sqrt{2}}(B_x - iB_y)$	$g_{\|\|}B_z$	0
$\langle -1\|$	$g_\perp\frac{1}{\sqrt{2}}(B_x + iB_y)$	0	$-g_{\|\|}B_z$

We can now identify these expressions with the actual matrix elements in the basis of the three D_3 components, keeping in mind the relationship between the complex and real triplet basis, as given in Eq. (7.39). One obtains:

$$\langle 0|\mathcal{H}_{Ze}|+1\rangle = -\frac{1}{\sqrt{2}}\langle A_1|\mathcal{H}|E_x + iE_y\rangle = \frac{1}{\sqrt{2}}\big[-a+d+i(-b-c)\big]$$
$$\langle 0|\mathcal{H}_{Ze}|-1\rangle = \frac{1}{\sqrt{2}}\langle A_1|\mathcal{H}|E_x - iE_y\rangle = \frac{1}{\sqrt{2}}\big[a+d+i(b-c)\big]$$
$$\langle \pm 1|\mathcal{H}_{Ze}|\pm 1\rangle = \frac{1}{2}\big[\langle x|\mathcal{H}|x\rangle + \langle y|\mathcal{H}|y\rangle \pm i\big(\langle x|\mathcal{H}|y\rangle - \langle y|\mathcal{H}|x\rangle\big)\big] = \pm f$$

From these equations the parameters may be identified as follows:

$$\begin{aligned} a &= 0 \\ b &= -g_{\perp}B_y \\ c &= 0 \\ d &= g_{\perp}B_x \\ e &= 0 \\ f &= g_{||}B_z \end{aligned}$$

The Zeeman Hamiltonian does not include the zero-field splitting between the A_1 and E states. This can be rendered by a second-order spin operator, which transforms as the octahedral $E_g\theta$ quadrupole component:

$$\mathcal{H}_{ZF} = \frac{D}{3\hbar^2}\left(2\tilde{S}_z^2 - \tilde{S}_x^2 - \tilde{S}_y^2\right) = \frac{D}{\hbar^2}\left(\tilde{S}_z^2 - \frac{1}{3}\tilde{S}^2\right)$$

One then obtains

$$D = 3\Delta$$

7.5 The action of the components of the fictitious spin operator on the Γ_8 basis is dictated by the general expressions for the action of the spin operators on the $S = \frac{3}{2}$ basis functions. It is verified that the spin-Hamiltonian that generates the J_p part of the matrix precisely corresponds to

$$\mathcal{H}_p = J_p \mathbf{B} \cdot \tilde{\mathbf{S}}$$

The fictitious spin operator indeed transforms as a T_1 operator and has the tensorial rank of a p-orbital. However, as we have shown, the full Hamiltonian also includes a J_f part, which involves an f-like operator. To mimic this part by a spin Hamiltonian, one thus will need a symmetrized triple product of the fictitious spin, which will embody an f-tensor, transforming in the octahedral symmetry as the T_1 irrep. These f-functions can be found in Table 7.1 and are of type $z(5z^2 - 3r^2)$. But beware! To find the corresponding spin operator, it is not sufficient simply to substitute the Cartesian variables by the corresponding spinor components, i.e., z by $\tilde{S}_z$, etc.; indeed, while products of x, y, and z are commutative, the products of the corresponding operators are not. Hence, when constructing the octupolar product of the spin components, products of noncommuting operators must be fully symmetrized. For the f_{z^3} function, this is the case for the functions $3zx^2$ and $3xy^2$, which are parts of $3zr^3$. As an example, the operator analogue of $3zx^2$ reads

$$3zx^2 \rightarrow \tilde{S}_z\tilde{S}_x\tilde{S}_x + \tilde{S}_x\tilde{S}_z\tilde{S}_x + \tilde{S}_x\tilde{S}_x\tilde{S}_z$$

One then has for the operator equivalent of $3z(x^2 + y^2)$:

$$\begin{aligned}&\tilde{S}_z\tilde{S}_x\tilde{S}_x + \tilde{S}_x\tilde{S}_z\tilde{S}_x + \tilde{S}_x\tilde{S}_x\tilde{S}_z + \tilde{S}_z\tilde{S}_y\tilde{S}_y + \tilde{S}_y\tilde{S}_z\tilde{S}_y + \tilde{S}_y\tilde{S}_y\tilde{S}_z\\ &\quad = 3\tilde{S}_z\left(\tilde{S}_x^2 + \tilde{S}_y^2\right) + i\hbar(\tilde{S}_x\tilde{S}_y - \tilde{S}_y\tilde{S}_x) = 3\tilde{S}_z\left(\tilde{S}_x^2 + \tilde{S}_y^2\right) - \hbar^2\tilde{S}_z\end{aligned}$$

where we have used the commutation relation for the spin-operators:

$$S_xS_y - S_yS_x = i\hbar S_z$$

The octupolar spin operator will then be of type

$$\begin{aligned}\mathcal{H}_f = \frac{\mu_B}{\hbar^3}g_f B_z\left(\tilde{S}_z^3 - \frac{3}{5}\tilde{S}_z\tilde{S}^2 + \frac{1}{5}\hbar^2\tilde{S}_z\right) + B_x\left(\tilde{S}_x^3 - \frac{3}{5}\tilde{S}_x\tilde{S}^2 + \frac{1}{5}\hbar^2\tilde{S}_x\right)\\ + B_y\left(\tilde{S}_y^3 - \frac{3}{5}\tilde{S}_y\tilde{S}^2 + \frac{1}{5}\hbar^2\tilde{S}_y\right)\end{aligned}$$

In order to identify the parameter correspondence, let us work out the action of this operator on the quartet functions. As an example for a magnetic field along the z-direction, the matrix is diagonal, and its elements (in units of μ_B) are given by

$$\begin{aligned}\left\langle \pm\frac{3}{2}\middle|\mathcal{H}_f\middle|\pm\frac{3}{2}\right\rangle &= \pm g_f B_z\frac{3}{2}\left(\frac{9}{4} - \frac{45}{20} + \frac{1}{5}\right) = \pm\frac{3}{10}g_f B_z\\ \left\langle \pm\frac{1}{2}\middle|\mathcal{H}_f\middle|\pm\frac{1}{2}\right\rangle &= \mp\frac{9}{10}g_f B_z\end{aligned}$$

By comparing these elements to the results in Table 7.8 we can identify the parameter correspondence as

$$J_f = -\frac{3}{10}g_f \tag{13}$$

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