

Appendix A Direct Product Tables

These tables give the symmetry species of the product of two functions with the indicated symmetry species, for each point group. Although these are all immediately derivable from the character tables for each point group (for which, see any of the references listed in chapter 6), the direct product tables should suffice for most ordinary applications, such as determining selection rules, and so on. Also tabulated are the symmetry species of the components of the electromagnetic transition operators, as follows:

electric dipole: x, y, z ;

magnetic dipole: R_x, R_y, R_z ;

electric quadrupole: $x^2 + y^2, x^2 - y^2, z^2, xy, xz, yz$.

1.

C_1	A	Operators
A	A	All

2.

C_2	A	B	Operators
A	A	B	$z, R_z, x^2, y^2, z^2, xy$
B	B	A	x, y, R_x, R_y, xz, yz

3.

C_3	A	E	Operators
A	A	E	$z, R_z, x^2 + y^2, z^2$
E	E	$2A \oplus E$	$x, y, R_x, R_y, x^2 - y^2, xy, xz, yz$

4.

C_4	A	B	E	Operators
A	A	B	E	$z, R_z, x^2 + y^2, z^2$
B	B	A	E	$x^2 - y^2, xy$
E	E	E	$2A \oplus 2B$	x, y, R_x, R_y, xz, yz

5.

C_{2v}	A_1	A_2	B_1	B_2	Operators
A_1	A_1	A_2	B_1	B_2	z, x^2, y^2, z^2
A_2	A_2	A_1	B_2	B_1	R_z, xy
B_1	B_1	B_2	A_1	A_2	x, R_y, xz
B_2	B_2	B_1	A_2	A_1	y, R_x, yz

6.

C_{3v}	A_1	A_2	E	Operators
A_1	A_1	A_2	E	$z, x^2 + y^2, z^2$
A_2	A_2	A_1	E	R_z
E	E	E	$A_1 \oplus A_2 \oplus E$	$x, y, R_x, R_y, x^2 - y^2, xy, xz, yz$

Appendix A

7.

C_{4v}
A_1
A_2
B_1
B_2
E

8.

C_{5v}
A_1
A_2
E_1
E_2

9.

C_{6v}	A
A_1	A
A_2	A
B_1	B
B_2	B
E_1	E
E_2	E

10.

$C_3 = C_1$
A'
A''

11.

C_{2h}
A_g
A_u
B_g
B_u

12.

C_{3h}
A'
A''
E'
E''

functions with
 igh these are all
 oint group (for
 t product tables
 nining selection
 the components

7. C_{4v}	A_1	A_2	B_1	B_2	E	Operators
A_1	A_1	A_2	B_1	B_2	E	$z, x^2 + y^2, z^2$
A_2	A_2	A_1	B_2	B_1	E	R_z
B_1	B_1	B_2	A_1	A_2	E	$x^2 - y^2$
B_2	B_2	B_1	A_2	A_1	E	xy
E	E	E	E	E	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$	x, y, R_x, R_y, xz, yz

8. C_{5v}	A_1	A_2	E_1	E_2	Operators
A_1	A_1	A_2	E_1	E_2	$z, x^2 + y^2, z^2$
A_2	A_2	A_1	E_2	E_1	R_z
E_1	E_1	E_2	$A_1 \oplus A_2 \oplus E_2$	$E_1 \oplus E_2$	x, y, R_x, R_y, xz, yz
E_2	E_2	E_1	$E_1 \oplus E_2$	$A_1 \oplus A_2 \oplus E_1$	$x^2 - y^2, xy$

9. C_{6v}	A_1	A_2	B_1	B_2	E_1	E_2	Operators
A_1	A_1	A_2	B_1	B_2	E_1	E_2	$z, x^2 + y^2, z^2$
A_2	A_2	A_1	B_2	B_1	E_1	E_2	R_z
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_2	E_2	E_1	$A_1 \oplus A_2 \oplus E_2$	$B_1 \oplus B_2 \oplus E_1$	x, y, R_x, R_y, xz, yz
E_2	E_2	E_1	E_1	E_2	$B_1 \oplus B_2 \oplus E_1$	$A_1 \oplus A_2 \oplus E_2$	$x^2 - y^2, xy$

10. $C_s = C_{1h}$	A'	A''	Operators
A'	A'	A''	$x, y, R_z, x^2, y^2, z^2, xy$
A''	A''	A'	z, R_x, R_y, xz, yz

11. C_{2h}	A_g	A_u	B_g	B_u	Operators
A_g	A_g	A_u	B_g	B_u	R_z, x^2, y^2, z^2, xy
A_u	A_u	A_g	B_u	B_g	z
B_g	B_g	B_u	A_g	A_u	R_x, R_y, xz, yz
B_u	B_u	B_g	A_u	A_g	x, y

12. C_{3h}	A'	A''	E'	E''	Operators
A'	A'	A''	E'	E''	$R_z, x^2 + y^2, z^2$
A''	A''	A'	E''	E'	z
E'	E'	E''	$2A' \oplus E'$	$2A'' \oplus E''$	$x, y, x^2 - y^2, xy$
E''	E''	E'	$2A'' \oplus E''$	$2A' \oplus E'$	R_x, R_y, xz, yz

z^2, z^2
 $x^2 - y^2, xy, xz, yz$

Operators
 $z, R_z, x^2 + y^2, z^2$
 $x^2 - y^2, xy$
 x, y, R_x, R_y, xz, yz

Operators
 z, x^2, y^2, z^2
 R_x, xy
 x, R_y, xz
 y, R_x, yz

z^2
 $z, x^2 - y^2, xy, xz, yz$

n care
 of clas
 rest is i
 of radi
 ulation
 their inter

mainly v
 ave been
 istent no
 a review
 d and ato
 tional. v
 ic molec
 y then le
 polyator
 essor of

Rydberg
 aviolet (b
 ortion of t
 he I₂ mol
 piece).

13.

C_{24}	A_g	A_u	B_g	B_u	E_g	E_u	Operators
A_g	A_g	A_u	B_g	B_u	E_g	E_u	$R_z, x^2 + y^2, z^2$
A_u	A_u	A_g	B_u	B_g	E_u	E_g	z
B_g	B_g	B_u	A_g	A_u	E_g	E_u	$x^2 - y^2, xy$
B_u	B_u	B_g	A_u	A_g	E_u	E_g	
E_g	E_g	E_u	E_g	E_u	$2A_g \oplus 2B_g$	$2A_u \oplus 2B_u$	R_x, R_y, xz, yz
E_u	E_u	E_g	E_u	E_g	$2A_u \oplus 2B_u$	$2A_g \oplus 2B_g$	x, y

14.

D_2	A_1	B_1	B_2	B_3	Operators
A_1	A_1	B_1	B_2	B_3	x^2, y^2, z^2
B_1	B_1	A_1	B_3	B_2	z, R_z, xy
B_2	B_2	B_3	A_1	B_1	y, R_y, xz
B_3	B_3	B_2	B_1	A_1	x, R_x, yz

15.

D_3	A_1	A_2	E	Operators
A_1	A_1	A_2	E	$x^2 + y^2, z^2$
A_2	A_2	A_1	E	z, R_z
E	E	E	$A_1 \oplus A_2 \oplus E$	$x, y, R_x, R_y, xz, yz, x^2 - y^2, xy$

16.

D_4	A_1	A_2	B_1	B_2	E	Operators
A_1	A_1	A_2	B_1	B_2	E	$x^2 + y^2, z^2$
A_2	A_2	A_1	B_2	B_1	E	z, R_z
B_1	B_1	B_2	A_1	A_2	E	$x^2 - y^2$
B_2	B_2	B_1	A_2	A_1	E	xy
E	E	E	E	E	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$	x, y, R_x, R_y, xz, yz

17.

D_5	A_1	A_2	E_1	E_2	Operators
A_1	A_1	A_2	E_1	E_2	$x^2 + y^2, z^2$
A_2	A_2	A_1	E_1	E_2	z, R_z
E_1	E_1	E_1	$A_1 \oplus A_2 \oplus E_2$	$E_1 \oplus E_2$	x, y, R_x, R_y, xz, yz
E_2	E_2	E_2	$E_1 \oplus E_2$	$A_1 \oplus A_2 \oplus E_1$	$x^2 - y^2, xy$

18.

D_6	A_1	A_2	B_1	B_2	E_1	E_2	Operators
A_1	A_1	A_2	B_1	B_2	E_1	E_2	$x^2 + y^2, z^2$
A_2	A_2	A_1	B_2	B_1	E_1	E_2	z, R_z
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_1	$A_1 \oplus A_2 \oplus E_2$	$B_1 \oplus B_2 \oplus E_1$	x, y, R_x, R_y, xz, yz
E_2	E_2	E_2	E_1	E_2	$B_1 \oplus B_2 \oplus E_1$	$A_1 \oplus A_2 \oplus E_1$	$x^2 - y^2, xy$

19.

D_{24}
A_1
A_2
B_1
B_2
E

20. D_{3d} t with for t

21. D_{2h} t with for t

22.

D_{3h}
A_1'
A_2'
A_1''
A_2''
E'
E''

23. D_{4h} t with the g (tabl

24.

O, T_d
A_1
A_2
E

F_1

F_2

	Operators
	$R_z, x^2 + y^2, z^2$
	z
	$x^2 - y^2, xy$
$A_u \oplus 2B_u$	R_x, R_y, xz, yz
$A_g \oplus 2B_g$	x, y

Operators
$x^2 + y^2, z^2$
z, R_z
$x, y, R_x, R_y, xz, yz, x^2 - y^2, xy$

	Operators
	$x^2 + y^2, z^2$
	z, R_z
	$x^2 - y^2$
	xy
$B_1 \oplus B_2$	x, y, R_x, R_y, xz, yz

	Operators
	$x^2 + y^2, z^2$
	z, R_z
	x, y, R_x, R_y, xz, yz
	$x^2 - y^2, xy$
$B E_2$	
$A_2 \oplus E_1$	

	Operators
	$x^2 + y^2, z^2$
	z, R_z
$B_1 \oplus B_2 \oplus E_1$	x, y, R_x, R_y, xz, yz
$A_1 \oplus A_2 \oplus E_1$	$x^2 - y^2, xy$

19. D_{2d}	A_1	A_2	B_1	B_2	E	Operators
A_1	A_1	A_2	B_1	B_2	E	$x^2 + y^2, z^2$
A_2	A_2	A_1	B_2	B_1	E	R_z
B_1	B_1	B_2	A_1	A_2	E	$x^2 - y^2$
B_2	B_2	B_1	A_2	A_1	E	z, xy
E	E	E	E	E	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$	x, y, R_x, R_y, xz, yz

20. D_{3d} has the same product rules and operator species as D_3 (table 15), with the addition of $g \otimes g = g, u \otimes u = g$, and $u \otimes g = u$. See table 11 for the $g-u$ characters of the operators.

21. D_{2h} has the same product rules and operator species as D_2 (table 14), with the addition of $g \otimes g = g, u \otimes u = g$, and $u \otimes g = u$. See table 11 for the $g-u$ characters of the operators.

22. D_{3h}	A'_1	A'_2	A''_1	A''_2	E'	E''	Operators
A'_1	A'_1	A'_2	A''_1	A''_2	E'	E''	$x^2 + y^2, z^2$
A'_2	A'_2	A'_1	A''_2	A''_1	E'	E''	R_z
A''_1	A''_1	A''_2	A'_1	A'_2	E''	E'	z
A''_2	A''_2	A''_1	A'_2	A'_1	E''	E'	$x, y, x^2 - y^2, xy$
E'	E'	E'	E''	E''	$A'_1 \oplus A'_2 \oplus E'$	$A''_1 \oplus A''_2 \oplus E''$	R_x, R_y, xz, yz
E''	E''	E''	E'	E'	$A''_1 \oplus A''_2 \oplus E''$	$A'_1 \oplus A'_2 \oplus E'$	

23. D_{4h} has the same product rules and operator species as D_4 (table 16), with the addition of $u \otimes u = g, g \otimes g = g, u \otimes g = u$. See table 11 for the $g-u$ character of the operator. D_{6h} is similarly derived from D_6 (table 18).

24. O, T_d	A_1	A_2	E	F_1	F_2	Operators
A_1	A_1	A_2	E	F_1	F_2	$x^2 + y^2 + z^2$
A_2	A_2	A_1	E	F_2	F_1	
E	E	E	$\left\{ \begin{matrix} A_1 \oplus A_2 \\ \oplus E \end{matrix} \right.$	$F_1 \oplus F_2$	$F_1 \oplus F_2$	$2z^2 - x^2 - y^2, \sqrt{3}(x^2 - y^2)$
F_1	F_1	F_2	$F_1 \oplus F_2$	$\left\{ \begin{matrix} A_1 \oplus E \\ \oplus F_1 \\ \oplus F_2 \end{matrix} \right.$	$\left\{ \begin{matrix} A_2 \oplus E \\ \oplus F_1 \\ \oplus F_2 \end{matrix} \right.$	$\{ R_x, R_y, R_z \}$ $\{ x, y, z(O) \}$
F_2	F_2	F_1	$F_1 \oplus F_2$	$\left\{ \begin{matrix} A_2 \oplus E \\ \oplus F_1 \\ \oplus F_2 \end{matrix} \right.$	$\left\{ \begin{matrix} A_1 \oplus E \\ \oplus F_1 \\ \oplus F_2 \end{matrix} \right.$	$\{ x, y, z(T_d) \}$ $\{ xz, xy, yz(O) \}$

25. O_h has the same product rules and operator species as O (table 24), with the addition of $g \otimes g = g$, $u \otimes u = g$, and $u \otimes g = u$. See table 11 for the $u-g$ character of the operators.

26. $C_{\infty v}$	Σ^+	Σ^-	Π	Δ	...	Operators
Σ^+	Σ^+	Σ^-	Π	Δ	...	$x^2 + y^2, z^2, z$
Σ^-	Σ^-	Σ^+	Π	Δ	...	R_z
Π	Π	Π	$\Sigma^+ \oplus \Sigma^- \oplus \Delta$	$\Pi \oplus \Phi$...	x, y, R_x, R_y, xz, yz
Δ	Δ	Δ	$\Pi \oplus \Phi$	$\Sigma^+ \oplus \Sigma^- \oplus \Gamma$...	$x^2 - y^2, xy$
...

27. $D_{\infty h}$	Σ_g^+	Σ_u^+	Σ_g^-	Σ_u^-	Π_g	Π_u
Σ_g^+	Σ_g^+	Σ_u^+	Σ_g^-	Σ_u^-	Π_g	Π_u
Σ_u^+	Σ_u^+	Σ_g^+	Σ_u^-	Σ_g^-	Π_u	Π_g
Σ_g^-	Σ_g^-	Σ_u^-	Σ_g^+	Σ_u^+	Π_g	Π_u
Σ_u^-	Σ_u^-	Σ_g^-	Σ_u^+	Σ_g^+	Π_u	Π_g
Π_g	Π_g	Π_u	Π_g	Π_u	$\Sigma_g^+ \oplus \Sigma_g^- \oplus \Delta_g$	$\Sigma_u^+ \oplus \Sigma_u^- \oplus \Delta_u$
Π_u	Π_u	Π_g	Π_u	Π_g	$\Sigma_u^+ \oplus \Sigma_u^- \oplus \Delta_u$	$\Sigma_g^+ \oplus \Sigma_g^- \oplus \Delta_g$
Δ_g	Δ_g	Δ_u	Δ_g	Δ_u	$\Pi_g \oplus \Phi_g$	$\Pi_u \oplus \Phi_u$
Δ_u	Δ_u	Δ_g	Δ_u	Δ_g	$\Pi_u \oplus \Phi_u$	$\Pi_g \oplus \Phi_g$
...

$D_{\infty h}$	Δ_g	Δ_u	...	Operators
Σ_g^+	Δ_g	Δ_u	...	$z^2, x^2 + y^2$
Σ_u^+	Δ_u	Δ_g	...	z
Σ_g^-	Δ_g	Δ_u	...	R_z
Σ_u^-	Δ_u	Δ_g
Π_g	$\Pi_g \oplus \Phi_g$	$\Pi_u \oplus \Phi_u$...	R_x, R_y, xz, yz
Π_u	$\Pi_u \oplus \Phi_u$	$\Pi_g \oplus \Phi_g$...	x, y
Δ_g	$\Sigma_g^+ \oplus \Sigma_g^- \oplus \Gamma_g$	$\Sigma_u^+ \oplus \Sigma_u^- \oplus \Gamma_u$...	$x^2 - y^2, xy$
Δ_u	$\Sigma_u^+ \oplus \Sigma_u^- \oplus \Gamma_u$	$\Sigma_g^+ \oplus \Sigma_g^- \oplus \Gamma_g$
...

Appendix B

Newtonian mechanics
 many problems
 Lagrange's equations
 relation of coordinates
 often simple
 elliptical. It is
 brings out this
 to simple form
 minimizing
 for example,
 vertical in a
 forces exerted
 that their effect
 allow us to
 that remove
 forces of constraint

Let us define
 $L \equiv T - V$
 a function

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) -$$

where q_i and
 will be shown

1 Some

We begin

$$\mathbf{v} = (\dot{x}, \dot{y},$$

thus \mathbf{v} has
 derivatives
 and x, y

1. This appendix
 mechanics
 University