APPENDIX IV

RESOLUTION OF SPECIES OF SYMMETRIC POINT GROUPS INTO THOSE OF POINT GROUPS OF LOWER SYMMETRY

TABLE 58

RESOLUTION OF SPECIES OF ATOMS INTO THOSE OF MOLECULES OF VARIOUS POINT GROUPS

Atomic species	Molecular species				
	O_h, (O [a])	T_d	$D_{\infty h}$, ($C_{\infty v}$ [a])	D_{6h}, (D_6 [a], C_{6v} [b])	D_{4h}, (D_4 [a], C_{4v} [b])
S_g	A_{1g}	A_1	Σ_g^+	A_{1g}	A_{1g}
S_u	A_{1u}	A_2	Σ_u^-	A_{1u}	A_{1u}
P_g	F_{1g}	F_1	$\Sigma_g^- + \Pi_g$	$A_{2g} + E_{1g}$	$A_{2g} + E_g$
P_u	F_{1u}	F_2	$\Sigma_u^+ + \Pi_u$	$A_{2u} + E_{1u}$	$A_{2u} + E_u$
D_g	$E_g + F_{2g}$	$E + F_2$	$\Sigma_g^+ + \Pi_g + \Delta_g$	$A_{1g} + E_{1g} + E_{2g}$	$A_{1g} + B_{1g} + B_{2g} + E_g$
D_u	$E_u + F_{2u}$	$E + F_1$	$\Sigma_u^- + \Pi_u + \Delta_u$	$A_{1u} + E_{1u} + E_{2u}$	$A_{1u} + B_{1u} + B_{2u} + E_u$
F_g	$A_{2g} + F_{1g} + F_{2g}$	$A_2 + F_1 + F_2$	$\Sigma_g^- + \Pi_g + \Delta_g + \Phi_g$	$A_{2g} + B_{1g} + B_{2g} + E_{1g} + E_{2g}$	$A_{2g} + B_{1g} + B_{2g} + 2E_g$
F_u	$A_{2u} + F_{1u} + F_{2u}$	$A_1 + F_1 + F_2$	$\Sigma_u^+ + \Pi_u + \Delta_u + \Phi_u$	$A_{2u} + B_{1u} + B_{2u} + E_{1u} + E_{2u}$	$A_{2u} + B_{1u} + B_{2u} + 2E_u$
G_g	$A_{1g} + E_g + F_{1g} + F_{2g}$	$A_1 + E + F_1 + F_2$	$\Sigma_g^+ + \Pi_g + \Delta_g + \Phi_g + \Gamma_g$	$A_{1g} + B_{1g} + B_{2g} + E_{1g} + 2E_{2g}$	$2A_{1g} + A_{2g} + B_{1g} + B_{2g} + 2E_g$
G_u	$A_{1u} + E_u + F_{1u} + F_{2u}$	$A_2 + E + F_1 + F_2$	$\Sigma_u^- + \Pi_u + \Delta_u + \Phi_u + \Gamma_u$	$A_{1u} + B_{1u} + B_{2u} + E_{1u} + 2E_{2u}$	$2A_{1u} + A_{2u} + B_{1u} + B_{2u} + 2E_u$

TABLE 58 (*continued*)

Molecular Species

Atomic species	D_{3h}, (D_{3d}[c], D_3[d], C_{3h}[e])	C_{3v}	D_{2d}	D_{2h}, (D_2)[a]	C_{2v}	C_s
S_g	A_1'	A_1	A_1	A_g	A_1	A'
S_u	A_1''	A_2	B_1	A_u	A_2	A''
P_g	$A_2'+E''$	A_2+E	A_2+E	$B_{1g}+B_{2g}+B_{3g}$	$A_2+B_1+B_2$	$A'+2A''$
P_u	$A_2''+E'$	A_1+E	B_2+E	$B_{1u}+B_{2u}+B_{3u}$	$A_1+B_1+B_2$	$2A'+A''$
D_g	$A_1'+E'+E''$	A_1+2E	$A_1+B_1+B_2+E$	$2A_g+B_{1g}+B_{2g}+B_{3g}$	$2A_1+A_2+B_1+B_2$	$3A'+2A''$
D_u	$A_1''+E'+E''$	A_2+2E	$A_1+A_2+B_1+E$	$2A_u+B_{1u}+B_{2u}+B_{3u}$	$A_1+2A_2+B_1+B_2$	$2A'+3A''$
F_g	$A_1''+A_2'+A_2''+E'+E''$	A_1+2A_2+2E	$A_2+B_1+B_2+2E$	$A_g+2B_{1g}+2B_{2g}+2B_{3g}$	$A_1+2A_2+2B_1+2B_2$	$3A'+4A''$
F_u	$A_1'+A_2'+A_2''+E'+E''$	$2A_1+A_2+2E$	$A_1+A_2+B_2+2E$	$A_u+2B_{1u}+2B_{2u}+2B_{3u}$	$2A_1+A_2+2B_1+2B_2$	$4A'+3A''$
G_g	$A_1'+A_1''+A_2''+2E'+E''$	$2A_1+A_2+3E$	$2A_1+A_2+B_1+B_2+2E$	$3A_g+2B_{1g}+2B_{2g}+2B_{3g}$	$3A_1+2A_2+2B_1+2B_2$	$5A'+4A''$
G_u	$A_1'+A_1''+A_2'+E'+2E''$	A_1+2A_2+3E	$A_1+A_2+2B_1+B_2+2E$	$3A_u+2B_{1u}+2B_{2u}+2B_{3u}$	$2A_1+3A_2+2B_1+2B_2$	$4A'+5A''$

[a] For these point groups disregard the subscripts g and u.
[b] Substitute A_1 for A_{1g} and A_{2u}, and A_2 for A_{2g} and A_{1u}, and disregard the subscripts g and u in the remaining species.
[c] Disregard $'$ and $''$ and add g and u to agree with that in the corresponding atomic species.
[d] Disregard $'$ and $''$.
[e] Disregard the difference between A_1 and A_2.

Table 59

RESOLUTION OF SPECIES OF LINEAR MOLECULES (POINT GROUPS $D_{\infty h}$, $C_{\infty v}$) INTO THOSE OF MOLECULES OF LOWER SYMMETRY

The z axis in the linear case is assumed to lie in the internuclear axis. For the axial point groups it is assumed to coincide with the main symmetry axis, but for the point groups D_{2h}, C_{2v}, C_{2h} and C_s the correlation is given for several assumptions about the relative positions of the linear axis and the axis of the molecule to be formed.

Linear[a] molecule	D_{6h}, (D_6)[a]	C_{6v}	D_{4h},(D_4)[a]	D_{3h}, (D_3)[bc]	C_{3v}	D_{2d}	D_{2h}		C_{2v}			C_{2h}, (C_2)[a]		C_s	
							$z\to z$	$z\to x$	$z\to z$	$z\to y$	$z\to x$	$z\to z$	$z\to x,y$	$\sigma_h\to\sigma$	$\sigma_v\to\sigma$
Σ_g^+	A_{1g}	A_1	A_{1g}	A_1'	A_1	A_1	A_g	A_g	A_1	A_1	A_1	A_g	A_g	A'	A'
Σ_u^+	A_{2u}	A_1	A_{2u}	A_2''	A_1	B_2	B_{1u}	B_{3u}	A_1	B_2	B_1	A_u	B_u	A''	A'
Σ_g^-	A_{2g}	A_2	A_{2g}	A_2'	A_2	A_2	B_{1g}	B_{3g}	A_2	B_1	B_2	A_g	B_g	A'	A''
Σ_u^-	A_{1u}	A_2	A_{1u}	A_2''	A_2	B_1	A_u	A_u	A_2	A_2	A_2	A_u	A_u	A''	A''
Π_g	E_{1g}	E_1	E_g	E''	E	E	$B_{2g}+B_{3g}$	$B_{1g}+B_{2g}$	B_1+B_2	A_2+B_2	A_2+B_1	$2B_g$	A_g+B_g	$2A''$	$A'+A''$
Π_u	E_{1u}	E_1	E_u	E'	E	E	$B_{2u}+B_{3u}$	$B_{1u}+B_{2u}$	B_1+B_2	A_1+B_1	A_1+B_2	$2B_u$	A_u+B_u	$2A'$	$A'+A''$
Δ_g	E_{2g}	E_2	$B_{1g}+B_{2g}$	E'	E	B_1+B_2	A_g+B_{1g}	A_g+B_{3g}	A_1+A_2	A_1+B_1	A_1+B_2	$2A_g$	A_g+B_g	$2A'$	$A'+A''$
Δ_u	E_{2u}	E_2	$B_{1u}+B_{2u}$	E''	E	A_1+A_2	A_u+B_{1u}	A_u+B_{3u}	A_1+A_2	A_2+B_2	A_2+B_1	$2A_u$	A_u+B_u	$2A''$	$A'+A''$
Φ_g	$B_{1g}+B_{2g}$	B_1+B_2	E_g	$A_1''+A_2''$	A_1+A_2	E	$B_{2g}+B_{3g}$	$B_{1g}+B_{2g}$	B_1+B_2	A_2+B_2	A_2+B_1	$2B_g$	A_g+B_g	$2A''$	$A'+A''$
Φ_u	$B_{1u}+B_{2u}$	B_1+B_2	E_u	$A_1'+A_2'$	A_1+A_2	E	$B_{2u}+B_{3u}$	$B_{1u}+B_{2u}$	B_1+B_2	A_1+B_1	A_1+B_2	$2B_u$	A_u+B_u	$2A'$	$A'+A''$
Γ_g	E_{2g}	E_2	$A_{1g}+A_{2g}$	E'	E	A_1+A_2	A_g+B_{1g}	A_g+B_{3g}	A_1+A_2	A_1+B_1	A_1+B_2	$2A_g$	A_g+B_g	$2A'$	$A'+A''$
Γ_u	E_{2u}	E_2	$A_{1u}+A_{2u}$	E''	E	B_1+B_2	A_u+B_{1u}	A_u+B_{3u}	A_1+A_2	A_2+B_2	A_2+B_1	$2A_u$	A_u+B_u	$2A''$	$A'+A''$

[a] For $C_{\infty v}$, D_6, D_4, C_2 disregard the subscripts g and u.
[b] For D_3 disregard $'$ and $''$.
[c] For D_{3d} disregard $'$ and $''$ and add g and u to agree with linear case.

TABLE 60

RESOLUTION OF SPECIES OF POINT GROUPS C_{2v}, D_{2h}, D_{3h}, D_{4h}, T_d INTO THOSE OF POINT GROUPS OF LOWER SYMMETRY

C_{2v}	C_s $\sigma(xz)\to\sigma$	C_s $\sigma(yz)\to\sigma$
A_1	A'	A'
A_2	A''	A''
B_1	A'	A''
B_2	A''	A'

D_{2h}	C_{2h} $z\to z$	C_{2v} $y\to y, z\to z$	C_s $\sigma(yz)\to\sigma$
A_g	A_g	A_1	A'
A_u	A_u	A_2	A''
B_{1g}	A_g	A_2	A''
B_{1u}	A_u	A_1	A'
B_{2g}	B_g	B_1	A''
B_{2u}	B_u	B_2	A'
B_{3g}	B_g	B_2	A'
B_{3u}	B_u	B_1	A''

D_{3h}	C_{3v}	C_s $\sigma_v\to\sigma$	C_{2v} $\sigma_h\to\sigma_v('yz)$
A_1'	A_1	A'	A_1
A_1''	A_2	A''	A_2
A_2'	A_2	A''	B_2
A_2''	A_1	A'	B_1
E'	E	$A' + A''$	$A_1 + B_2$
E''	E	$A' + A''$	$A_2 + B_1$

D_{4h}	C_{4v}	D_{2d}	D_{2h} $z\to z$
A_{1g}	A_1	A_1	A_g
A_{1u}	A_2	B_1	A_u
A_{2g}	A_2	A_2	B_{1g}
A_{2u}	A_1	B_2	B_{1u}
B_{1g}	B_1	B_1	A_g
B_{1u}	B_2	A_1	A_u
B_{2g}	B_2	B_2	B_{1g}
B_{2u}	B_1	A_2	B_{1u}
E_g	E	E	$B_{2g} + B_{3g}$
E_u	E	E	$B_{2u} + B_{3u}$

T_d	D_{2d}	C_{3v}	C_{2v}
A_1	A_1	A_1	A_1
A_2	B_1	A_2	A_2
E	$A_1 + B_1$	E	$A_1 + A_2$
F_1	$A_2 + E$	$A_2 + E$	$A_2 + B_1 + B_2$
F_2	$B_2 + E$	$A_1 + E$	$A_1 + B_1 + B_2$