APPENDIX 18-1: CHARACTER TABLES OF SOME SPIN DOUBLE GROUPS

Table 18-16

The group $C_s(\mathrm{M})^2$

$C_s(\mathrm{M})^2$:	E	E^*	R	
	1	2	1	
Equiv. rot.:	R^0	$R_c{}^\pi$	$R^{2\pi}$	
A' :	1	1	1	
A'' :	1	−1	1	
$E_{1/2}$:	2	0	−2	: sep

Table 18-17

The group $C_i(\mathrm{M})^2$

$C_i(\mathrm{M})^2$:	E	$(12)(34)(56)(78)^*$	R	$R(12)(34)(56)(78)^*$
	1	1	1	1
Equiv. rot.:	R^0	R^0	$R^{2\pi}$	$R^{2\pi}$
A_g:	1	1	1	1
A_u:	1	−1	1	−1
$E_{g/2}$:	2	2	−2	−2
$E_{u/2}$:	2	−2	−2	2

The characters in $E_{g/2}$ and $E_{u/2}$ have been doubled since they come from type two corepresentations [Wigner (1959) page 343], also called case (b) [Dimmock and Wheeler (1964) page 733].

Table 18-18

The group $C_2(\mathrm{M})^2$

$C_2(\mathrm{M})^2$:	E	$(12)(34)$	R	
	1	2	1	
Equiv. rot.:	R^0	$R_b{}^\pi$	$R^{2\pi}$	
A:	1	1	1	
B:	1	−1	1	
$E_{1/2}$:	2	0	−2	: sep

Table 18-19
The group $C_{2v}(M)^2$

$C_{2v}(M)^2$:	E	(12)	E^*	$(12)^*$	R
	1	2	2	2	1
Equiv. rot.:	R^0	$R_b{}^\pi$	$R_c{}^\pi$	$R_a{}^\pi$	$R^{2\pi}$
A_1:	1	1	1	1	1
A_2:	1	1	−1	−1	1
B_1:	1	−1	−1	1	1
B_2:	1	−1	1	−1	1
$E_{1/2}$:	2	0	0	0	−2

Table 18-20
The group $C_{3v}(M)^2$

$C_{3v}(M)^2$:	E	(123)	$(23)^*$	R	$R(123)$	
	1	2	6	1	2	
Equiv. rot.:	R^0	$R_z^{2\pi/3}$	$R_{\pi/2}^{\pi}$	$R^{2\pi}$	$R_z^{8\pi/3}$	
A_1:	1	1	1	1	1	
A_2:	1	1	−1	1	1	
E:	2	−1	0	2	−1	
$E_{1/2}$:	2	1	0	−2	−1	
$E_{3/2}$:	2	−2	0	−2	2	: sep

Table 18-21
The group $\boldsymbol{D}_{2h}(M)^2$

	E	$(12)(34)$	$(13)(24)(56)$	$(14)(23)(56)$	E^*	$(12)(34)^*$	$(13)(24)(56)^*$	$(14)(23)(56)^*$	R	$R(14)(23)(56)^*$
$D_{2h}(M)^2$:	1	2	2	2	2	2	2	1	1	1
Equiv. rot.:	R^0	$R_a{}^\pi$	$R_b{}^\pi$	$R_c{}^\pi$	$R_c{}^\pi$	$R_b{}^\pi$	$R_a{}^\pi$	R^0	$R^{2\pi}$	$R^{2\pi}$
A_g:	1	1	1	1	1	1	1	1	1	1
A_u:	1	1	1	1	−1	−1	−1	−1	1	−1
B_{1g}:	1	1	−1	−1	−1	−1	1	1	1	1
B_{1u}:	1	1	−1	−1	1	1	−1	−1	1	−1
B_{2g}:	1	−1	1	−1	−1	1	−1	1	1	1
B_{2u}:	1	−1	1	−1	1	−1	1	−1	1	−1
B_{3g}:	1	−1	−1	1	1	−1	−1	1	1	1
B_{3u}:	1	−1	−1	1	−1	1	1	−1	1	−1
$E_{g/2}$:	2	0	0	0	0	0	0	2	−2	−2
$E_{u/2}$:	2	0	0	0	0	0	0	−2	−2	2

Table 18-22
The group $\boldsymbol{C}_{2h}(M)^2$

	E	$(12)(34)(56)$	E^*	$(12)(34)(56)^*$	R	$R(12)(34)(56)^*$	
$C_{2h}(M)^2$:	1	2	2	1	1	1	
Equiv. rot.:	R^0	$R_c{}^\pi$	$R_c{}^\pi$	R^0	$R^{2\pi}$	$R^{2\pi}$	
A_g:	1	1	1	1	1	1	
A_u:	1	1	−1	−1	1	−1	
B_g:	1	−1	−1	1	1	1	
B_u:	1	−1	1	−1	1	−1	
$E_{g/2}$:	2	0	0	2	−2	−2	: sep
$E_{u/2}$:	2	0	0	−2	−2	2	: sep

Table 18-23
The group $\boldsymbol{D}_{3h}(M)^2$

$\boldsymbol{D}_{3h}(M)^2$:	E	(123)	(23)	E^*	$(123)^*$	$(23)^*$	R	$R(123)$	$R(123)^*$
	1	2	6	2	2	6	1	2	2
Equiv. rot.:	R^0	$R_z^{2\pi/3}$	R_0^{π}	R_z^{π}	$R_z^{-\pi/3}$	$R_{\pi/2}^{\pi}$	$R^{2\pi}$	$R_z^{8\pi/3}$	$R_z^{5\pi/3}$
A_1':	1	1	1	1	1	1	1	1	1
A_1'':	1	1	1	−1	−1	−1	1	1	−1
A_2':	1	1	−1	1	1	−1	1	1	1
A_2'':	1	1	−1	−1	−1	1	1	1	−1
E':	2	−1	0	2	−1	0	2	−1	−1
E'':	2	−1	0	−2	1	0	2	−1	1
$E_{1/2}$:	2	1	0	0	$\sqrt{3}$	0	−2	−1	$-\sqrt{3}$
$E_{3/2}$:	2	−2	0	0	0	0	−2	2	0
$E_{5/2}$:	2	1	0	0	$-\sqrt{3}$	0	−2	−1	$\sqrt{3}$

Table 18-24
The group $\boldsymbol{G}_6{}^2$. Example: CH_3OH^+ when the axes are tied to the OH group

$\boldsymbol{G}_6{}^2$:	E	(123)	$(23)^*$	R	$R(123)$	
	1	2	6	1	2	
Equiv. rot.:	R^0	R^0	$R_c{}^{\pi}$	$R^{2\pi}$	$R^{2\pi}$	
A_1:	1	1	1	1	1	
A_2:	1	1	−1	1	1	
E:	2	−1	0	2	−1	
$E_{a/2}$:	2	−1	0	−2	1	
$E_{1/2}$:	2	2	0	−2	−2	: sep

Table 18-25

The group $G_{12}{}^2$. Example: $CH_3NO_2^+$ when the axes are tied to the NO_2 group

	E	(123)	$(23)^*$	(45)	(123)(45)	$(23)(45)^*$	R	$R(123)$	$R(123)(45)$
G_{12}^2 :	1	2	6	2	2	6	1	2	2
Equiv. rot.:	R^0	R^0	$R_c{}^\pi$	$R_a{}^\pi$	$R_a{}^\pi$	$R_b{}^\pi$	$R^{2\pi}$	$R^{2\pi}$	$R_a^{3\pi}$
A_1' :	1	1	1	1	1	1	1	1	1
A_1'' :	1	1	1	−1	−1	−1	1	1	−1
A_2' :	1	1	−1	1	1	−1	1	1	1
A_2'' :	1	1	−1	−1	−1	1	1	1	−1
E' :	2	−1	0	2	−1	0	2	−1	−1
E'' :	2	−1	0	−2	1	0	2	−1	1
$E_{a/2}$:	2	−1	0	0	$\sqrt{3}$	0	−2	+1	$-\sqrt{3}$
$E_{1/2}$:	2	2	0	0	0	0	−2	−2	0
$E_{b/2}$:	2	−1	0	0	$-\sqrt{3}$	0	−2	+1	$\sqrt{3}$

Table 18-26

The character table of the spin double group for $CH_3NO_2^+$ obtained when the axes are tied to the CH_3 rotor

	E	(123)	$(12)^*$	(45)	(123)(45)	$(12)(45)^*$	R	$R(123)$	$R(45)$	$R(123)(45)$	
	1	2	6	1	2	6	1	2	1	2	
Equiv. rot.:	R^0	$R_z^{2\pi/3}$	$R_{\pi/6}^{\pi}$	R^0	$R_z^{2\pi/3}$	$R_{\pi/6}^{\pi}$	$R^{2\pi}$	$R_z^{8\pi/3}$	$R^{2\pi}$	$R_z^{8\pi/3}$	
A_1' :	1	1	1	1	1	1	1	1	1	1	
A_1'' :	1	1	1	−1	−1	−1	1	1	−1	−1	
A_2' :	1	1	−1	1	1	−1	1	1	1	1	
A_2'' :	1	1	−1	−1	−1	1	1	1	−1	−1	
E' :	2	−1	0	2	−1	0	2	−1	2	−1	
E'' :	2	−1	0	−2	1	0	2	−1	−2	1	
$E_{1/2}'$:	2	1	0	2	1	0	−2	−1	−2	−1	
$E_{1/2}''$:	2	−1	0	−2	1	0	−2	1	2	−1	
$E_{3/2}'$:	2	−2	0	2	−2	0	−2	2	−2	2	: sep
$E_{3/2}''$:	2	−2	0	−2	2	0	−2	2	2	−2	: sep

TABLE 52

POINT GROUPS $\boldsymbol{D}_\infty$, $\boldsymbol{C}_{\infty v}$; $\boldsymbol{D}_{\infty h}$

$\boldsymbol{D}_\infty$ / $\boldsymbol{C}_{\infty v}$	I / I	$2C_\infty^\varphi$ / $2C_\infty^\varphi$	$2C_\infty^{2\varphi}$ / $2C_\infty^{2\varphi}$	$2C_\infty^{3\varphi}$ / $2C_\infty^{3\varphi}$	... / ...	∞C_2 / $\infty\sigma_v$	R / R	$2C_\infty^\varphi R$ / $2C_\infty^\varphi R$	... / ...	
Σ^+	1	1	1	1		1	1	1		T_z
Σ^-	1	1	1	1		−1	1	1		R_z
Π	+2	$2\cos\varphi$	$2\cos 2\varphi$	$2\cos 3\varphi$	...	0	+2	$2\cos\varphi$	...	$T_{x,y}$; $R_{x,y}$
Δ	+2	$2\cos 2\varphi$	$2\cos 2\cdot 2\varphi$	$2\cos 3\cdot 2\varphi$	...	0	+2	$2\cos 2\varphi$	...	
Φ	+2	$2\cos 3\varphi$	$2\cos 2\cdot 3\varphi$	$2\cos 3\cdot 3\varphi$	...	0	+2	$2\cos 3\varphi$	...	
. .	.	.	.	.	.	.	.	.	.	
$E_{\frac{1}{2}}$	+2	$2\cos\frac{1}{2}\varphi$	$2\cos\varphi$	$2\cos 3\cdot\frac{1}{2}\varphi$	...	0	−2	$-2\cos\frac{1}{2}\varphi$	...	
$E_{\frac{3}{2}}$	+2	$2\cos\frac{3}{2}\varphi$	$2\cos 3\varphi$	$2\cos 3\cdot\frac{3}{2}\varphi$	...	0	−2	$-2\cos\frac{3}{2}\varphi$	...	
$E_{\frac{5}{2}}$	+2	$2\cos\frac{5}{2}\varphi$	$2\cos 5\varphi$	$2\cos 3\cdot\frac{5}{2}\varphi$	...	0	−2	$-2\cos\frac{5}{2}\varphi$	...	
. .	.	.	.	.	.	.	.	.	.	

$\boldsymbol{D}_{\infty h} \equiv \boldsymbol{C}_{\infty v} \times \boldsymbol{C}_i$ (see Vol. II, p. 119)

TABLE 53

POINT GROUPS $\boldsymbol{O}$, $\boldsymbol{T}_d$; $\boldsymbol{O}_h$

$\boldsymbol{O}$ / $\boldsymbol{T}_d$ [a]		I / I	$8C_3$ / $8C_3$	$6C_2$ / $6\sigma_d$	$6C_4$ / $6S_4$	$3C_4^2 \equiv 3C_2''$ / $3S_4^2 \equiv 3C_2$	R / R	$8C_3^2$ / $8C_3^2$	$6C_4^3$ / $6S_4^3$	
A_1	Γ_1	1	1	1	1	1	1	1	1	
A_2	Γ_2	1	1	−1	−1	1	1	1	−1	
E	Γ_3	2	−1	0	0	2	2	−1	0	
F_1 (T_1)	Γ_4	3	0	−1	1	−1	3	0	1	$T_{x,y,z}$ for $\boldsymbol{O}$; $R_{x,y,z}$
F_2 (T_2)	Γ_5	3	0	1	−1	−1	3	0	−1	$T_{x,y,z}$ for $\boldsymbol{T}_d$
$E_{\frac{1}{2}}$	Γ_6	2	1	0	$\sqrt{2}$	0	−2	−1	$-\sqrt{2}$	
$E_{\frac{3}{2}}$	Γ_7	2	1	0	$-\sqrt{2}$	0	−2	−1	$\sqrt{2}$	
$G_{\frac{1}{2}}$	Γ_8	4	−1	0	0	0	−4	1	0	

$\boldsymbol{O}_h \equiv \boldsymbol{O} \times \boldsymbol{C}_i$ (see Vol. II, p. 123)

[a] Alternative species designations used by some authors.