

APPENDIX A

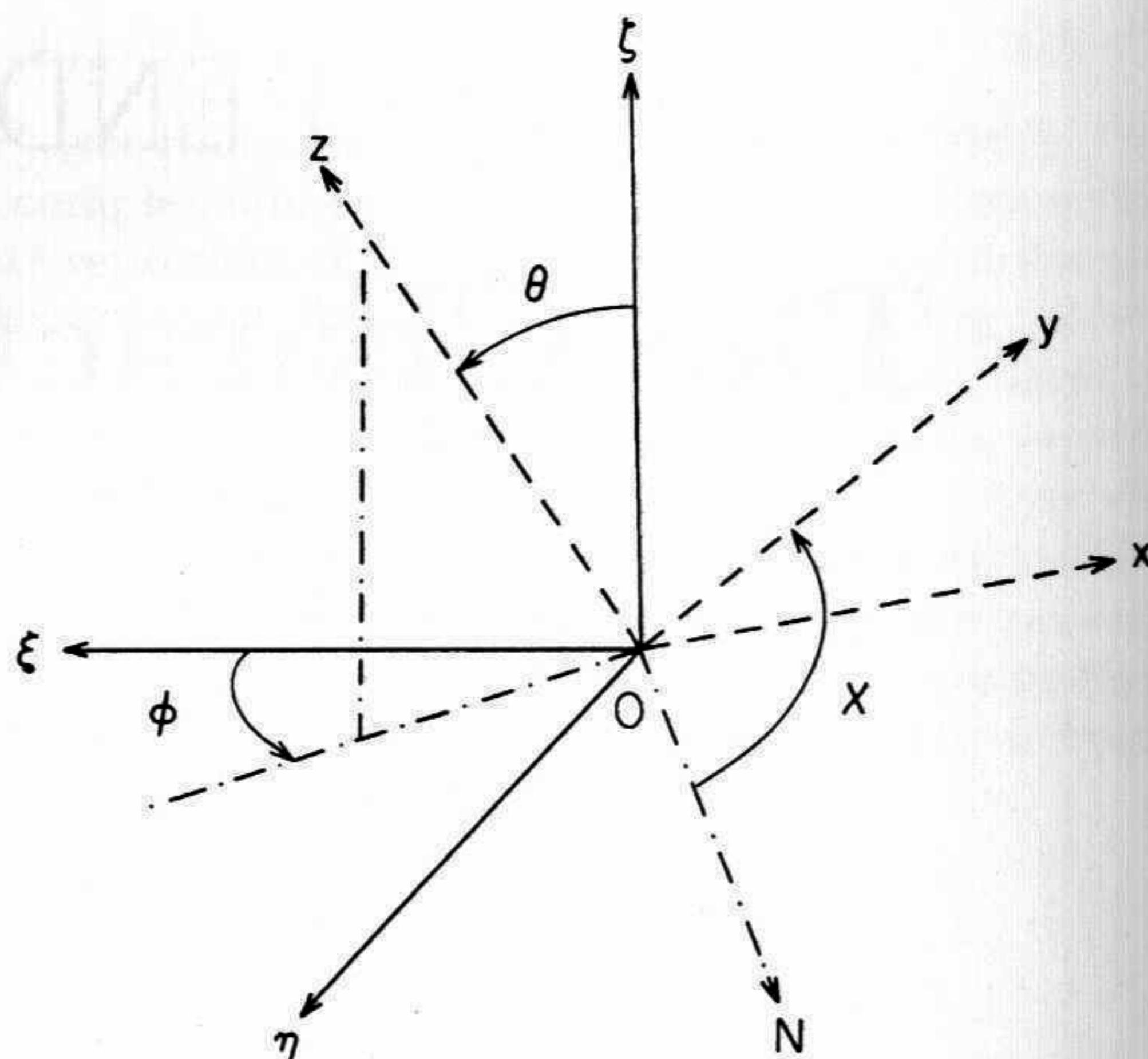
The Character Tables

This Appendix gives the character tables of the most common molecular symmetry (MS) groups and extended molecular symmetry (EMS) groups. The MS group is defined in Chapter 3. The EMS group is necessary for the classification of the vibronic states, and other basis states, of linear molecules and of nonrigid molecules (like dimethylacetylene) that have identical coaxial internal rotors. The EMS group is defined in Eqs. (17-99)–(17-112) for linear molecules, and in Sections 15.4.4–15.4.6 for nonrigid molecules that have identical coaxial internal rotors. The latter EMS groups contain the special symmetry operation E' which is the rotation of either of the two internal rotors through 2π radians, and which does nothing to the space fixed coordinates.

For a rigid nonlinear molecule the MS group is isomorphic to the molecular point group, and in such a case the name of the MS group is taken to be that of the point group followed by (M), e.g., the MS group of CH_3F is called $C_{3v}(\text{M})$. For a linear rigid molecule the EMS group is isomorphic to the molecular point group and is called $C_{\infty v}(\text{EM})$ or $D_{\infty h}(\text{EM})$ as appropriate; the MS group of

a linear molecule is called $C_{\infty v}(M)$ or $D_{\infty h}(M)$ but these are not isomorphic to the $C_{\infty v}$ or $D_{\infty h}$ point groups. For a nonrigid molecule the MS group is called G_n , where n is the order of the group, and the EMS group for a molecule whose MS group is G_n is called $G_n(EM)$. For rigid molecules the irreducible representations are named in the same way as for the (isomorphic) point group. The irreducible representations are ordered in each symmetry group according to established convention; the convention is necessary to ensure a consistent numbering system for the normal vibrations. The normal vibrations are numbered according to their symmetry species, and then within each symmetry species from highest to lowest wavenumber.

Fig. A-1. The definition of the Euler angles (θ, ϕ, χ) that relate the orientation of the molecule fixed (x, y, z) axes to the (ξ, η, ζ) axes. The origin of both axis systems is at the nuclear center of mass O , and the node line ON is directed so that a right handed screw is driven along ON in its positive direction by twisting it from ζ to z through θ where $0 \leq \theta \leq \pi$. ϕ and χ have the ranges 0 to 2π . χ is measured from the node line.



In each character table one element from each class is given and the number of elements in the class is indicated underneath the element. If the MS or EMS group is isomorphic to the molecular point group (this only happens for rigid molecules), the appropriate elements in each class of the molecular point group are given (this shows the effects of the MS or EMS group element on the vibronic variables), and the names of the irreducible representations are taken from the molecular point group. The equivalent rotation (Equiv. rot.) of the MS or EMS group element written for each class is also given. The equivalent rotations of an asymmetric top molecule are called R_a^π , R_b^π , or R_c^π to indicate rotations through π radians about the a , b , or c axis respectively. For a symmetric top molecule the equivalent rotations are called R_α^π or R_z^β as defined in Table A-1 which is a copy of Table 12-1. Knowing the equivalent rotations one can classify the components of the rovibronic angular momentum operator \hat{J}_α (see Table A-1). For further convenience we also give in Fig. A-1 a copy of Fig. 10-1 which defines the Euler angles.

The species obtained for the \hat{J}_α are indicated by placing the \hat{J}_α to the right of the appropriate irreducible representation. The rotational coordinate R_α [see Eq. (10-112)] transforms in the same way as \hat{J}_α under permutations and

Table A-1

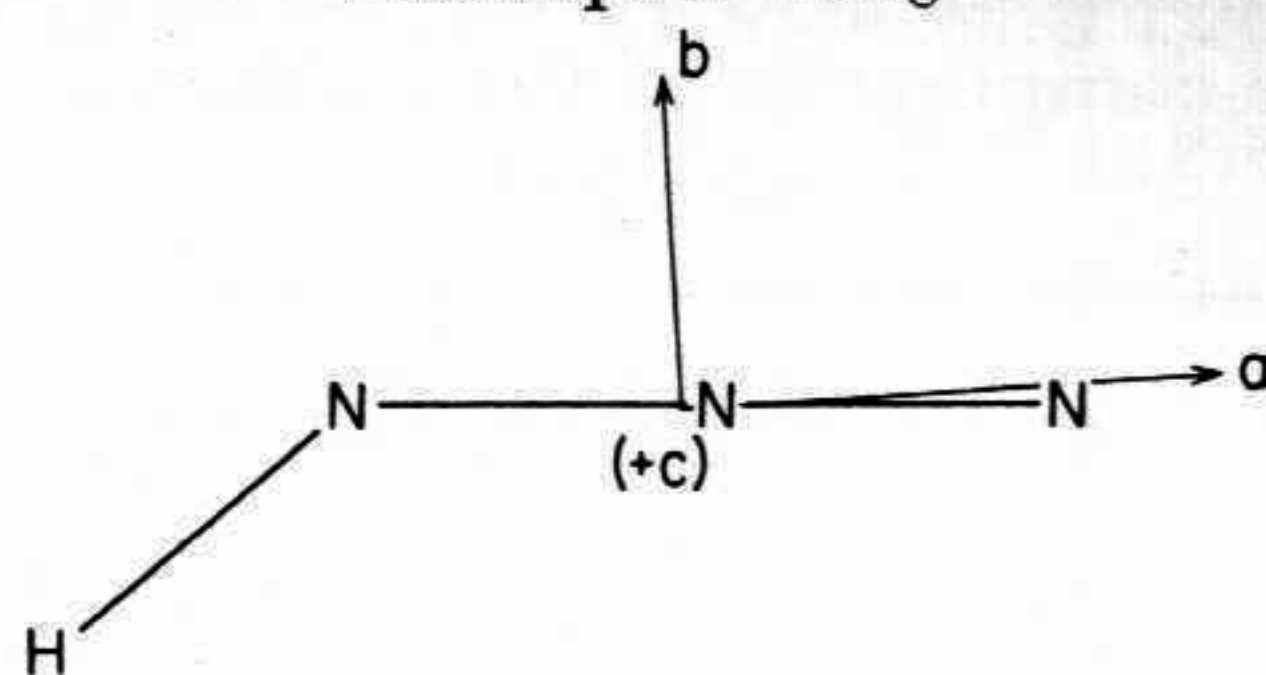
The transformation properties^a of the Euler angles and of the components of the rovibronic angular momentum \hat{J}

	R_α^π	R_z^β
θ	$\pi - \theta$	θ
ϕ	$\phi + \pi$	ϕ
χ	$2\pi - 2\alpha - \chi$	$\chi + \beta$
\hat{J}_x	$\hat{J}_x \cos 2\alpha + \hat{J}_y \sin 2\alpha$	$\hat{J}_x \cos \beta + \hat{J}_y \sin \beta$
\hat{J}_y	$\hat{J}_x \sin 2\alpha - \hat{J}_y \cos 2\alpha$	$-\hat{J}_x \sin \beta + \hat{J}_y \cos \beta$
\hat{J}_z	$-\hat{J}_z$	\hat{J}_z

^a R_α^π is a rotation of the molecule fixed (x, y, z) axes through π radians about an axis in the xy plane making an angle α with the x axis (α is measured in the right handed sense about the z axis), and R_z^β is a rotation of the molecule fixed (x, y, z) axes through β radians about the z axis (β is measured in the right handed sense about the z axis). The expressions for the \hat{J}_α are given in Eqs. (10-84)-(10-86).

permutation-inversions. The translational coordinate T_α [see Eq. (10-111)] transforms in the same way as \hat{J}_α under a nuclear permutation but with opposite sign under a permutation-inversion (see Table 12-20), and the molecule fixed dipole moment components μ_α transform in the same way as the T_α [see Eq. (14-36)]. The species of the T_α , and of the components $\alpha_{\gamma\delta}$ of the electronic polarizability, given by the species of $T_\gamma T_\delta$ [see Eq. (14-138)], are also indicated by placing them the right of the appropriate irreducible representation. For molecules with a single internal rotation coordinate we have indicated, when possible, the symmetry of the torsional momentum operator \hat{J}_ρ . Finally the dipole representation Γ^* that has character +1 for the permutations and -1 for the permutation-inversions is indicated; allowed transitions are connected by this symmetry species as discussed in Chapter 14 [see Eq. (14-8)]. electric

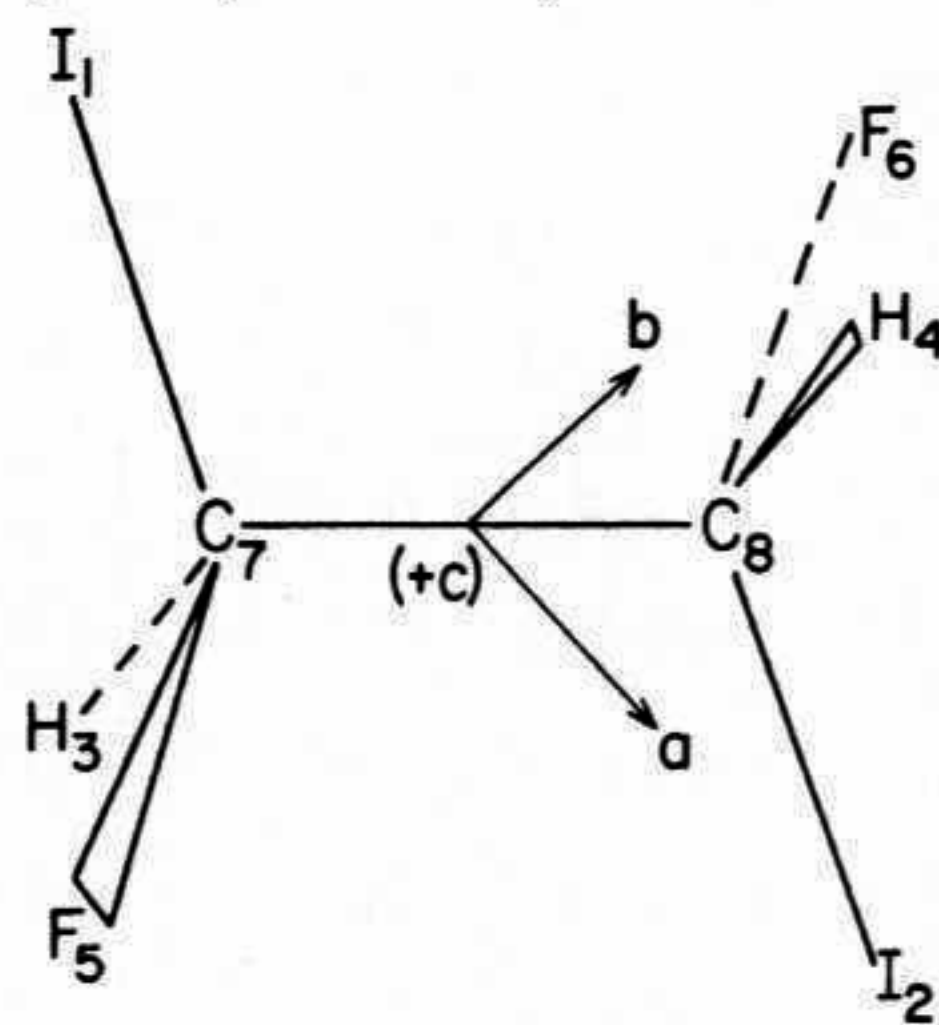
Table A-2
The group $C_s(M)$
Example: HN_3



$C_s(M)$:	E	E^*	
	1	1	
C_s :	E	σ_{ab}	
Equiv. rot.:	R^0	R_c^π	
A' :	1	1	: $T_a, T_b, \hat{J}_c, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}, \alpha_{ab}$
A'' :	1	-1	: $T_c, \hat{J}_a, \hat{J}_b, \alpha_{ac}, \alpha_{bc}, \Gamma^*$

Table A-3

The Group $C_i(M)$
Example: Trans $\text{C}(\text{HIF})\text{CHIF}$ (without torsional tunneling)

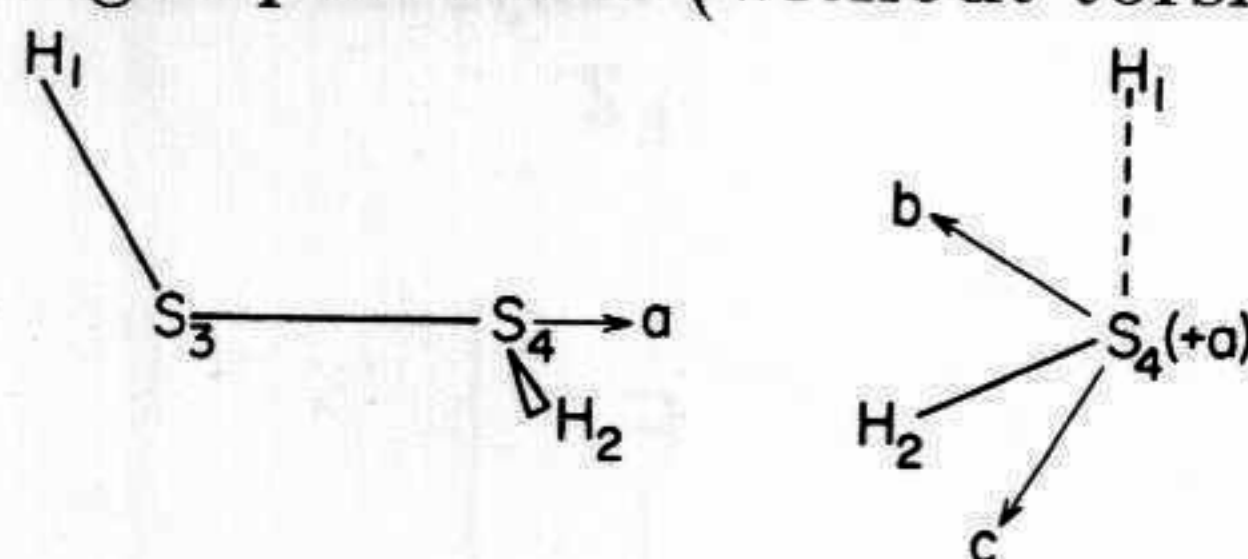


$C_i(M)$:	E	$(12)(34)(56)(78)^*$	
	1	1	
C_i :	E	i	
Equiv. rot.:	R^0	R^0	
A_g :	1	1	: $\hat{J}_a, \hat{J}_b, \hat{J}_c, \alpha$
A_u :	1	-1	: T_a, T_b, T_c, Γ^*

Table A-4

The group $C_2(M)$

Example: Hydrogen persulfide (without torsional tunneling)

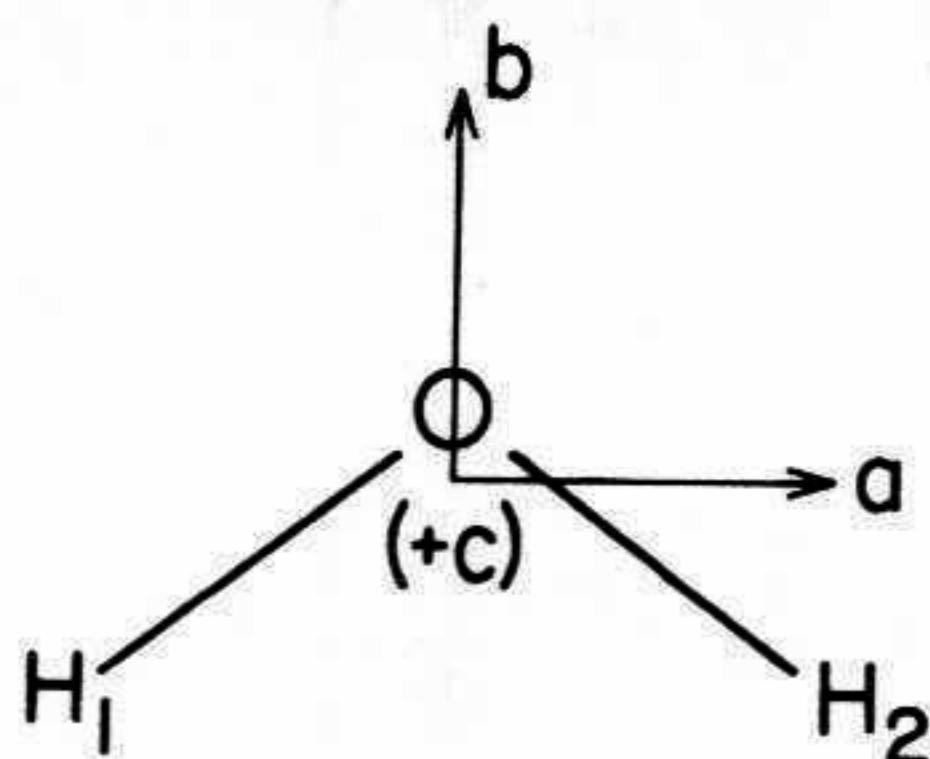


$C_2(M)$:	E	$(12)(34)$		
	1	1		
C_2 :	E	C_{2b}		
Equiv. rot.:	R^0	R_b^π		
A :	1	1	:	$T_b, \hat{J}_b, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}, \alpha_{ac}, \Gamma^*$
B :	1	-1	:	$T_a, T_c, \hat{J}_a, \hat{J}_c, \alpha_{ab}, \alpha_{bc}$

Table A-5

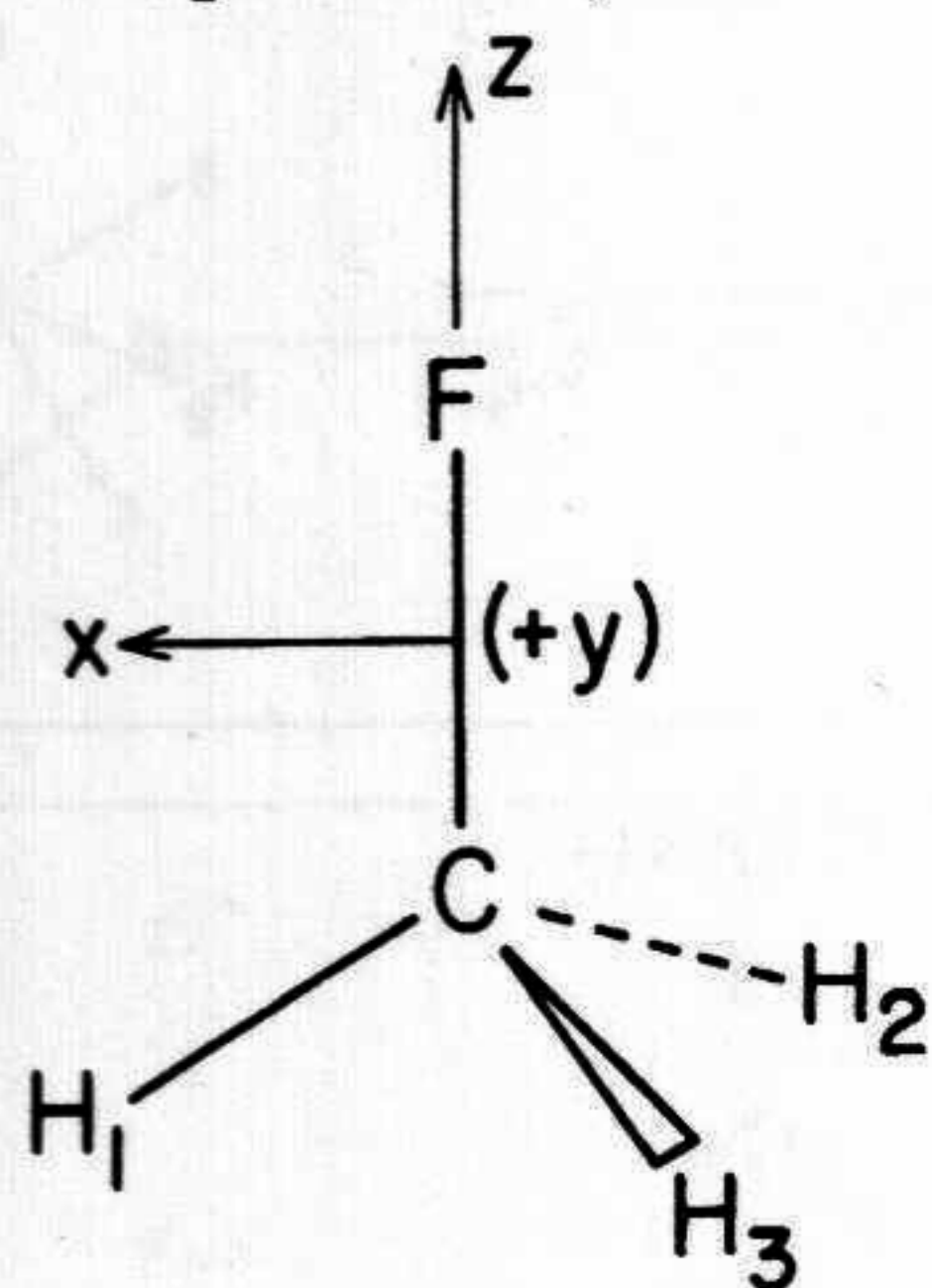
The group $C_{2v}(M)$

Example: Water



$C_{2v}(M)$:	E	(12)	E^*	$(12)^*$	
	1	1	1	1	
C_{2v} :	E	C_{2b}	σ_{ab}	σ_{bc}	
Equiv. rot.:	R^0	R_b^π	R_c^π	R_a^π	
A_1 :	1	1	1	1	:
A_2 :	1	1	-1	-1	:
B_1 :	1	-1	-1	1	:
B_2 :	1	-1	1	-1	:
					$T_b, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}$
					$\hat{J}_b, \alpha_{ac}, \Gamma^*$
					$T_c, \hat{J}_a, \alpha_{bc}$
					$T_a, \hat{J}_c, \alpha_{ab}$

Table A-6
The group $C_{3v}(M)$
Example: Methyl fluoride

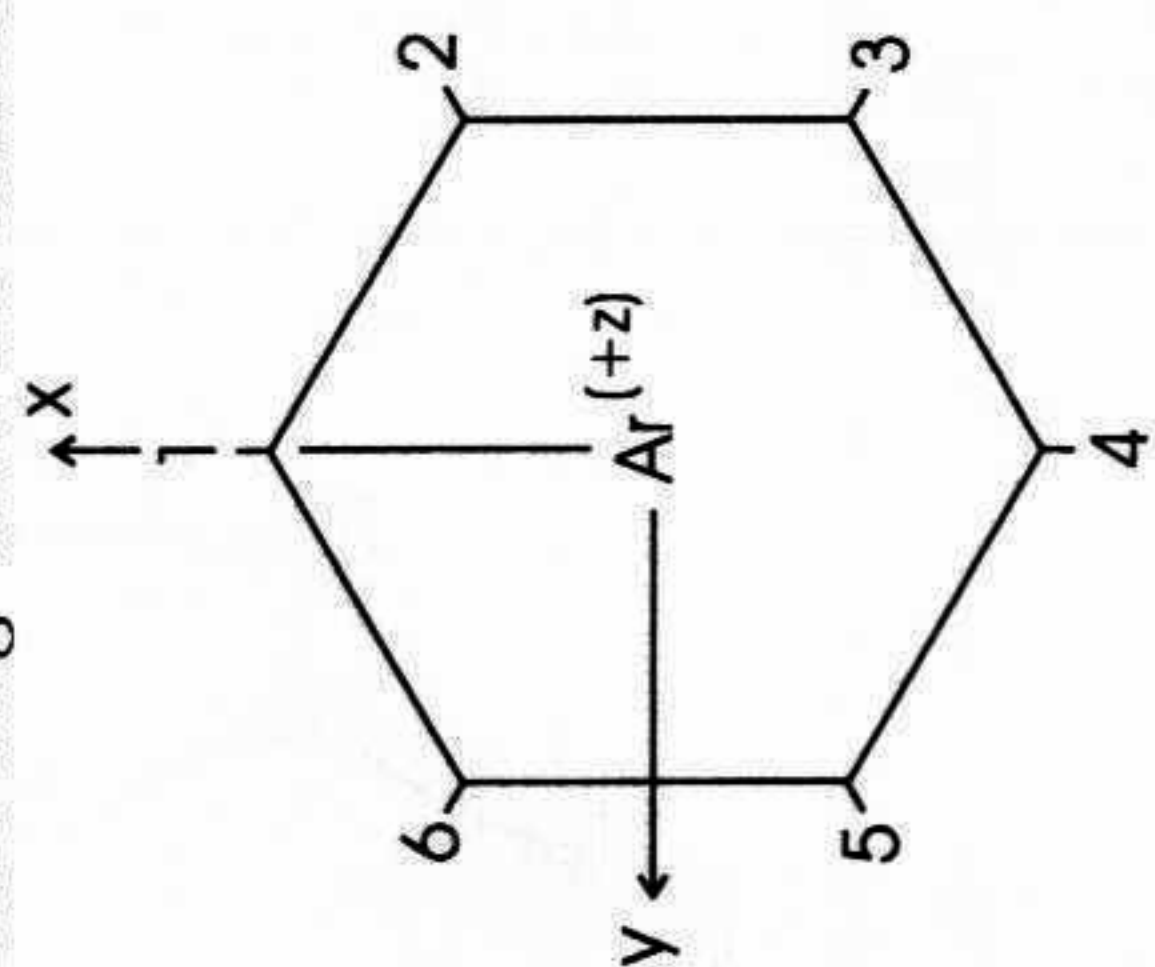


$C_{3v}(M)$:	E	(123)	$(23)^*$	
	1	2	3	
C_{3v} :	E	$2C_3$	$3\sigma_v$	
Equiv. rot.:	R^0	$R_z^{2\pi/3}$	$R_{\pi/2}^\pi$	
A_1 :	1	1	1	: $T_z, \alpha_{zz}, \alpha_{xx} + \alpha_{yy}$
A_2 :	1	1	-1	: \hat{J}_z, Γ^*
E :	2	-1	0	: $(T_x, T_y), (\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz}), (\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

Table A-7

The group $C_{6v}(M)$ Example: Benzene-argon dimer^a

(The argon atom is above the benzene ring with no tunneling to the other side of the ring).



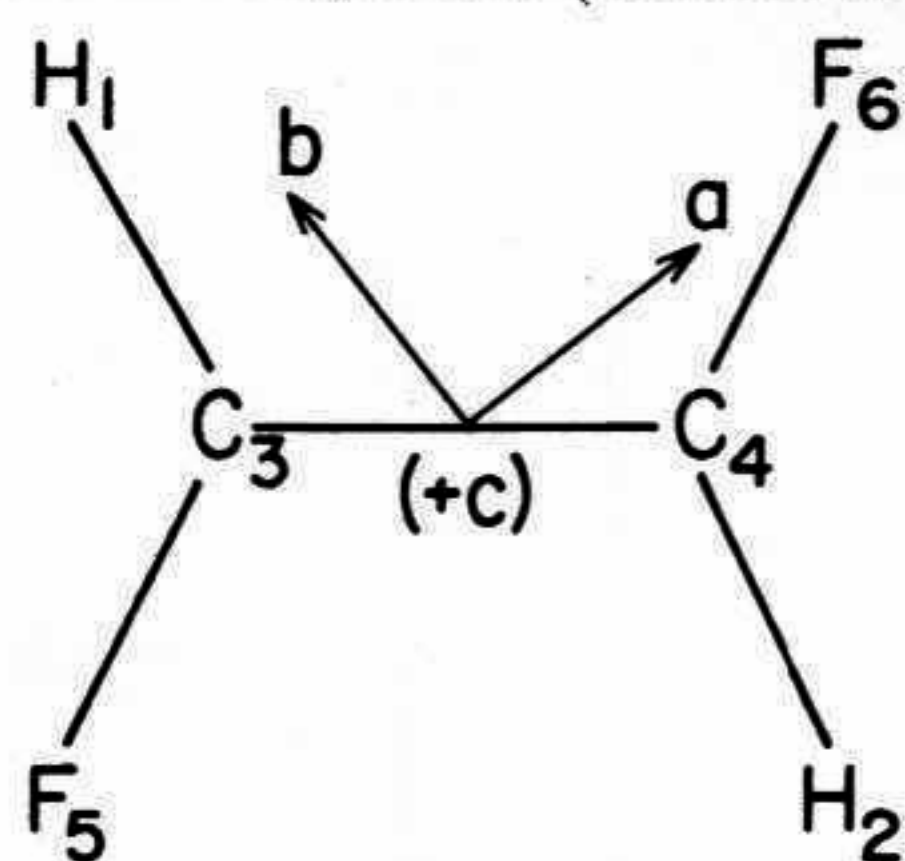
$C_{6v}(M)$:	E	(123456)	$(135)(246)$	$(14)(25)(36)$	$(26)(35)^*$	$(14)(23)(56)^*$
	1	2	2	1	3	3
C_{6v} :	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Equiv. rot.:	R^0	$R_z^{\pi/3}$	$R_z^{2\pi/3}$	R_z^{π}	$R_{\pi/2}^{\pi}$	R_0^{π}
A_1 :	1	1	1	1	1	1
A_2 :	1	1	1	1	-1	-1
B_1 :	1	-1	1	-1	1	-1
B_2 :	1	-1	1	-1	-1	1
E_1 :	2	1	-1	-2	0	0
E_2 :	2	-1	-1	2	0	0
						$: T_z, \alpha_{zz}, \alpha_{xx} + \alpha_{yy}$ $: \hat{J}_z, \Gamma^*$
						$: (T_x, T_y), (\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$ $: (\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$

^a See van der Avoird (1993). The pairs of bonded CH nuclei of the benzene moiety are labeled 1 through 6.

Table A-8

The group $C_{2h}(M)$

Example: Trans-difluoroethylene (without torsional tunneling)

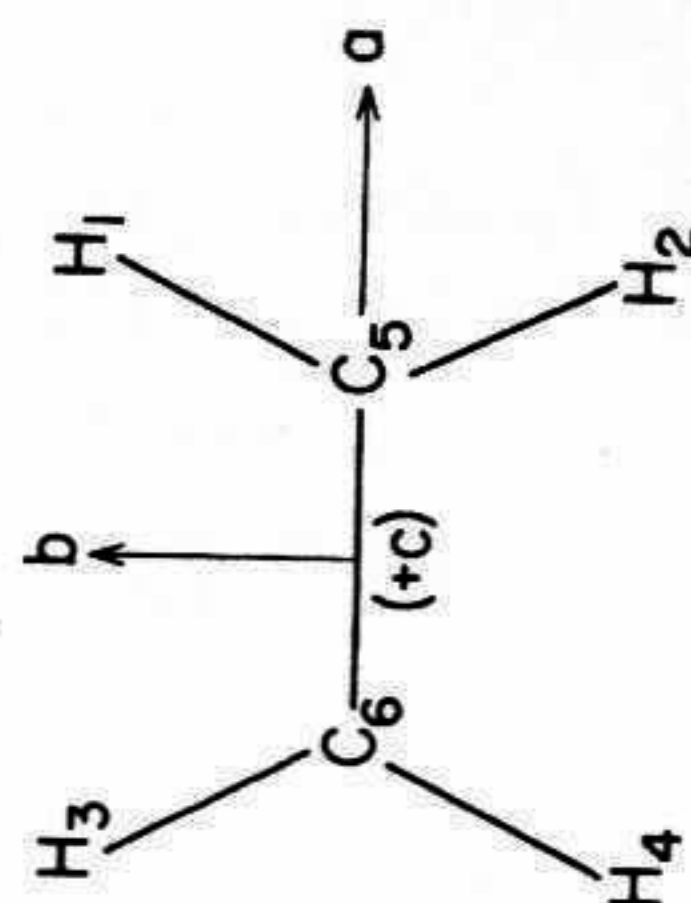


$C_{2h}(M):$	E	$(12)(34)(56)$	E^*	$(12)(34)(56)^*$	
	1	1	1	1	
$C_{2h}:$	E	C_{2c}	σ_{ab}	i	
Equiv. rot.:	R^0	R_c^π	R_c^π	R^0	
$A_g:$	1	1	1	1	: $\hat{J}_c, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}, \alpha_{ab}$
$A_u:$	1	1	-1	-1	: T_c, Γ^*
$B_g:$	1	-1	-1	1	: $\hat{J}_a, \hat{J}_b, \alpha_{ac}, \alpha_{bc}$
$B_u:$	1	-1	1	-1	: T_a, T_b

Table A-9

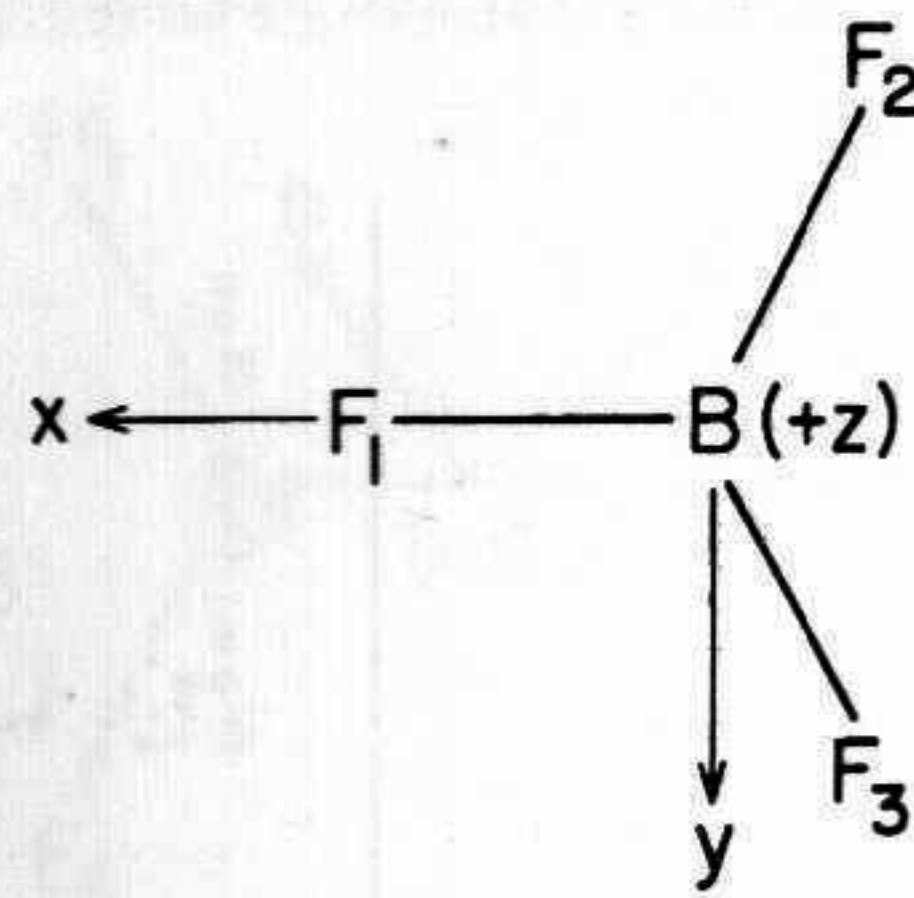
The group $D_{2h}(M)$

Example: Ethylene (without torsional tunneling)



	E	$(12)(34)$	$(13)(24)(56)$	$(14)(23)(56)$	E^*	$(12)(34)^*$	$(13)(24)(56)^*$	$(14)(23)(56)^*$	R^0
$D_{2h}(M):$	1	1	1	1	1	1	1	1	1
$D_{2h}: E$	C_{2a}	C_{2b}	C_{2c}	σ_{ab}	σ_{ac}	σ_{bc}	i		
Equiv. rot.:	R_a^π	R_b^π	R_c^π	R_c^π	R_b^π	R_a^π	R^0		
$A_g:$	1	1	1	1	1	1	1	1	$\alpha_{aa}, \alpha_{bb}, \alpha_{cc}$
$A_u:$	1	1	1	1	-1	-1	-1	-1	Γ^*
$B_{1g}:$	1	1	-1	-1	-1	-1	1	1	f_a, α_{bc}
$B_{1u}:$	1	1	-1	-1	1	1	-1	-1	T_a
$B_{2g}:$	1	-1	1	-1	-1	1	-1	1	f_b, α_{ac}
$B_{2u}:$	1	-1	1	-1	1	-1	1	-1	T_b
$B_{3g}:$	1	-1	-1	1	1	-1	-1	1	f_c, α_{ab}
$B_{3u}:$	1	-1	-1	1	-1	1	-1	-1	T_c

Table A-10
The group $D_{3h}(M)$
Example: Boron trifluoride



$D_{3h}(M)$:	E	(123)	(23)	E^*	$(123)^*$	$(23)^*$	
	1	2	3	1	2	3	
D_{3h} :	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	
Equiv. rot.:	R^0	$R_z^{2\pi/3}$	R_0^π	R_z^π	$R_z^{-\pi/3}$	$R_{\pi/2}^\pi$	
A_1' :	1	1	1	1	1	1	: $\alpha_{zz}, \alpha_{xx} + \alpha_{yy}$
A_1'' :	1	1	1	-1	-1	-1	: Γ^*
A_2' :	1	1	-1	1	1	-1	: \hat{J}_z
A_2'' :	1	1	-1	-1	-1	1	: T_z
E' :	2	-1	0	2	-1	0	: $(T_x, T_y), (\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E'' :	2	-1	0	-2	1	0	: $(\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$

Un exemple pour la détermination de la représentation de J_x, J_y, J_z

→ Pour J_z

selon la table 12.1, p. 266, J_x se transforme de la façon suivante :

$$J_z \rightarrow -J_z \text{ par } R_\alpha^\pi \quad ; \quad J_z \rightarrow J_z \text{ par } R_z^\beta$$

donc sous :

$$E = R^0 : J_z \rightarrow J_z, (123) = R_z^{2\pi/3} : J_z \rightarrow J_z, (23) = R_0^\pi : J_z \rightarrow -J_z$$

$$E^* = R_z^\pi : J_z \rightarrow J_z, (123)^* = R_z^{-\pi/3} : J_z \rightarrow J_z, (23)^* = R_{\pi/2}^\pi : J_z \rightarrow -J_z$$

le caractère est donc $(1, 1, -1, 1, 1, -1) = A_2'$

→ Pour J_x, J_y

Selon la table 12.1, J_x, J_y forment une base à 2 dimensions

qui a pour caractère $\chi_\alpha = 0$ sous R_α^π ; $\chi_\beta = 2\cos(\beta)$ sous R_z^β

puisque les matrices de transformations sont

$$D[R_\alpha^\pi] = \begin{pmatrix} \cos(2\alpha) & \sin(2\alpha) \\ \sin(2\alpha) & -\cos(2\alpha) \end{pmatrix} \quad ; \quad D[R_z^\beta] = \begin{pmatrix} \cos(\beta) & \sin(\beta) \\ -\sin(\beta) & \cos(\beta) \end{pmatrix}$$

donc sous :

$$E = R^0 : \chi^E = 2, (123) = R_z^{2\pi/3} ; \chi^{(123)} = 2\cos(2\pi/3) = -1, (23) = R_0^\pi ; \chi^{(23)} = 0$$

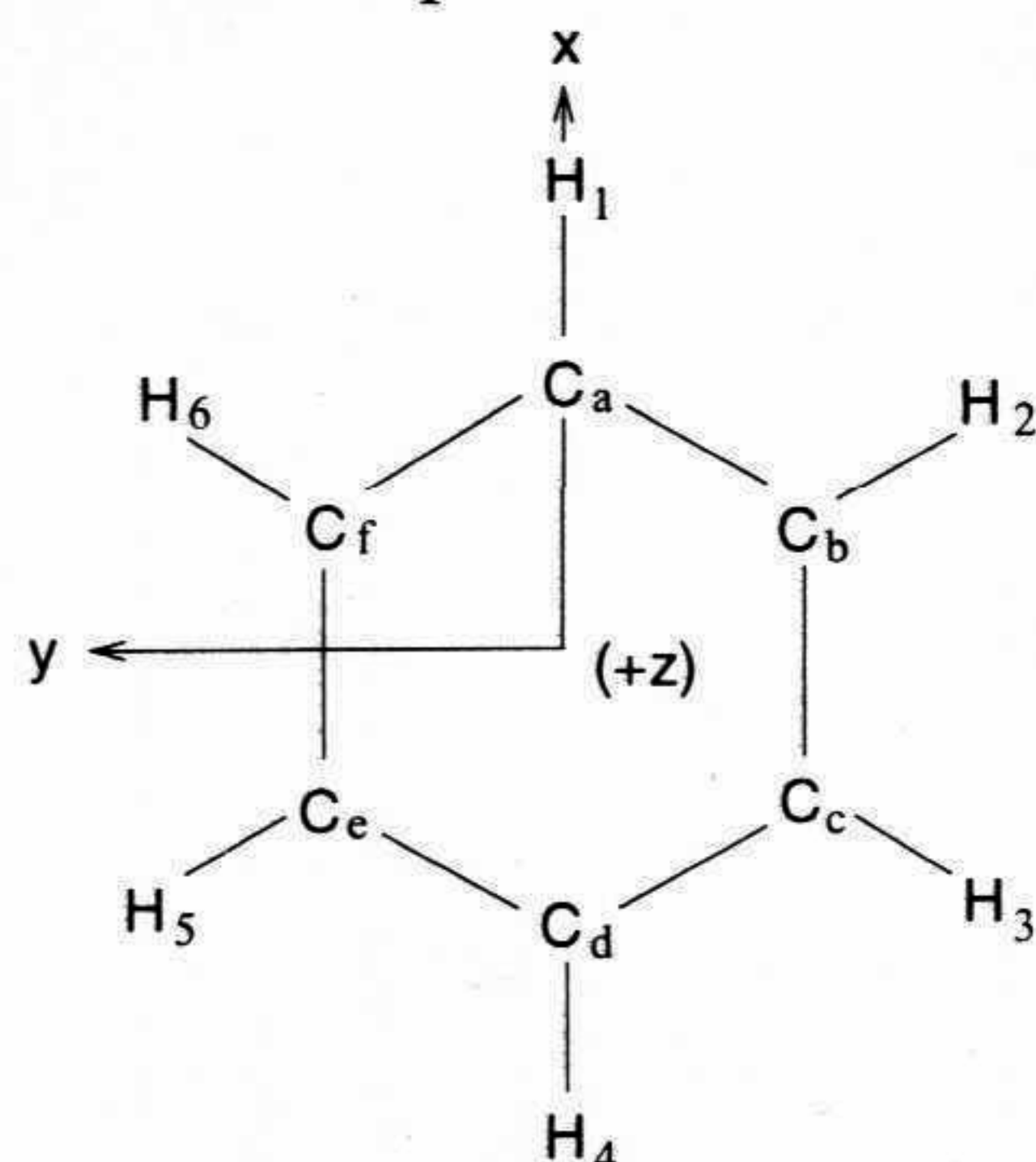
$$E^* = R_z^\pi : \chi^{E^*} = 2\cos(\pi) = -2, (123)^* = R_z^{-\pi/3} ; \chi^{(123)^*} = 2\cos(-\pi/3) = 1, (23)^* = R_{\pi/2}^\pi ; \chi^{(23)^*} = 0$$

le caractère est donc $(2, -1, 0, -2, 1, 0) = E''$

* La même démarche peut être faite pour T_x, T_y, T_z , mais nous savons selon la p. 316 nous savons que T_α se transforme comme J_α sous P et comme $-J_\alpha$ sous P^* .

* De la même façon (voir p. 316) R_α se transforme comme J_α pour tout P .

Table A-11
The group $D_{6h}(M)$
Example: Benzene

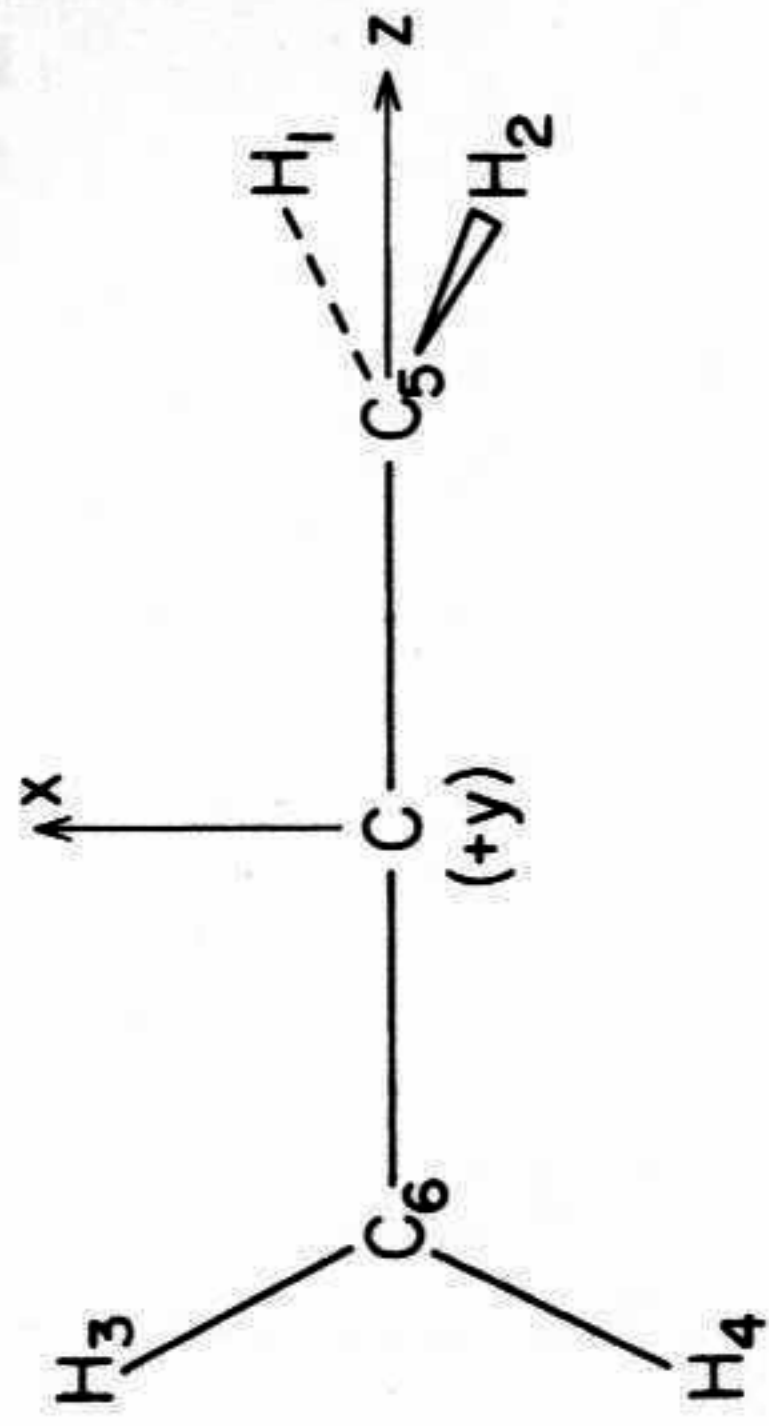


$D_{6h}(M)$:	E	$(123456)(abcdef)$	$(135)(246)(ace)(bdf)$	$(14)(25)(36)(ad)(be)(cf)$	$(26)(35)(bf)(ce)$	$(14)(23)(56)(ad)(bc)(ef)$	$(14)(25)(36)(ad)(be)(cf)^*$	$(135)(246)(ace)(bdf)^*$	$(123456)(abcdef)^*$	E^*	$(14)(23)(56)(ad)(bc)(ef)^*$	$(26)(35)(bf)(ce)^*$	
D_{6h} :	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$	
Equiv. rot.:	R^0	$R_z^{\pi/3}$	$R_z^{2\pi/3}$	R_z^π	R_0^π	$R_{\pi/2}^\pi$	R^0	$R_z^{5\pi/3}$	$R_z^{4\pi/3}$	R_z^π	R_0^π	$R_{\pi/2}^\pi$	
A_{1g} :	1	1	1	1	1	1	1	1	1	1	1	1	: $\alpha_{zz},$ $\alpha_{xx} + \alpha_{yy}$
A_{1u} :	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	: Γ^*
A_{2g} :	1	1	1	1	-1	-1	1	1	1	1	-1	-1	: \hat{J}_z
A_{2u} :	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	: T_z
B_{1g} :	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	
B_{1u} :	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	
B_{2g} :	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	
E_{1g} :	2	1	-1	-2	0	0	2	1	-1	-2	0	0	: $(\hat{J}_x, \hat{J}_y),$ $(\alpha_{xz}, \alpha_{yz})$
E_{1u} :	2	1	-1	-2	0	0	-2	-1	1	2	0	0	: (T_x, T_y)
E_{2g} :	2	-1	-1	2	0	0	2	-1	-1	2	0	0	: $(\alpha_{xy},$ $\alpha_{xx} - \alpha_{yy})$
E_{2u} :	2	-1	-1	2	0	0	-2	1	1	-2	0	0	

Table A-12

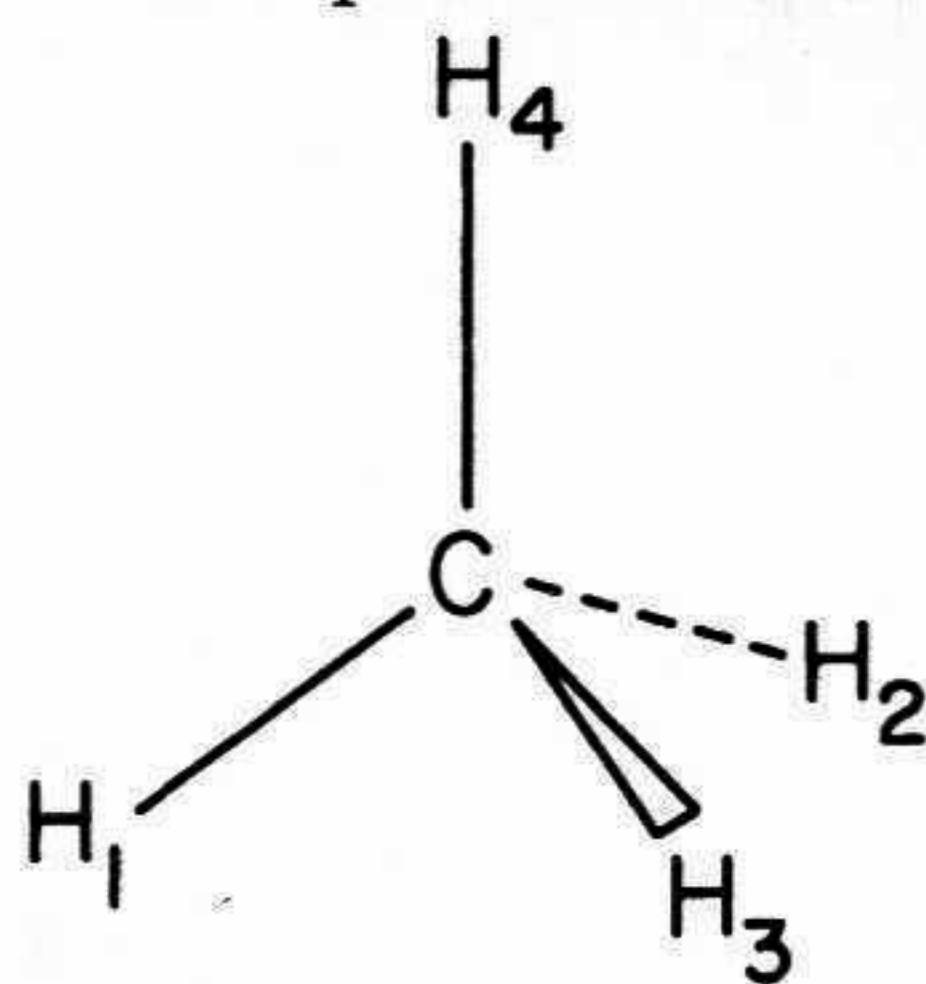
The group $D_{2d}(M)$

Example: Allene (without torsional tunneling)



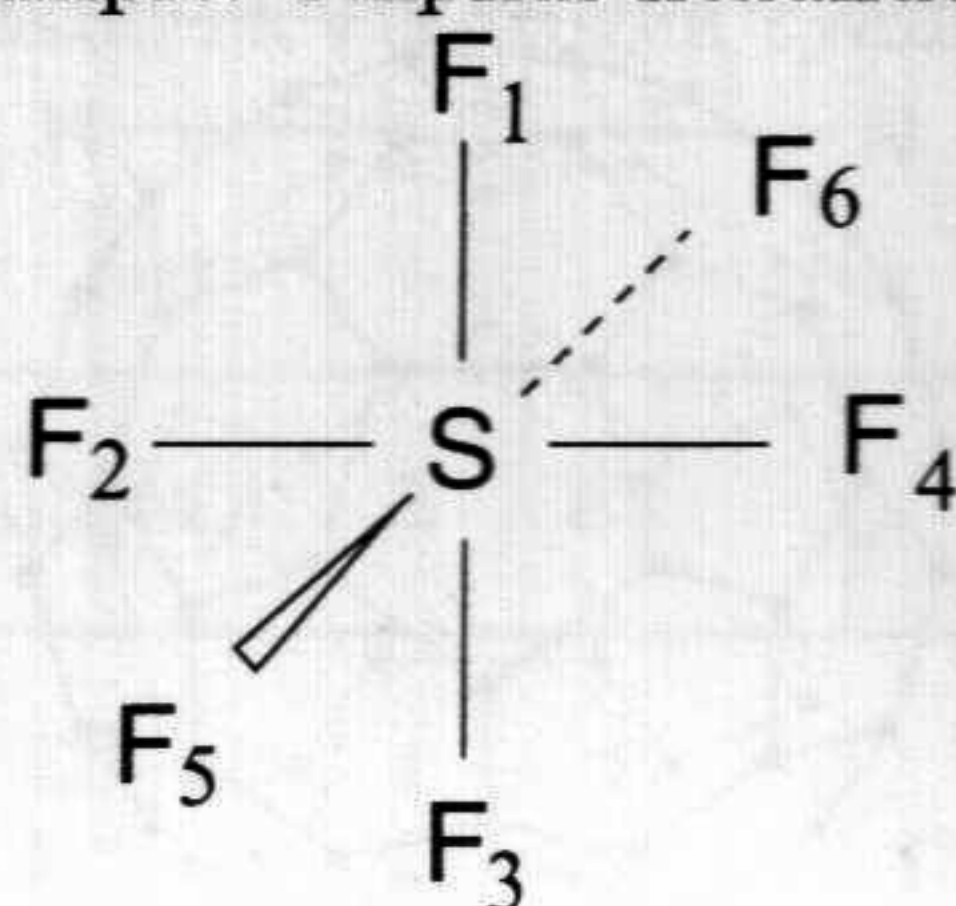
$D_{2d}(M):$	E	$(1423)(56)^*$	$(12)(34)$	$(13)(24)(56)$	$(34)^*$
	1	2	1	2	2
$D_{2d}:$	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$
Equiv. rot.:	R^0	$R_z^{3\pi/2}$	R_z^π	$R_{3\pi/4}^\pi$	R_0^π
$A_1:$	1	1	1	1	1
$A_2:$	1	1	1	-1	-1
$B_1:$	1	-1	1	1	-1
$B_2:$	1	-1	1	-1	1
$E:$	2	0	-2	0	0
					$:\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$ $:\hat{J}_z$ $:\alpha_{xx} - \alpha_{yy}, \Gamma^*$ $:T_z, \alpha_{xy}$ $:(T_x, T_y), (\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$

Table A-14
The group $T_d(M)$
Example: Methane



$T_d(M):$	E	(123)	$(14)(23)$	$(1423)^*$	$(23)^*$	
	1	8	3	6	6	
$T_d:$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	
$A_1:$	1	1	1	1	1	: $\alpha_{xx} + \alpha_{yy} + \alpha_{zz}$
$A_2:$	1	1	1	-1	-1	: Γ^*
$E:$	2	-1	2	0	0	: $(\alpha_{xx} + \alpha_{yy} - 2\alpha_{zz}, \alpha_{xx} - \alpha_{yy})$
$F_1:$	3	0	-1	1	-1	: $(\hat{J}_x, \hat{J}_y, \hat{J}_z)$
$F_2:$	3	0	-1	-1	1	: $(T_x, T_y, T_z), (\alpha_{xy}, \alpha_{yz}, \alpha_{xz})$

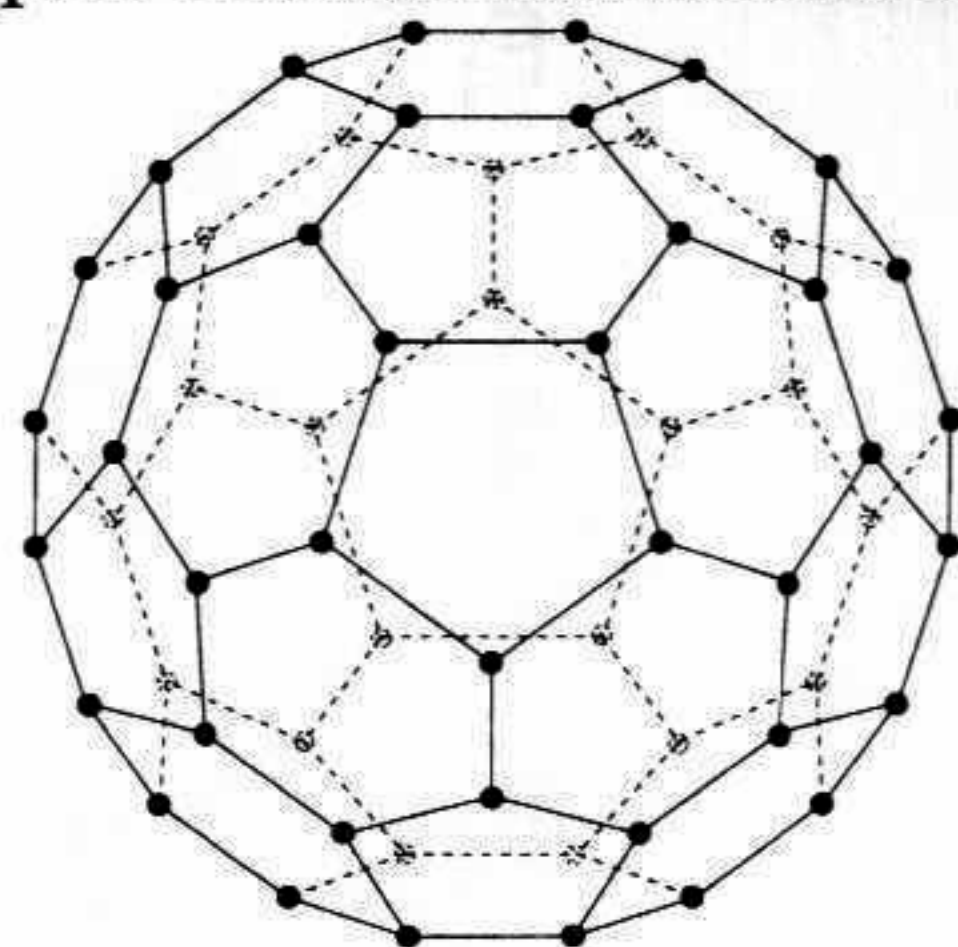
Table A-15
 The group $O_h(M)$
 Example: Sulphur hexafluoride



$O_h(M)$:	E	$(145)(263)$	$(13)(26)(45)$	(1234)	$(13)(24)$	$(13)(24)(56)^*$	$(125346)^*$	$(25)(46)^*$	$(1432)(56)^*$	$(56)^*$
	1	8	6	6	3	1	8	6	6	3
O_h :	E	$8C_3$	$6C_2$	$6C_4$	$3C_2$	i	$8S_6$	$6\sigma_d$	$6S_4$	$3\sigma_h$

A_{1g} :	1	1	1	1	1	1	1	1	1	1	:	$\alpha_{zz} + \alpha_{xx} + \alpha_{yy}$
A_{1u} :	1	1	1	1	1	-1	-1	-1	-1	-1	:	Γ^*
A_{2g} :	1	1	-1	-1	1	1	1	-1	-1	1		
A_{2u} :	1	1	-1	-1	1	-1	-1	1	1	-1		
E_g :	2	-1	0	0	2	2	-1	0	0	2	:	$(2\alpha_{zz} - \alpha_{xx} - \alpha_{yy},$ $\alpha_{xx} - \alpha_{yy})$
E_u :	2	-1	0	0	2	-2	1	0	0	-2		
F_{1g} :	3	0	-1	1	-1	3	0	-1	1	-1	:	$(\hat{J}_x, \hat{J}_y, \hat{J}_z)$
F_{1u} :	3	0	-1	1	-1	-3	0	1	-1	1	:	(T_x, T_y, T_z)
F_{2g} :	3	0	1	-1	-1	3	0	1	-1	-1	:	$(\alpha_{xz}, \alpha_{yz}, \alpha_{xy})$
F_{2u} :	3	0	1	-1	-1	-3	0	-1	1	1		

Table A-16
 The group $I_h(M)$
 Example: Buckminsterfullerene C_{60}



$I_h(M):$	E	C_2	C_3	C_4	C_5	\hat{O}_i	C_7	C_8	C_9	C_{10}
	1	12	12	20	15	1	12	12	20	15

$I_h:$	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}^3$	$12S_{10}$	$20S_6$	15σ
--------	-----	---------	-----------	---------	---------	-----	--------------	------------	---------	------------

$A_g:$	1	1	1	1	1	1	1	1	1	1	:	$\alpha_{zz} + \alpha_{xx} + \alpha_{yy}$
$A_u:$	1	1	1	1	1	-1	-1	-1	-1	-1	:	Γ^*
$F_{1g}:$	3	η^+	η^-	0	-1	3	η^+	η^-	0	-1	:	$(\hat{J}_x, \hat{J}_y, \hat{J}_z)$
$F_{1u}:$	3	η^+	η^-	0	-1	-3	$-\eta^+$	$-\eta^-$	0	1	:	(T_x, T_y, T_z)
$F_{2g}:$	3	η^-	η^+	0	-1	3	η^-	η^+	0	-1		
$F_{2u}:$	3	η^-	η^+	0	-1	-3	$-\eta^-$	$-\eta^+$	0	1		
$G_g:$	4	-1	-1	1	0	4	-1	-1	1	0		
$G_u:$	4	-1	-1	1	0	-4	1	1	-1	0		
$H_g:$	5	0	0	-1	1	5	0	0	-1	1	:	$(2\alpha_{zz} - \alpha_{xx} - \alpha_{yy},$ $\alpha_{xx} - \alpha_{yy},$ $\alpha_{xz}, \alpha_{yz}, \alpha_{xy})$
$H_u:$	5	0	0	-1	1	-5	0	0	1	-1		

$\eta^\pm = (1 \pm \sqrt{5})/2$. Each of the MS group operations involves the 60 indices labeling the nuclei in C_{60} [see Fig. 8-2] and we do not show the operations here. The elements in each class are described as follows:

C_2 Each operation is a product of 12 five-cycles ($abcde$).

C_3 Each operation is a product of 12 five-cycles ($abcde$).

C_4 Each operation is a product of 20 three-cycles (abc).

C_5 Each operation is a product of 30 transpositions (ab).

\hat{O}_i The product of 30 transpositions (ab) and the inversion E^* [see Eq. (8-37)].

$C_7 = C_2 \hat{O}_i$. Each operation is the product of six ten-cycles ($abcdefghij$) and the inversion E^* .

$C_8 = C_3 \hat{O}_i$. Each operation is the product of six ten-cycles ($abcdefghij$) and the inversion E^* .

$C_9 = C_4 \hat{O}_i$. Each operation is the product of 10 six-cycles ($abcdef$) and the inversion E^* .

$C_{10} = C_5 \hat{O}_i$. Each operation is the product of ²⁸30 transpositions (ab) and the inversion E^* .

$C_k = C_j \hat{O}_i$ indicates that the elements in C_k are obtained by combining each element in C_j with \hat{O}_i [see Section 8.4.3]. From Fig. 8-2 the reader can construct the expressions for the MS group operations of C_{60} .

Table A-17

The group $C_{\infty v}(M)$
 Example: Hydrogen cyanide
 H — C — N

$C_{\infty v}(M):$	E	E^*		
$\Sigma^+, +:$	1	1		
$\Sigma^-, -:$	1	-1	:	Γ^*

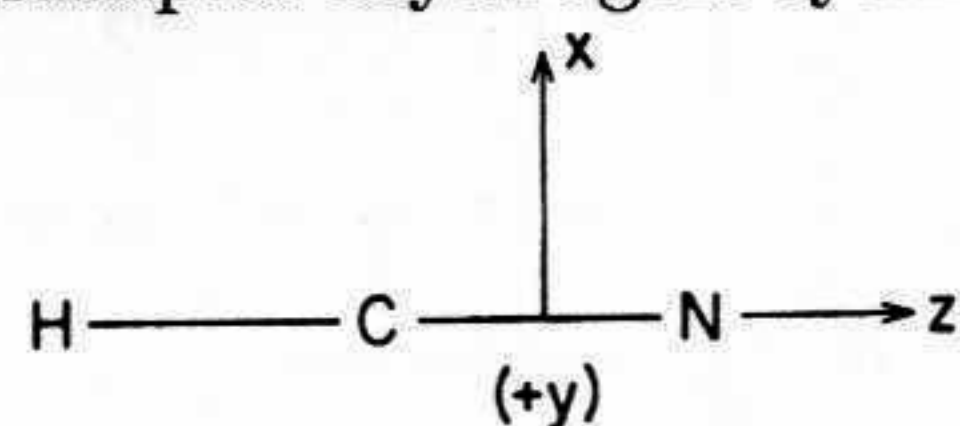
Table A-18

The group $D_{\infty h}(M)$
 Example: Carbon dioxide
 O₁ — C — O₂

$D_{\infty h}(M):$	E	(12)	E^*	(12)*	
$\Sigma_g^+, +s:$	1	1	1	1	
$\Sigma_u^+, +a:$	1	-1	1	-1	
$\Sigma_g^-, -a:$	1	-1	-1	1	
$\Sigma_u^-, -s:$	1	1	-1	-1	: Γ^*

Table A-19

The group^a $C_{\infty v}(EM)$
 Example: Hydrogen cyanide



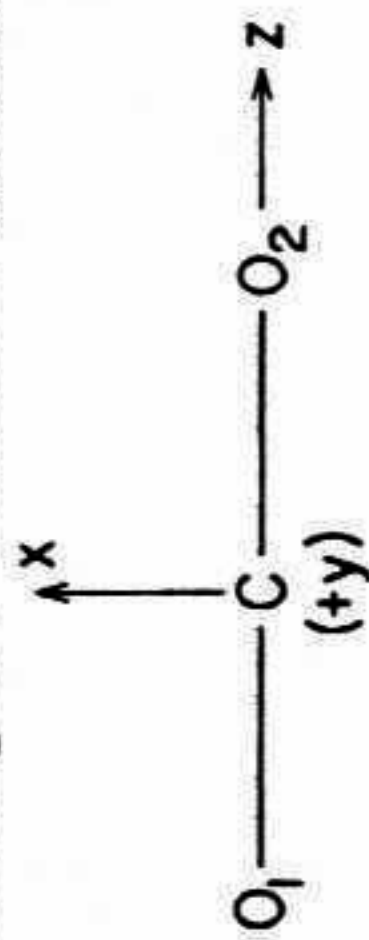
$C_{\infty v}(EM)$	E_0	E_ϵ	...	∞E_ϵ^*	
	1	2	...	∞	
$C_{\infty v}:$	E	$2C_\infty^\epsilon$...	$\infty \sigma_v^{(\epsilon/2)}$	
Equiv. rot.:	R^0	$R_z^{-\epsilon}$...	$R_{(\pi+\epsilon)/2}^\pi$	
$(+)\Sigma^+:$	1	1	...	1	: $T_z, \alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$(-)\Sigma^-:$	1	1	...	-1	: \hat{J}_z, Γ^*
$\Pi:$	2	$2 \cos \epsilon$...	0	: $(T_x, T_y), (\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$
$\Delta:$	2	$2 \cos 2\epsilon$...	0	: $(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
\vdots	\vdots	\vdots	...	\vdots	

^a The xyz axes are the $x'y'z'$ axes introduced in Chapter 17 for the isomorphic Hamiltonian.

Table A-20

The group^a $D_{\infty h}$ (EM)

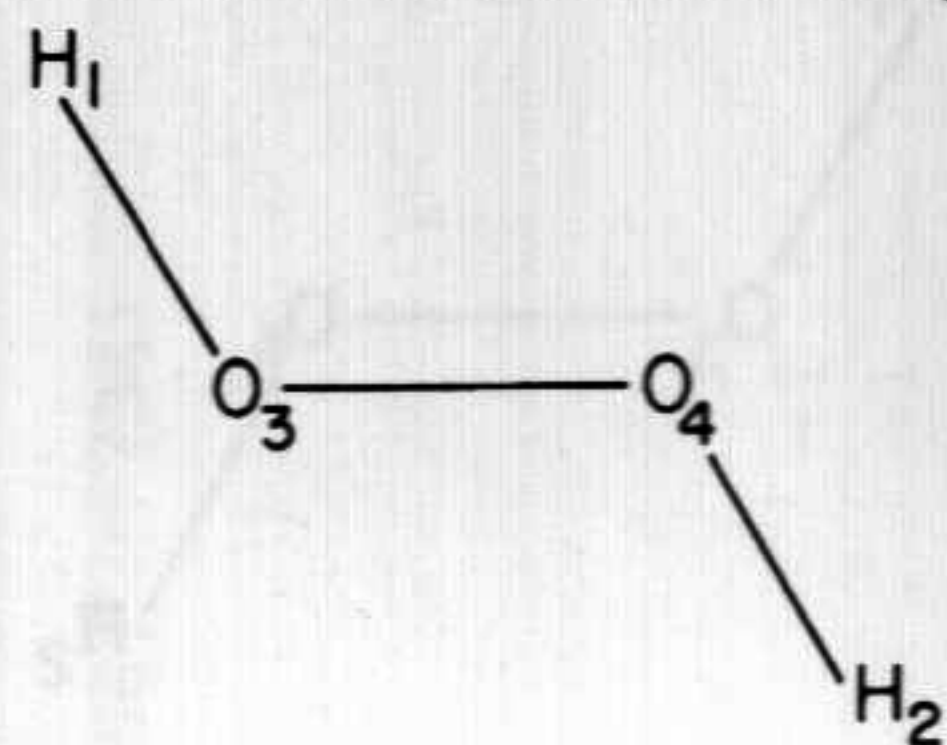
Example: Carbon dioxide



$D_{\infty h}$ (EM):	E_0	E_ϵ	∞E_ϵ^*	$(12)_\pi^*$	$(12)_{\pi+\epsilon}^*$	\dots	$\infty(12)_\epsilon$
	1	2	∞	1	2	\dots	∞
$D_{\infty h}$:	E	$2C_{\infty}^\epsilon$	\dots	i	$2S_{\infty}^{\pi+\epsilon}$	\dots	$\infty C_2^{(\epsilon/2)}$
Equiv. rot.:	R^0	R_z^-	\dots	R^0	R_z^-	\dots	$R_{\epsilon/2}^\pi$
$(+s)\Sigma_g^+$:	1	1	\dots	1	1	\dots	$\alpha_{xx} + \alpha_{yy}, \alpha_{zz}$
$(+a)\Sigma_u^+$:	1	1	\dots	-1	-1	\dots	T_z
$(-a)\Sigma_g^-$:	1	1	\dots	1	1	\dots	\hat{J}_z
$(-s)\Sigma_u^-$:	1	1	\dots	-1	-1	\dots	Γ^*
Π_g :	2	$2\cos\epsilon$	\dots	2	$2\cos\epsilon$	\dots	$(\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$
Π_u :	2	$2\cos\epsilon$	\dots	-2	$-2\cos\epsilon$	\dots	(T_x, T_y)
Δ_g :	2	$2\cos 2\epsilon$	\dots	2	$2\cos 2\epsilon$	\dots	$(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
Δ_u :	2	$2\cos 2\epsilon$	\dots	-2	$-2\cos 2\epsilon$	\dots	
\vdots	\vdots	\vdots	\dots	\vdots	\vdots	\dots	\vdots
\vdots	\vdots	\vdots	\dots	\vdots	\vdots	\dots	\vdots

^a The xyz axes are the $x'y'z'$ axes introduced in Chapter 17 for the isomorphic Hamiltonian.

Table A-21
The group G_4
Example: Hydrogen peroxide
(with torsional tunneling)



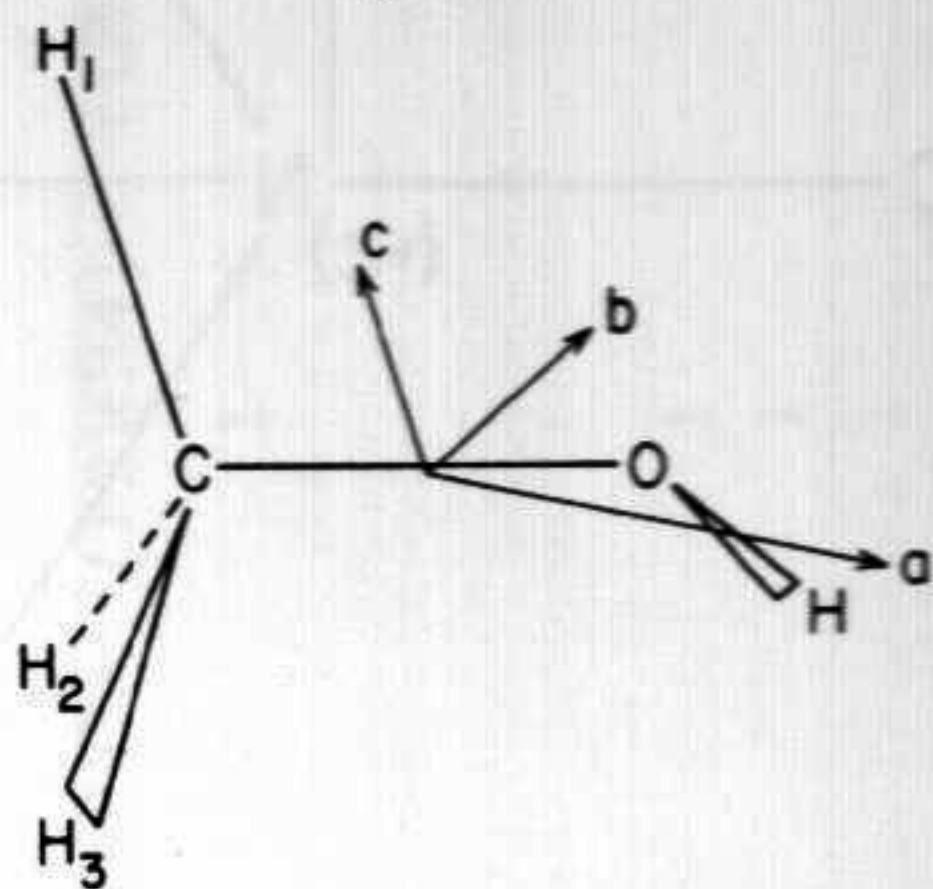
Γ_1^a	Γ_2^b	$G_4 :$ $\Gamma_3^c :$	E	$(12)(34)$	E^*	$(12)(34)^*$	
			1	1	1	1	
A^+	A_g	$A_1 :$	1	1	1	1	
A^-	A_u	$A_2 :$	1	1	-1	-1	Γ^*
B^-	B_g	$B_1 :$	1	-1	-1	1	
B^+	B_u	$B_2 :$	1	-1	1	-1	

^a Γ_1 notation based on effects of $(12)(34)$ and E^* .

^b Γ_2 notation based on C_{2h} notation.

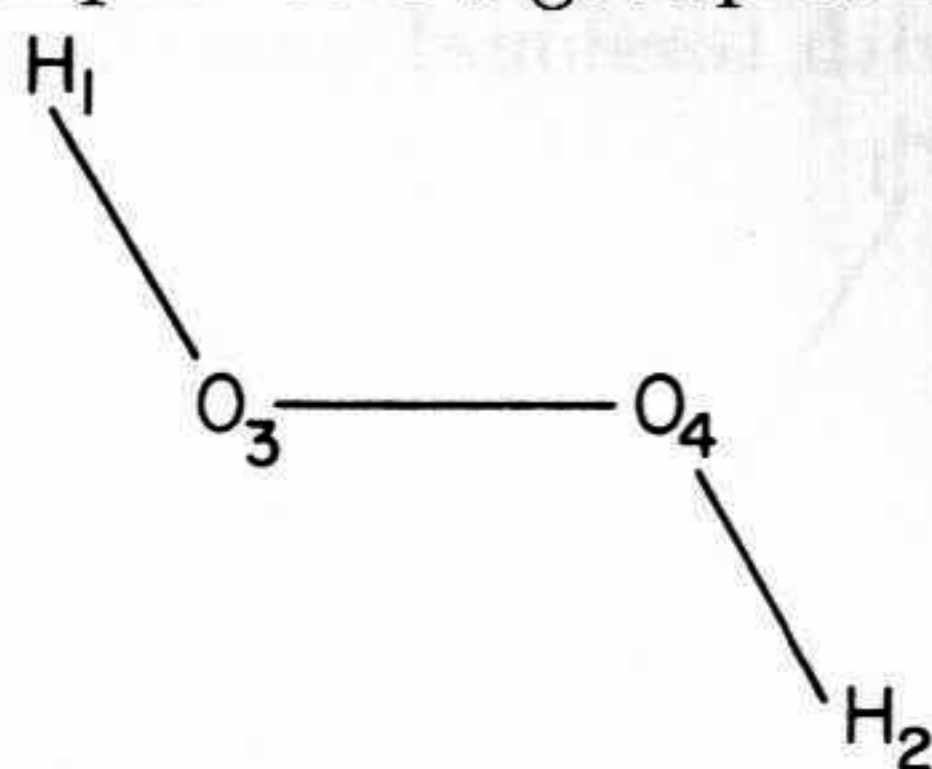
^c Γ_3 notation based on C_{2v} notation.

Table A-22
The group G_6
Example: Methanol (with torsional tunneling)



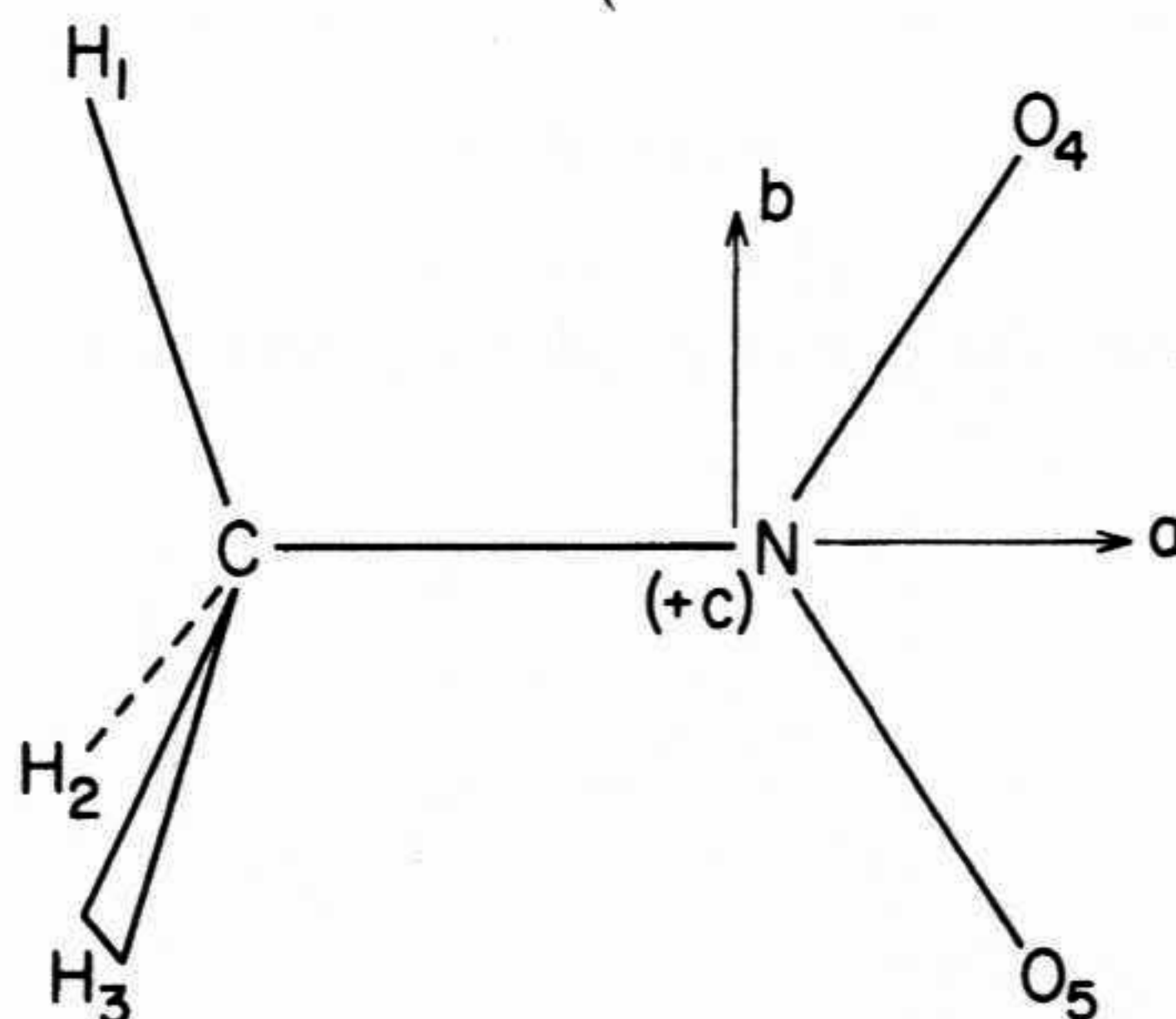
$G_6 :$	E	(123)	$(23)^*$	
	1	2	3	
Equiv. rot.:	R^0	R^0	R_c^π	
$A_1 :$	1	1	1	$T_a, T_b, \hat{J}_c, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}, \alpha_{ab}$
$A_2 :$	1	1	-1	$T_c, \hat{J}_a, \hat{J}_b, \hat{J}_\rho, \alpha_{ac}, \alpha_{bc}, \Gamma^*$
$E :$	2	-1	0	

Table A-23
The group G_8
Example: CNPI group of H_2O_2



G_8 :	E	$(12)(34)$	E^*	$(12)(34)^*$	(12)	(34)	$(12)^*$	$(34)^*$	
A_1'	1	1	1	1	1	1	1	1	
A_1''	1	1	1	1	-1	-1	-1	-1	
A_2'	1	1	-1	-1	1	1	-1	-1	Γ^*
A_2''	1	1	-1	-1	-1	-1	1	1	
B_1'	1	-1	-1	1	1	-1	-1	1	
B_1''	1	-1	-1	1	-1	1	1	-1	
B_2'	1	-1	1	-1	1	-1	1	-1	
B_2''	1	-1	1	-1	-1	1	-1	1	

Table A-24
The group G_{12}
Example: Nitromethane (with torsional tunneling)

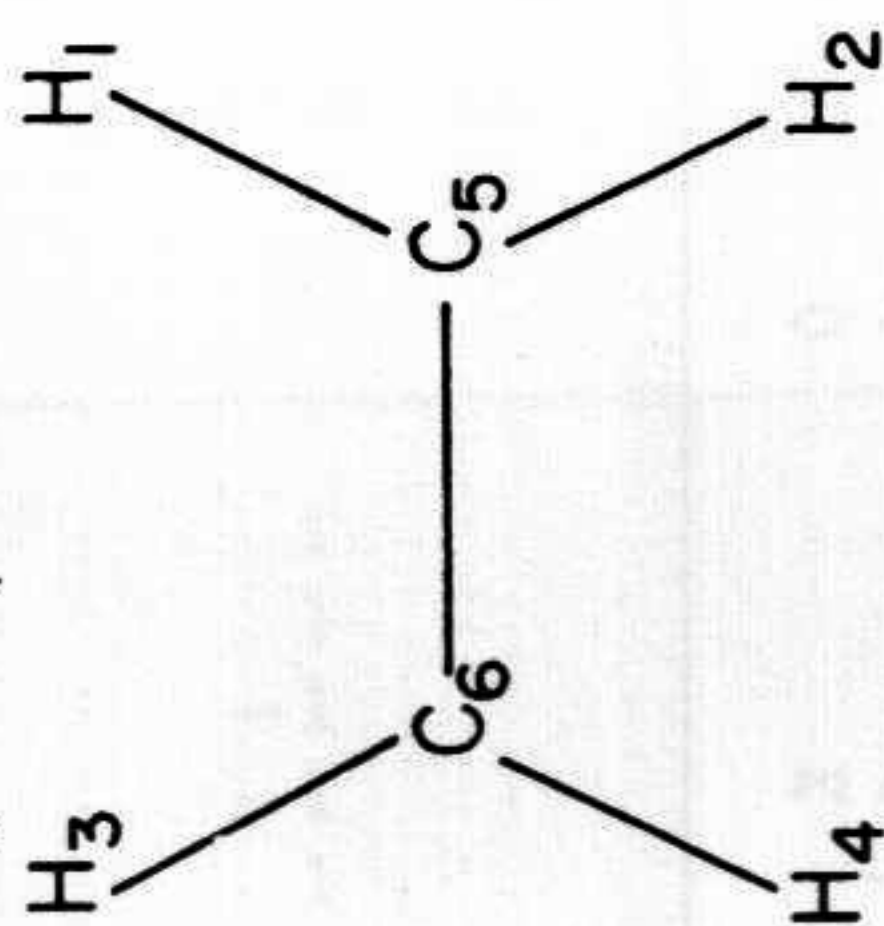


G_{12} :	E	(123)	$(23)^*$	(45)	$(123)(45)$	$(23)(45)^*$	
	1	2	3	1	2	3	
Equiv. rot.:	R^0	R^0	R_c^π	R_a^π	R_a^π	R_b^π	
A_1'	1	1	1	1	1	1	$T_a, \alpha_{aa}, \alpha_{bb}, \alpha_{cc}$
A_1''	1	1	1	-1	-1	-1	$T_b, \hat{J}_c, \alpha_{ab}$
A_2'	1	1	-1	1	1	-1	$\hat{J}_a, \hat{J}_\rho, \alpha_{bc}, \Gamma^*$
A_2''	1	1	-1	-1	-1	1	$T_c, \hat{J}_b, \alpha_{ac}$
E'	2	-1	0	2	-1	0	
E''	2	-1	0	-2	1	0	

Table A-25

The group G_{16}

Example: Ethylene (with torsional tunneling)



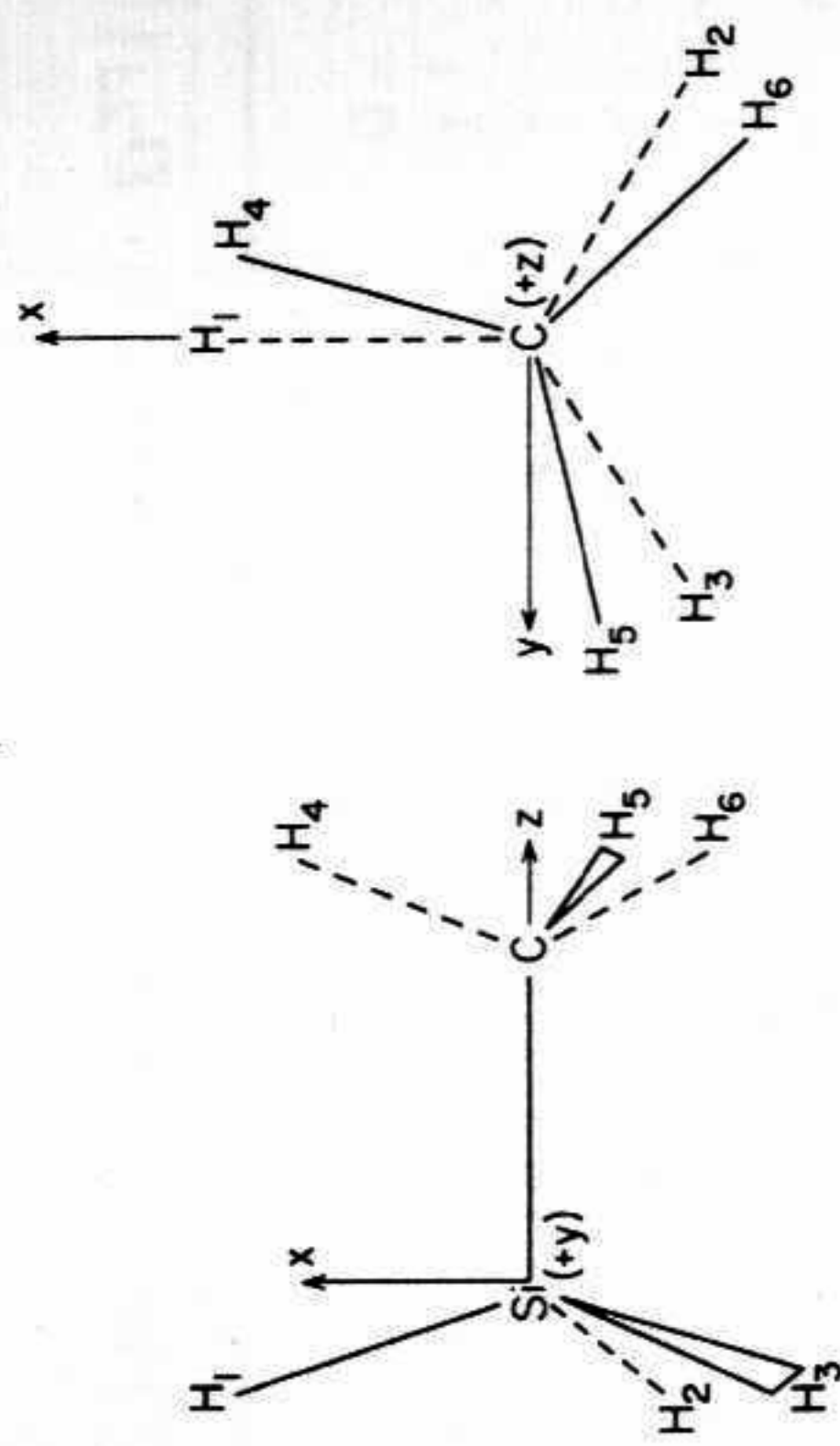
		E	(1423)(56)*	(12)(34)	(13)(24)(56)	(34)*	E^*	(1423)(56)	(12)(34)*	(13)(24)(56)*	(34)	
G_{16}	:	1	2	1	2	2	1	2	1	2	2	
MW ^c	LH ^b											
A_1^+	:	1	1	1	1	1	1	1	1	1	1	
A_2^+	:	1	1	-1	-1	-1	1	1	1	-1	-1	
B_1^+	:	1	-1	1	1	-1	1	-1	1	1	-1	
B_2^+	:	1	-1	1	-1	1	1	-1	1	-1	1	
E^+	:	2	0	-2	0	0	2	0	-2	0	0	
A_1^-	:	1	1	1	1	1	-1	-1	-1	-1	-1	
A_2^-	:	1	1	-1	-1	-1	-1	-1	-1	-1	-1	
B_1^-	:	1	-1	1	1	-1	-1	1	-1	-1	1	
B_2^-	:	1	-1	1	-1	1	-1	1	-1	1	-1	
E^-	:	2	0	-2	0	0	-2	0	2	0	0	
											Γ^*	

^aNotation from Merer and Watson (1973). This correlates appropriately to $D_{2d}(M)$ (see Table A-12).^bNotation from Longuet-Higgins (1963).

Table A-26

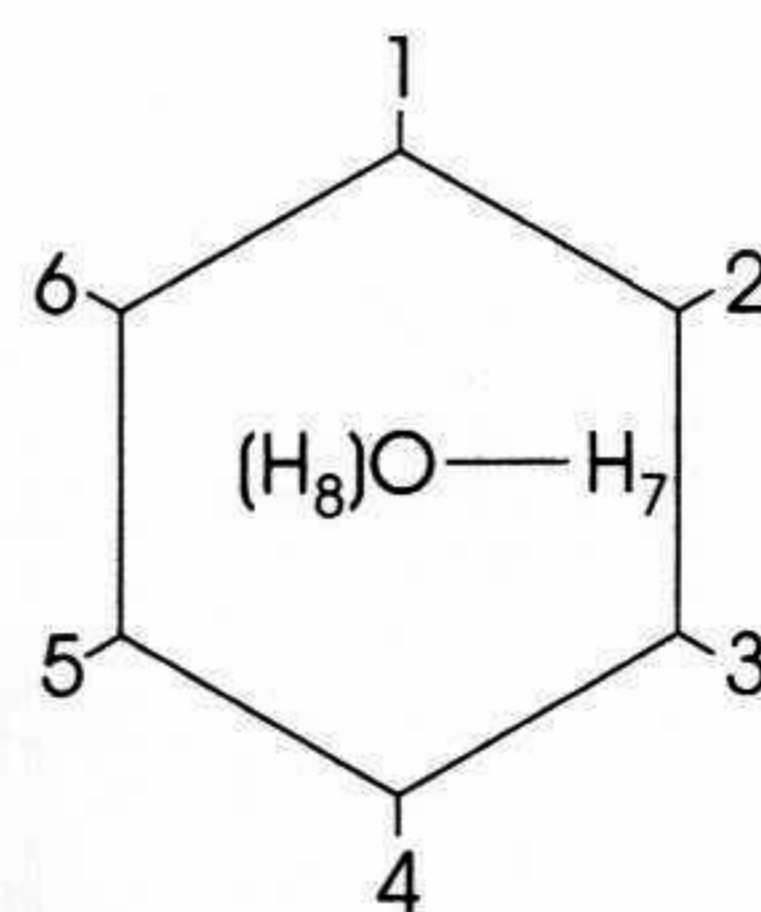
The group G_{18}

Example: Methylsilane (with torsional tunneling)



G_{18}	E	(456)	(123)	$(123)(456)$	$(123)(465)$	$(23)(56)^*$
	1	2	2	2	2	9
Equiv. rot.:	R^0	R^0	$R_z^{2\pi/3}$	$R_z^{2\pi/3}$	$R_z^{2\pi/3}$	$R_{\pi/2}^{\pi}$
A_1 :	1	1	1	1	1	$T_z, \alpha_{zz}, \alpha_{xx} + \alpha_{yy}$
A_2 :	1	1	1	1	1	$\hat{J}_z, \hat{J}_\rho, \Gamma^*$
E_1 :	2	2	-1	-1	0	$(T_x, T_y), (\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz}), (\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
E_2 :	2	-1	2	-1	0	
E_3 :	2	-1	-1	-1	0	
E_4 :	2	-1	-1	2	0	

Table A-27
 The group G_{24}
 Example: Benzene-water dimer^a
 (The water moiety is above the benzene ring
 and we assume that (123456) and (78) are
 feasible; see page 49).

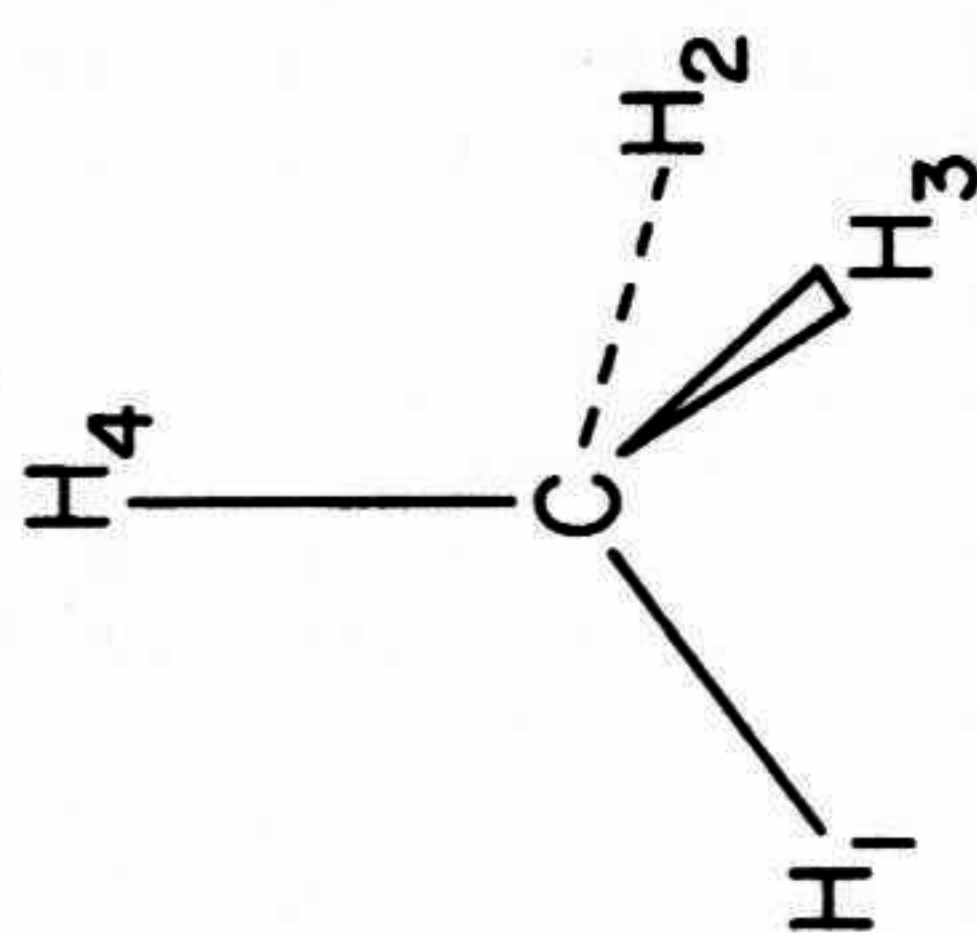


	E	(123456)	(135)(246)	(14)(25)(36)	(26)(35)*	(14)(23)(56)*
G_{24} :	1	2	2	1	3	3
A_{1s} :	1	1	1	1	1	1
A_{2s} :	1	1	1	1	-1	-1
B_{1s} :	1	-1	1	-1	1	-1
B_{2s} :	1	-1	1	-1	-1	1
E_{1s} :	2	1	-1	-2	0	0
E_{2s} :	2	-1	-1	2	0	0
A_{1a} :	1	1	1	1	1	1
A_{2a} :	1	1	1	1	-1	-1
B_{1a} :	1	-1	1	-1	1	-1
B_{2a} :	1	-1	1	-1	-1	1
E_{1a} :	2	1	-1	-2	0	0
E_{2a} :	2	-1	-1	2	0	0
	(78)	(123456)(78)	(135)(246)(78)	(14)(25)(36)(78)	(26)(35)(78)*	(14)(23)(56)(78)*
	1	2	2	1	3	3
	1	1	1	1	1	1
	1	1	1	1	-1	-1
	1	-1	1	-1	1	-1
	1	-1	1	-1	-1	1
	2	1	-1	-2	0	0
	2	-1	-1	2	0	0
	-1	-1	-1	-1	-1	-1
	-1	-1	-1	-1	1	1
	-1	1	-1	1	-1	1
	-1	1	-1	1	1	-1
	-2	-1	1	2	0	0
	-2	1	1	-2	0	0

: Γ^*

^aSee Table 9 of Gregory and Clary (1996), but we use s/a instead of +/-, and we exchange B_1 and B_2 labels (see Table A-7). Pairs of bonded CH nuclei are labeled 1 through 6.

Table A-29

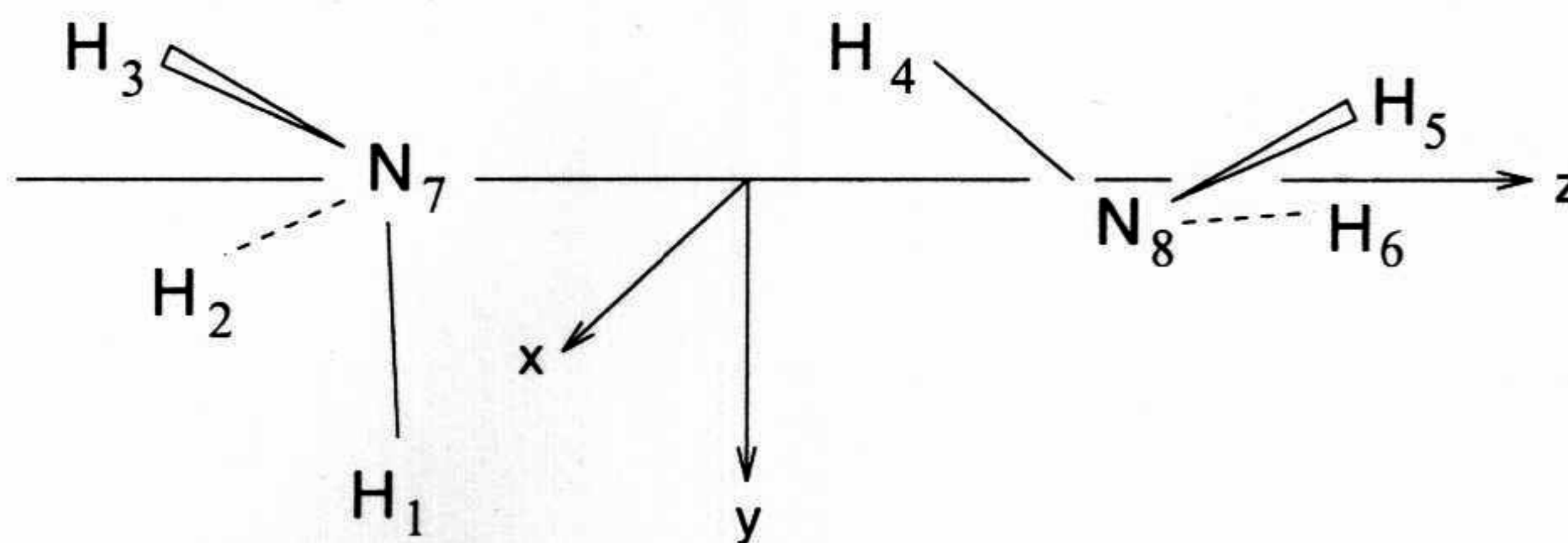
The group G_{48} Example: CNPI group of CH_4 

G_{48}	E	(123)	(14)(23)	(1423)*	(23)*	E^*	(123)*	(14)(23)*	(1423)	(23)
	1	8	3	6	6	1	8	3	6	6
A_1^+	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	2	0	0	2	-1	2	0	0
F_1^+	3	0	-1	1	-1	3	0	-1	1	-1
F_2^+	3	0	-1	-1	1	3	0	-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
E^-	2	-1	2	0	0	-2	1	-2	0	0
F_1^-	3	0	-1	1	-1	-3	0	1	-1	1
F_2^-	3	0	-1	-1	1	-3	0	1	1	-1
										Γ^*

Table A-30

The group G_{144}

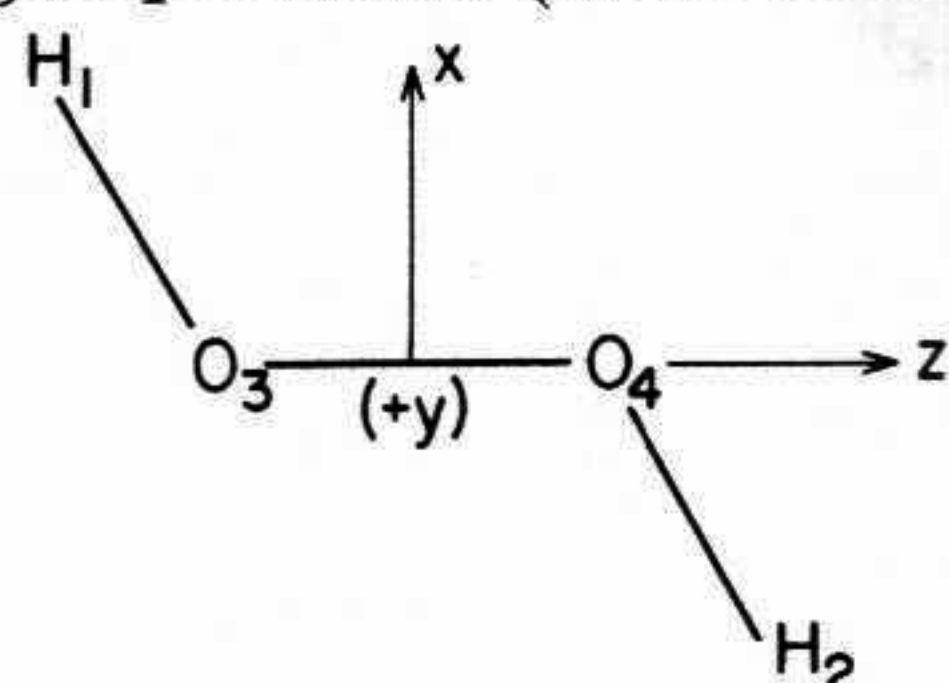
Example: Ammonia dimer (with moiety inversion)



G_{144} :	E	(12)	$(12)(45)$	(123)	$(14)(25)(36)(78)$	$(12)(456)$	$(123)(456)$	$(14)(2536)(78)$	$(142536)(78)$	E^*	$(12)^*$	$(12)(45)^*$	$(123)^*$	$(14)(25)(36)(78)^*$	$(12)(456)^*$	$(123)(456)^*$	$(14)(2536)(78)^*$	$(142536)(78)^*$
	1	6	9	4	6	12	4	18	12	1	6	9	4	6	12	4	18	12
A_1^+	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2^+	1	-1	1	1	-1	-1	1	1	-1	1	-1	1	1	-1	-1	1	1	-1
B_1^+	1	1	1	1	-1	1	1	-1	-1	1	1	1	1	-1	1	1	-1	-1
B_2^+	1	-1	1	1	1	-1	1	-1	1	1	-1	1	1	1	-1	1	-1	1
E^+	2	0	-2	2	0	0	2	0	0	2	0	-2	2	0	0	2	0	0
G_1^+	4	2	0	1	0	-1	-2	0	0	4	2	0	1	0	-1	-2	0	0
G_2^+	4	-2	0	1	0	1	-2	0	0	4	-2	0	1	0	1	-2	0	0
G_3^+	4	0	0	-2	-2	0	1	0	1	4	0	0	-2	-2	0	1	0	1
G_4^+	4	0	0	-2	2	0	1	0	-1	4	0	0	-2	2	0	1	0	-1
A_1^-	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1
A_2^-	1	-1	1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	-1	-1	1
B_1^-	1	1	1	1	-1	1	1	-1	-1	-1	-1	-1	-1	1	-1	-1	1	1
B_2^-	1	-1	1	1	1	-1	1	-1	1	-1	1	-1	-1	-1	1	-1	1	-1
E^-	2	0	-2	2	0	0	2	0	0	-2	0	2	-2	0	0	-2	0	0
G_1^-	4	2	0	1	0	-1	-2	0	0	-4	-2	0	-1	0	1	2	0	0
G_2^-	4	-2	0	1	0	1	-2	0	0	-4	2	0	-1	0	-1	2	0	0
G_3^-	4	0	0	-2	-2	0	1	0	1	-4	0	0	2	2	0	-1	0	-1
G_4^-	4	0	0	-2	2	0	1	0	-1	-4	0	0	2	-2	0	-1	0	1

The labeling of the irreducible representations is as given by Odutola, Dyke, Howard, and Muenter (1979).

Table A-31
 The group $G_4(EM)$
 Example: Hydrogen peroxide (with torsional tunneling)^{a,b}



$G_4(EM)$:	E	a	b	ab	E'	$E'a$	$E'b$	$E'ab$	
Equiv. rot.:	R^0	$R_{\pi/2}^\pi$	R_{π}^π	R_z^π	R_z^π	R_{π}^π	$R_{3\pi/2}^\pi$	R^0	
A_{gs} :	1	1	1	1	1	1	1	1	: $\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
A_{us} :	1	1	-1	-1	1	1	-1	-1	: \hat{J}_ρ, Γ^*
B_{gs} :	1	-1	-1	1	1	-1	-1	1	: \hat{J}_z, α_{xy}
B_{us} :	1	-1	1	-1	1	-1	1	-1	: T_z
A_{gd} :	1	1	-1	-1	-1	-1	1	1	: \hat{J}_y, α_{xz}
A_{ud} :	1	1	1	1	-1	-1	-1	-1	: T_y
B_{gd} :	1	-1	1	-1	-1	1	-1	1	: \hat{J}_x, α_{yz}
B_{ud} :	1	-1	-1	1	-1	1	1	-1	: T_x

^aFor space fixed coordinates $a = (12)(34)$, $b = E^*$ and $E' = E$. See page 525.

^bFor the definitions of the Euler angle transformations see Table 15-11.

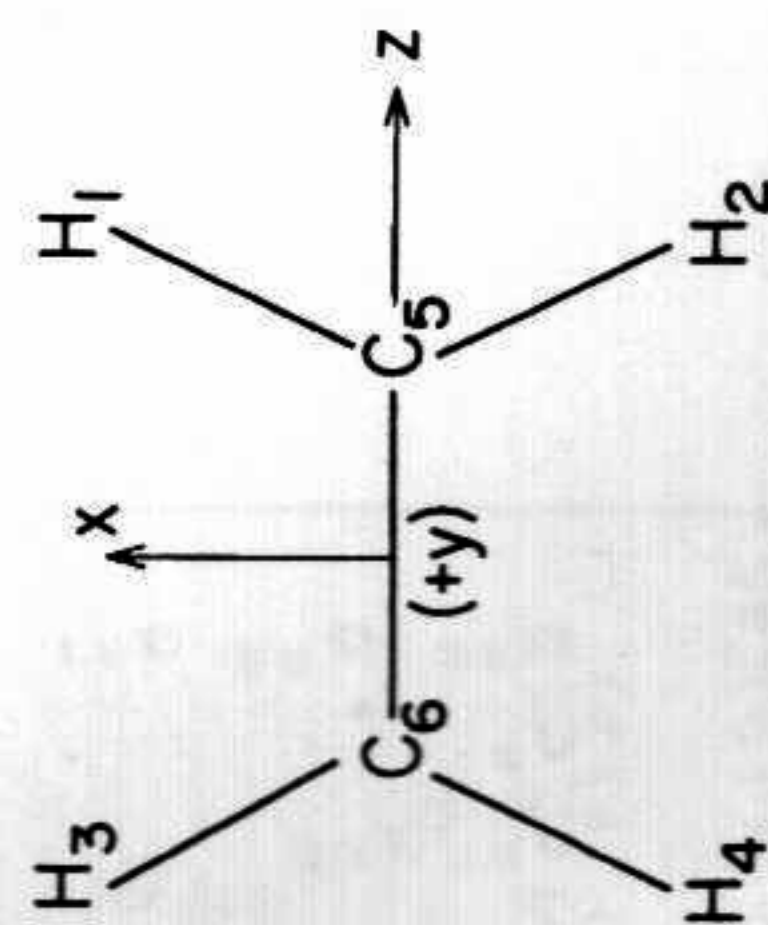


Table A-32

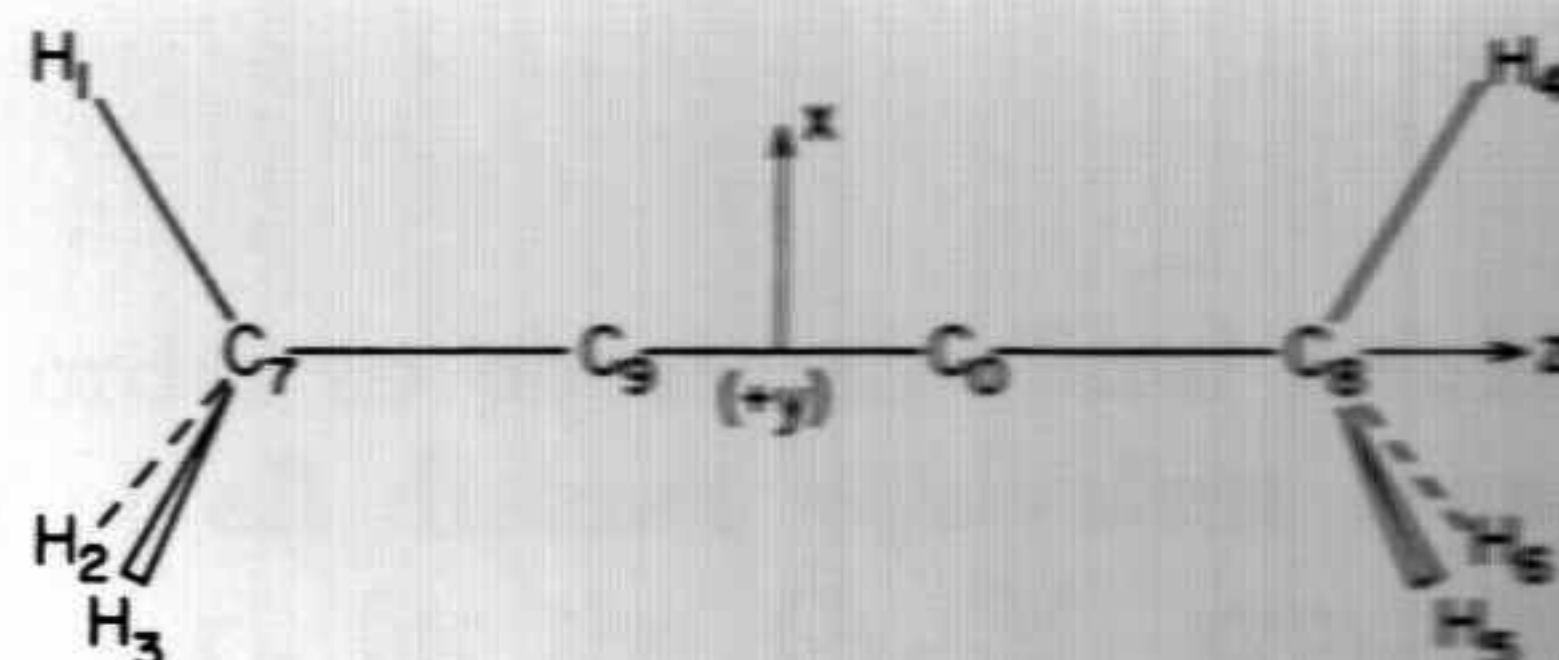
The group G_{16} (EM)Example: Ethylene (with torsional tunneling)^{a,b}

G_{16} (EM):	E	a	a^2	b	ab	c	ac	a^2c	bc	abc	E'	a^2E'	bE'	bcE'
	1	4	1	2	4	2	4	2	2	4	1	1	2	2
Equiv. rot.:	R^0	R_z^π	R_z^π	R_π^π	$R_{3\pi/4}^\pi$	R_π^π	$R_{3\pi/4}^\pi$	$R_{\pi/2}^\pi$	R^0	$R_z^{5\pi/2}$	R_z^π	$R^{2\pi}$	$R_{3\pi/2}^\pi$	R_z^π
A_{1g}^+	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_{1g}^+	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^+	2	0	-2	0	0	2	0	-2	0	0	2	-2	0	0
A_{1u}^-	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_{1u}^-	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^-	2	0	-2	0	0	-2	0	2	0	0	2	-2	0	0
E_1	2	0	2	2	0	0	0	0	0	0	-2	-2	-2	0
E_2	2	0	2	-2	0	0	0	0	0	0	-2	-2	2	0
E_g	2	0	-2	0	0	0	0	0	2	0	-2	2	0	-2
E_u	2	0	-2	0	0	0	0	0	-2	0	-2	2	0	2

$\alpha_{zz}, (\alpha_{xx} + \alpha_{yy})$
 $(\alpha_{xx} - \alpha_{yy})$
 T_z
 J_z
 Γ^*, J_ρ
 α_{xy}
 $(J_x, J_y), (\alpha_{xz}, \alpha_{yz})$
 (T_x, T_y)

^aFor space fixed coordinates $a = (1423)(56)^*$, $b = (13)(24)(56)$, $c = E^*$, and $E' = E$. See page 531.^bFor the definitions of the Euler angle transformations see Table 15-16.

Table A-33
 The group $G_{36}(\text{EM})$
 Example: Dimethylacetylene (with torsional tunneling)^{a,b}



$G_{36}(\text{EM})$:	E	ab	c	ab^5	a^4	b^2c	cd	b^4cd	d
	1	2	3	2	4	6	3	6	9
Equiv. rot.:	R^0	R^0	R_z^π	$R_z^{2\pi/3}$	$R_z^{4\pi/3}$	$R_z^{\pi/3}$	R_0^π	$R_{2\pi/3}^\pi$	$R_{\pi/2}^\pi$
A_{1s} :	1	1	1	1	1	1	1	1	1
A_{2s} :	1	1	1	1	1	1	-1	-1	-1
A_{3s} :	1	1	-1	1	1	-1	1	1	-1
A_{4s} :	1	1	-1	1	1	-1	-1	-1	1
E_{1s} :	2	2	2	-1	-1	-1	0	0	0
E_{2s} :	2	2	-2	-1	-1	1	0	0	0
E_{3s} :	2	-1	0	2	-1	0	2	-1	0
E_{4s} :	2	-1	0	2	-1	0	-2	1	0
G_s :	4	-2	0	-2	1	0	0	0	0
A_{1d} :	1	1	1	1	1	1	1	1	1
A_{2d} :	1	1	1	1	1	1	-1	-1	-1
A_{3d} :	1	1	-1	1	1	-1	1	1	-1
A_{4d} :	1	1	-1	1	1	-1	-1	-1	1
E_{1d} :	2	2	2	-1	-1	-1	0	0	0
E_{2d} :	2	2	-2	-1	-1	1	0	0	0
E_{3d} :	2	-1	0	2	-1	0	2	-1	0
E_{4d} :	2	-1	0	2	-1	0	-2	1	0
G_d :	4	-2	0	-2	1	0	0	0	0

E'	$E'ab$	$E'c$	$E'ab^5$	$E'a^4$	$E'b^2c$	$E'cd$	$E'b^4cd$	$E'd$	
1	2	3	2	4	6	3	6	9	
R_z^π	R_z^π	R^0	$R_z^{5\pi/3}$	$R_z^{\pi/3}$	$R_z^{4\pi/3}$	$R_{\pi/2}^\pi$	$R_{\pi/6}^\pi$	R_0^π	
1	1	1	1	1	1	1	1	1	: $(\alpha_{xx} + \alpha_{yy}), \alpha_{zz}$
1	1	1	1	1	1	-1	-1	-1	: \hat{J}_z
1	1	-1	1	1	-1	1	1	-1	: \hat{J}_ρ, Γ^*
1	1	-1	1	1	-1	-1	-1	1	: T_z
2	2	2	-1	-1	-1	0	0	0	: $(\alpha_{xx} - \alpha_{yy}, \alpha_{xy})$
2	2	-2	-1	-1	1	0	0	0	
2	-1	0	2	-1	0	2	-1	0	
2	-1	0	2	-1	0	-2	1	0	
4	-2	0	-2	1	0	0	0	0	
-1	-1	-1	-1	-1	-1	-1	-1	-1	
-1	-1	-1	-1	-1	-1	1	1	1	
-1	-1	1	-1	-1	1	-1	-1	1	
-1	-1	1	-1	-1	1	1	1	-1	
-2	-2	-2	1	1	1	0	0	0	: (T_x, T_y)
-2	-2	2	1	1	-1	0	0	0	: $(\hat{J}_x, \hat{J}_y), (\alpha_{xz}, \alpha_{yz})$
-2	1	0	-2	1	0	-2	1	0	
-2	1	0	-2	1	0	2	-1	0	
-4	2	0	2	-1	0	0	0	0	

^aFor space fixed coordinates $a = (123), b = (456), c = (14)(26)(35)(78)(90)^*, d = (23)(56)^*$, and $E' = E$. See page 520.

^bFor the definitions of the Euler angle transformations see Table 15-8.

APPENDIX *B*

The Correlation Tables

In this Appendix there are four types of correlation table.

In Table B-1 the representations $D^{(0)}$ through $D^{(3)}$ of the spin double group of the three-dimensional molecular rotational group $\mathbf{K}(\text{mol})^2$ are reduced onto the molecular rotation groups \mathbf{D}_∞^2 and \mathbf{D}_2^2 . The rotational states of a spherical top molecule can be labeled $D^{(J)}$ in $\mathbf{K}(\text{mol})^2$ according to the value of J . The rotational states of a symmetric top molecule can be labeled Σ^+ (or Σ^-), Π , Δ , . . . , in \mathbf{D}_∞^2 as $K = 0$ with J even (or $K = 0$ with J odd), $K = 1$, $K = 2$, . . . , respectively, and the rotational states of an asymmetric top molecule can be labeled A , B_a , B_b , and B_c in \mathbf{D}_2^2 as $K_a K_c$ is ee , eo , oo , and oe ($o = \text{odd}$ and $e = \text{even}$). Tables 12-15 and 12-16 were used in these reductions.

In Table B-2 the representations $D^{(0)}$ through $D^{(3)}$ of $\mathbf{K}(\text{mol})^2$ are reduced onto the representations of groups given in Appendices 18-1 and **A** by using the equivalent rotations of the elements of the group. We first reduce $\mathbf{K}(\text{mol})$ onto the equivalent rotation group of the MS (or EMS) group, and then make use of the isomorphism or homomorphism of the MS (or EMS)

group onto the equivalent rotation group in order to obtain the final result. The equivalent rotation group is the group of all distinct equivalent rotations of the MS (or EMS) group concerned; e.g., for the $C_{3v}(M)$ group it is $D_3 = \{E, R_z^{2\pi/3}, R_z^{4\pi/3}, R_{\pi/6}^\pi, R_{\pi/2}^\pi, R_{5\pi/6}^\pi\}$. From this table the symmetry Γ_{rot} of the rotational states with $J \leq 3$ of each molecule in its MS (or EMS) group can be obtained. The species of Hund's case (a) electron spin functions in these groups can be obtained from this table by identifying the representations of $K(\text{mol})^2$ with $D^{(S)}$.

In Table B-3 the correlations of the representations of the molecular point groups of bent and linear molecules are given for use in determining the correlation of the symmetry of the electronic states of a linear triatomic molecule with those obtained by bending the molecule.

In Table B-4 reverse correlation tables, with statistical weights, are given for some common nonrigid molecules. For a rigid methanol molecule the $C_s(M)$ group is $\{E, (23)^*\}$ if we take the rigid conformer as having O-C-H₁ coplanar with the C-O-H group. For a rigid methyl silane molecule the $C_{3v}(M)$ group of a conformer is $\{E, (123)(465), (132)(456), (12)(46)^*, (13)(45)^*, (23)(56)^*\}$ regardless of whether it is eclipsed or staggered. For a rigid acetone molecule in the conformation indicated in Table A-28 the $C_{2v}(M)$ group is $\{E, (14)(25)(36)(78), (23)(56)^*, (14)(26)(35)(78)^*\}$. The results in Table B-4 are of use when the tunneling splitting are small, and the statistical weights should help in the assignments of the states.

Table B-1

The correlation table of $K(\text{mol})^2$ with the molecular rotational groups D_∞^2 and D_2^2

$K(\text{mol})^2$	D_∞^2	D_2^2
$D^{(0)}$	Σ^+	A
$D^{(1/2)}$	$E_{1/2}$	$E_{1/2}$
$D^{(1)}$	$\Sigma^- \oplus \Pi$	$B_a \oplus B_b \oplus B_c$
$D^{(3/2)}$	$E_{1/2} \oplus E_{3/2}$	$2E_{1/2}$
$D^{(2)}$	$\Sigma^+ \oplus \Pi \oplus \Delta$	$2A \oplus B_a \oplus B_b \oplus B_c$
$D^{(5/2)}$	$E_{1/2} \oplus E_{3/2} \oplus E_{5/2}$	$3E_{1/2}$
$D^{(3)}$	$\Sigma^- \oplus \Pi \oplus \Delta \oplus \Phi$	$A \oplus 2B_a \oplus 2B_b \oplus 2B_c$

Table B-2

The correlation of $\mathbf{K}(\text{mol})^2$ with the spin double groups of MS and EMS groups

(i) Asymmetric top molecules

$\mathbf{K}(\text{mol})^2$	$C_s(\text{M})^2$	$C_1(\text{M})^2$	$C_2(\text{M})^2$	$C_{2v}(\text{M})^2$	$C_{2h}(\text{M})^2$	$D_{2h}(\text{M})^2$
$D^{(0)}$	A'	A_g	A	A_1	A_g	A_g
$D^{(1/2)}$	$E_{1/2}$	$E_{g/2}$	$E_{1/2}$	$E_{1/2}$	$E_{g/2}$	$E_{g/2}$
$D^{(1)}$	$A' \oplus 2A''$	$3A_g$	$A \oplus 2B$	$A_2 \oplus B_1 \oplus B_2$	$A_g \oplus 2B_g$	$B_{1g} \oplus B_{2g} \oplus B_{3g}$
$D^{(3/2)}$	$2E_{1/2}$	$2E_{g/2}$	$2E_{1/2}$	$2E_{1/2}$	$2E_{g/2}$	$2E_{g/2}$
$D^{(2)}$	$3A' \oplus 2A''$	$5A_g$	$3A \oplus 2B$	$2A_1 \oplus A_2 \oplus B_1 \oplus B_2$	$3A_g \oplus 2B_g$	$2A_g \oplus B_{1g} \oplus B_{2g} \oplus B_{3g}$
$D^{(5/2)}$	$3E_{1/2}$	$3E_{g/2}$	$3E_{1/2}$	$3E_{1/2}$	$3E_{g/2}$	$3E_{g/2}$
$D^{(3)}$	$3A' \oplus 4A''$	$7A_g$	$3A \oplus 4B$	$A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2$	$3A_g \oplus 4B_g$	$A_g \oplus 2B_{1g} \oplus 2B_{2g} \oplus 2B_{3g}$

Table B-2 continued
(ii) Symmetric top, spherical top, and linear molecules

$K(\text{mol})^2$	$D_{2d}(\text{M})^2$	$C_{3v}(\text{M})^2$	$D_{3h}(\text{M})^2$	$D_{3d}(\text{M})^2$
$D^{(0)}$	A_1	A_1	A_1'	A_{1g}
$D^{(1/2)}$	$E_{1/2}$	$E_{1/2}$	$E_{1/2}$	$E_{g/2}$
$D^{(1)}$	$A_2 \oplus E$	$A_2 \oplus E$	$A_2' \oplus E''$	$A_{2g} \oplus E_g$
$D^{(3/2)}$	$E_{1/2} \oplus E_{3/2}$	$E_{1/2} \oplus E_{3/2}$	$E_{1/2} \oplus E_{3/2}$	$E_{g/2} \oplus E_{3g/2}$
$D^{(2)}$	$A_1 \oplus B_1 \oplus B_2 \oplus E$	$A_1 \oplus 2E$	$A_1' \oplus E' \oplus E''$	$A_{1g} \oplus 2E_g$
$D^{(5/2)}$	$E_{1/2} \oplus 2E_{3/2}$	$2E_{1/2} \oplus E_{3/2}$	$E_{1/2} \oplus E_{3/2} \oplus E_{5/2}$	$2E_{g/2} \oplus E_{3g/2}$
$D^{(3)}$	$A_2 \oplus B_1 \oplus B_2 \oplus 2E$	$A_1 \oplus 2A_2 \oplus 2E$	$A_1'' \oplus A_2' \oplus A_2''$ $\oplus E' \oplus E''$	$A_{1g} \oplus 2A_{2g} \oplus 2E_g$

$K(\text{mol})^2$	$T_d(\text{M})^2$	$O_h(\text{M})^2$	$I_h(\text{M})^2$
$D^{(0)}$	A_1	A_{1g}	A_g
$D^{(1/2)}$	$E_{1/2}$	$E_{1g/2}$	$E_{1g/2}$
$D^{(1)}$	F_1	F_{1g}	F_{1g}
$D^{(3/2)}$	$G_{3/2}$	$G_{3g/2}$	$G_{3g/2}$
$D^{(2)}$	$E \oplus F_2$	$E_g \oplus F_{2g}$	H_g
$D^{(5/2)}$	$G_{3/2} \oplus E_{5/2}$	$G_{3g/2} \oplus E_{5g/2}$	$I_{5g/2}$
$D^{(3)}$	$A_2 \oplus F_1 \oplus F_2$	$A_{2g} \oplus F_{1g} \oplus F_{2g}$	$F_{2g} \oplus G_g$

$K(\text{mol})^2$	$C_{\infty v}(\text{EM})^2$	$D_{\infty h}(\text{EM})^2$
$D^{(0)}$	Σ^+	Σ_g^+
$D^{(1/2)}$	$E_{1/2}$	$E_{g/2}$
$D^{(1)}$	$\Sigma^- \oplus \Pi$	$\Sigma_g^- \oplus \Pi_g$
$D^{(3/2)}$	$E_{1/2} \oplus E_{3/2}$	$E_{g/2} \oplus E_{3g/2}$
$D^{(2)}$	$\Sigma^+ \oplus \Pi \oplus \Delta$	$\Sigma_g^+ \oplus \Pi_g \oplus \Delta_g$
$D^{(5/2)}$	$E_{1/2} \oplus E_{3/2} \oplus E_{5/2}$	$E_{g/2} \oplus E_{3g/2} \oplus E_{5g/2}$
$D^{(3)}$	$\Sigma^- \oplus \Pi \oplus \Delta \oplus \Phi$	$\Sigma_g^- \oplus \Pi_g \oplus \Delta_g \oplus \Phi_g$

Table B-2 continued
(iii) Nonrigid molecules

$K(\text{mol})^2$	G_6^2	G_{12}^2	G_{18}^2	G_{36}^2
$D^{(0)}$	A_1	A_1'	A_1	A_1
$D^{(1/2)}$	$E_{1/2}$	$E_{1/2}$	$E_{1/2}$	$E_{1/2}$
$D^{(1)}$	$A_1 \oplus 2A_2$	$A_2' \oplus A_1'' \oplus A_2''$	$A_2 \oplus E_1$	$A_2 \oplus A_3 \oplus A_4$
$D^{(3/2)}$	$2E_{1/2}$	$2E_{1/2}$	$E_{1/2} \oplus E_{3/2}$	$2E_{1/2}$
$D^{(2)}$	$3A_1 \oplus 2A_2$	$2A_1' \oplus A_2' \oplus A_1'' \oplus A_2''$	$A_1 \oplus 2E_1$	$2A_1 \oplus A_2 \oplus A_3 \oplus A_4$
$D^{(5/2)}$	$3E_{1/2}$	$3E_{1/2}$	$2E_{1/2} \oplus E_{3/2}$	$3E_{1/2}$
$D^{(3)}$	$3A_1 \oplus 4A_2$	$A_1' \oplus 2A_2' \oplus 2A_1'' \oplus 2A_2''$	$A_1 \oplus 2A_2 \oplus 2E_1$	$A_1 \oplus 2A_2 \oplus 2A_3 \oplus 2A_4$

$K(\text{mol})^2$	$G_4(\text{EM})^2$	$G_{16}(\text{EM})^2$	$G_{36}(\text{EM})^2$
$D^{(0)}$	A_1	A_1^+	A_1
$D^{(1/2)}$	$E_{g/2}$	$E_{g/2}$	$E_{1/2}$
$D^{(1)}$	$B_1 \oplus A_{2d} \oplus B_{2d}$	$A_2^- \oplus E_{3d}$	$A_2 \oplus E_{2d}$
$D^{(3/2)}$	$2E_{g/2}$	$E_{g/2} \oplus E_{3g/2}$	$E_{1/2} \oplus E_{3/2}$
$D^{(2)}$	$2A_1 \oplus B_1 \oplus A_{2d} \oplus B_{2d}$	$A_1^+ \oplus B_1^+ \oplus B_2^- \oplus E_{3d}$	$A_1 \oplus E_1 \oplus E_{2d}$
$D^{(5/2)}$	$3E_{g/2}$	$E_{g/2} \oplus 2E_{3g/2}$	$E_{1/2} \oplus E_{3/2} \oplus E_{5/2}$
$D^{(3)}$	$A_1 \oplus 2B_1 \oplus 2A_{2d} \oplus 2B_{2d}$	$A_2^- \oplus B_1^+ \oplus B_2^- \oplus 2E_{3d}$	$A_2 \oplus A_{3d} \oplus A_{4d} \oplus E_1 \oplus E_{2d}$

Table B-3

Correlation of species of electronic states of a linear triatomic molecule^a with species of electronic states obtained when molecule is bent^a

$D_{\infty h}$	C_{2v}	$C_{\infty v}$	C_s
Σ_g^+	A_1	Σ^+	A'
Σ_u^+	B_2	Σ^-	A''
Σ_g^-	B_1	Π	$A' \oplus A''$
Σ_u^-	A_2	Δ	$A' \oplus A''$
		\vdots	\vdots
Π_g	$A_2 \oplus B_2$		
Π_u	$A_1 \oplus B_1$		
Δ_g	$A_1 \oplus B_1$		
Δ_u	$A_2 \oplus B_2$		
\vdots	\vdots		

^a In $D_{\infty h}$ or $C_{\infty v}$.

^b In C_{2v} or C_s .

Table B-4

Reverse correlation Tables for nonrigid molecules with statistical weights (C = ¹²C, N = ¹⁴N, and O = ¹⁶O)

(i) NH ₃ ^a		(ii) CH ₃ OH ^b	
$C_{3v}(M)$	$D_{3h}(M)$	$C_s(M)$	G_6
$A_1(12)$	$A_1'(0) \oplus A_2''(12)$	$A'(8)$	$A_1(4) \oplus E(4)$
$A_2(12)$	$A_2'(12) \oplus A_1''(0)$	$A''(8)$	$A_2(4) \oplus E(4)$
$E(12)$	$E'(6) \oplus E''(6)$		

Table B-4 continued

(iii) SiH ₃ CH ₃ ^c		(iv) CH ₃ COCH ₃ ^d	
$C_{3v}(M)$	G_{18}	$C_{2v}(M)$	G_{36}
$A_1(24)$	$A_1(16) \oplus E_4(8)$	$A_1(28)$	$A_1(6) \oplus E_1(4) \oplus E_3(2) \oplus G(16)$
$A_2(24)$	$A_2(16) \oplus E_4(8)$	$A_2(28)$	$A_3(6) \oplus E_2(4) \oplus E_3(2) \oplus G(16)$
$E(40)$	$E_1(16) \oplus E_2(16) \oplus E_3(8)$	$B_1(36)$	$A_2(10) \oplus E_1(4) \oplus E_4(6) \oplus G(16)$
		$B_2(36)$	$A_4(10) \oplus E_2(4) \oplus E_4(6) \oplus G(16)$

(v) H₂O₂^e

$C_2(M)$	G_4	G_8
$A(2)$	$A_1(1) \oplus A_2(1)$	$A_1'(1) \oplus A_1''(0) \oplus A_2'(1) \oplus A_2''(0)$
$B(6)$	$B_1(3) \oplus B_2(3)$	$B_1'(0) \oplus B_1''(3) \oplus B_2'(0) \oplus B_2''(3)$

(vi) C₂H₄^f(vii) C₂H₆^g

$D_{2h}(M)$	G_{16}	$D_{3d}(M)$	G_{36}
$A_g(7)$	$A_1^+(1) \oplus B_1^+(6)$	$A_{1g}(8)$	$A_1(6) \oplus E_3(2)$
$A_u(7)$	$A_1^-(6) \oplus B_1^-(1)$	$A_{1u}(8)$	$A_3(6) \oplus E_3(2)$
$B_{1g}(3)$	$A_2^-(0) \oplus B_2^-(3)$	$A_{2g}(16)$	$A_2(10) \oplus E_4(6)$
$B_{1u}(3)$	$A_2^+(3) \oplus B_2^+(0)$	$A_{2u}(16)$	$A_4(10) \oplus E_4(6)$
$B_{2g}(3)$	$E^-(3)$	$E_g(20)$	$E_1(4) \oplus G(16)$
$B_{2u}(3)$	$E^+(3)$	$E_u(20)$	$E_2(4) \oplus G(16)$
$B_{3g}(3)$	$E^+(3)$		
$B_{3u}(3)$	$E^-(3)$		

(viii) CH₄^h

$T_d(M)$	G_{48}
$A_1(5)$	$A_1^+(0) \oplus A_1^-(5)$
$A_2(5)$	$A_2^+(5) \oplus A_2^-(0)$
$E(2)$	$E^+(1) \oplus E^-(1)$
$F_1(3)$	$F_1^+(3) \oplus F_1^-(0)$
$F_2(3)$	$F_2^+(0) \oplus F_2^-(3)$

^aSee Tables A-6 and A-10.^eSee Tables A-4, A-21, and A-23.^bSee Tables A-2 and A-22.^fSee Tables A-9, A-23, and 8-2.^cSee Tables A-6 and A-26.^gSee Tables A-13 and A-33.^dSee Tables A-5 and A-28.^hSee Tables A-14 and A-29.