UNIVERSITI SAINS MALAYSIA

PEPERIKSAAN KURSUS SEMASA CUTI PANJANG
ACADEMIC SESSION 2008/2009

JUNE 2009

JIK 317 – QUANTUM CHEMISTRY AND GROUP THEORY
[KIMIA KUANTUM DAN TEORI KUMPULAN]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains FIVE printed pages together with a 20 printed pages of **Appendix JIK 317** before you begin the examination.

Answer **FIVE** questions. You may answer **either** in Bahasa Malaysia or English.

All answers must be written in the answer booklet provided.

Each question is worth 20 marks and the mark for each sub question is given at the end of that question.

*Sila pastikan bahawa kertas peperiksaan ini mengandungi LIMA muka surat yang bercetak bersama dengan **Lampiran JIK 317** sebanyak 20 muka surat bercetak sebelum anda memulakan peperiksaan ini.*

*Jawab **LIMA** soalan. Anda dibenarkan menjawab soalan **sama ada** dalam Bahasa Malaysia atau Bahasa Inggeris.*

Setiap jawapan mesti dijawab di dalam buku jawapan yang disediakan.

Setiap soalan bernilai 20 markah dan markah subsoalan diperlihatkan di penghujung subsoalan itu.

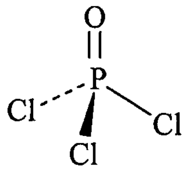
1. List the symmetry elements of the following molecules and classify each molecule into specific point group.

   Senaraikan unsur-unsur simetri bagi molekul-molekul berikut dan kelaskan setiap molekul kepada kumpulan titik tertentu.

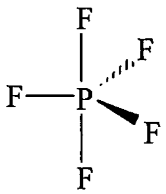
   (a)

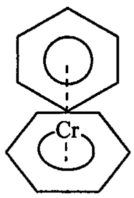
   (b)

   (c)

   (d)

   (staggered)

   (e) O = C = S

   [20 marks/*markah*]

2. (a) Reduce the following reducible representations.

Turunkan perwakilan-perwakilan terturunkan berikut :

(i)

C_2h	E	C_2	i	σ_h
Γ_{10}	8	0	6	2

(ii)

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_{11}	6	0	-2

(iii)

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
Γ_{12}	3	-3	1	-1

[10 marks/*markah*]

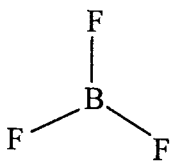
(b) Set up the correlation diagram for CH_4 molecule. Consider the 2s and 2p orbitals of carbon and the 1s orbital of each hydrogen atom.

Lukis gambar rajah korelasi bagi molekul CH_4. Atom karbon melibatkan orbital 2s dan 2p manakala setiap atom hidrogen melibatkan orbital 1s.

[10 marks/*markah*]

3. (a) Find the number, and symmetry species of the Raman and infrared active vibrations of boron trifluoride (D_{3h}). Show your calculation.

Kira bilangan dan spesies simetri spektrum Raman dan inframerah daripada getaran aktif molekul boron trifluorida (D_{3h}). Tunjukkan pengiraan anda.



[10 marks/*markah*]

(b) With appropriate calculation predict the hybrid orbital responsible for σ-bond at carbon atom in ethylene molecule, $CH_2 = CH_2$.

Dengan menunjukkan pengiraan yang berkaitan ramalkan orbital hibrid yang terlibat dengan ikatan-σ pada atom karbon dalam molekul etilena, $CH_2 = CH_2$.

[10 marks/*markah*]

4. Write out the results of experiment that produce the phenomenon known as the photoelectric effect. Which of those results cannot be explained using classical wave theory? How could the photoelectric effect phenomenon be explained by Einstein's hypothesis of quantization of light?

Tuliskan keputusan-keputusan eksperimen yang menghasilkan fenomena yang dikenali sebagai kesan fotoelektrik. Antara keputusan-keputusan itu, manakah yang tidak dapat dijelaskan dengan penggunaan teori klasik gelombang? Bagaimanakah hipotesis Einstein yang menyatakan bahawa cahaya adalah terkuantum berjaya menjelaskan fenomena ini?

[20 marks/*markah*]

5. (a) Write out the postulates of quantum mechanics.

Nyatakan postulat-postulat mekanik kuantum.

[15 marks/*markah*]

(b) A state of quantum system is given by

$$\psi = \phi_1 + 2\phi_2 + 3\phi_3 + 4\phi_4$$

Calculate the expectation value for measurement of energy, given that

$$\hat{H}\phi_1 = h\nu\phi_1$$
$$\hat{H}\phi_2 = 2h\nu\phi_2$$
$$\hat{H}\phi_3 = 3h\nu\phi_3$$
$$\hat{H}\phi_4 = 4h\nu\phi_4$$

Keadaan satu sistem kuantum diberikan oleh

$$\psi = \phi_1 + 2\phi_2 + 3\phi_3 + 4\phi_4$$

Kirakan nilai jangkaan bagi pengukuran tenaga, diberi bahawa

$$\hat{H}\phi_1 = h\nu\phi_1$$
$$\hat{H}\phi_2 = 2h\nu\phi_2$$
$$\hat{H}\phi_3 = 3h\nu\phi_3$$
$$\hat{H}\phi_4 = 4h\nu\phi_4$$

[5 marks/*markah*]

6. A particle of mass m is confined to a one-dimensional box of length L.

   Satu zarah berjisim m dihadkan dalam satu kotak satu dimensi yang panjangnya L.

   (a) Find the wavefunction of the particle in the box by solving the relevant Schroedinger equation, with appropriate boundary conditions.

   Dapatkan fungsi gelombang untuk zarah dalam kotak tersebut dengan menyelesaikan persamaan Schroedinger yang berkaitan, dengan syarat-syarat sempadan yang bersesuaian.

   [12 marks/*markah*]

   (b) Calculate the probability of finding the particle in the regions $0 \le x \le L/2$ and $L/2 \le x \le 3L/4$. Evaluate the expressions for general values of quantum number n obtained from 3(a).

   Kirakan kebarangkalian untuk mencari zarah tersebut dalam ruang $0 \le x \le L/2$ *dan* $L/2 \le x \le 3L/4$. *Tuliskan jawapan untuk nilai nombor kuantum n yang umum daripada 3(a).*

   [8 marks/*markah*]

- oooOooo -

APPENDIX JIK 317

QUANTUM CHEMISTRY AND GROUP THEORY

[CHARACTER TABLE]

Appendix

Character Tables for Some Chemically Important Symmetry Groups

C_s	E	σ_h		
A′	1	1	T_x, T_y, R_z	x^2, y^2, z^2, xy
A″	1	−1	T_z, R_x, R_y	yz, zx

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	x^2, y^2, z^2, xy, zx, yz
A_u	1	−1	T_x, T_y, T_z	

The C_n Groups

C_2	E	C_2		
A	1	1	T_z, R_z,	x^2, y^2, z^2, xy
B	1	−1	T_x, T_y, R_x, R_y	yz, zx

C_3	E	C_3	C_3^2		$\epsilon = \exp(2\pi i/3)$
A	1	1	1	T_z, R_z	x^2+y^2, z^2
E	$\left\{\begin{matrix}1\\1\end{matrix}\right.$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\left.\begin{matrix}\epsilon^*\\\epsilon\end{matrix}\right\}$	(T_x, T_y), (R_x, R_y)	(x^2-y^2, xy), (yz, zx)

The C_n Groups (continued)

C_4	E	C_4	C_2	C_4^3		
A	1	1	1	1	T_z, R_z	x^2+y^2, z^2
B	1	−1	1	−1		x^2-y^2, xy
E	1	i	−1	−i	(T_x, T_y);	(yz, zx)
	1	−i	−1	i	(R_x, R_y)	

C_5	E	C_5	C_5^2	C_5^3	C_5^4		$\epsilon = \exp(2\pi i/5)$
A	1	1	1	1	1	T_z, R_z	x^2+y^2, z^2
E_1	1	ϵ	ϵ^2	ϵ^{2*}	ϵ^*	(T_x, T_y), (R_x, R_y)	(yz, zx)
	1	ϵ^*	ϵ^{2*}	ϵ^2	ϵ		
E_2	1	ϵ^2	ϵ^*	ϵ	ϵ^{2*}		$(x^2-y^2$, xy)
	1	ϵ^{2*}	ϵ	ϵ^*	ϵ^2		

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5		$\epsilon = \exp(2\pi i/6)$
A	1	1	1	1	1	1	T_z, R_z	x^2+y^2, z^2
B	1	−1	1	−1	1	−1		
E_1	1	ϵ	$-\epsilon^*$	−1	$-\epsilon$	ϵ^*	(T_x, T_y),	(yz, zx)
	1	ϵ^*	$-\epsilon$	−1	$-\epsilon^*$	ϵ	(R_x, R_y)	
E_2	1	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$		$(x^2-y^2$, xy)
	1	$-\epsilon$	$-\epsilon^*$	1	$-\epsilon$	$-\epsilon^*$		

The C_n Groups (continued)

C_7	E	C_7	C_7^2	C_7^3	C_7^4	C_7^5	C_7^6		$\epsilon = \exp(2\pi i/7)$
A	1	1	1	1	1	1	1	T_z, R_z	x^2+y^2, z^2
E_1	1	ϵ	ϵ^2	ϵ^3	ϵ^{3*}	ϵ^{2*}	ϵ^*	(T_x, T_y),	(yz, zx)
	1	ϵ^*	ϵ^{2*}	ϵ^{3*}	ϵ^3	ϵ^2	ϵ	(R_x, R_y)	
E_2	1	ϵ^2	ϵ^{3*}	ϵ^*	ϵ	ϵ^3	ϵ^{2*}		(x^2-y^2, xy)
	1	ϵ^{2*}	ϵ^3	ϵ	ϵ^*	ϵ^{3*}	ϵ^2		
E_3	1	ϵ^3	ϵ^*	ϵ^2	ϵ^{2*}	ϵ	ϵ^{3*}		
	1	ϵ^{3*}	ϵ	ϵ^{2*}	ϵ^2	ϵ^*	ϵ^3		

C_8	E	C_8	C_4	C_2	C_4^3	C_8^3	C_8^5	C_8^7		$\epsilon = \exp(2\pi i/8)$
A	1	1	1	1	1	1	1	1	T_z, R_z	x^2+y^2, z^2
B	1	-1	1	1	1	-1	-1	-1		
E_1	1	ϵ	i	-1	$-i$	$-\epsilon^*$	$-\epsilon$	ϵ^*	(T_x, T_y),	(yz, zx)
	1	ϵ^*	$-i$	-1	i	$-\epsilon$	$-\epsilon^*$	ϵ	(R_x, R_y)	
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	$-i$	ϵ^*	ϵ	$-\epsilon^*$		
	1	$-\epsilon^*$	$-i$	-1	i	ϵ	ϵ^*	$-\epsilon$		

The D_n Groups

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	−1	−1	T_z, R_z	xy
B_2	1	−1	1	−1	T_y, R_y	zx
B_3	1	−1	−1	1	T_x, R_x	yz

D_3	E	$2C_3$	$3C_2$		
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	−1	T_z, R_z	
E	2	−1	0	$(T_x, T_y), (R_x, R_y)$	$(x^2-y^2, xy), (yz, zx)$

D_4	E	$2C_4$	$C_2\,(=C_4^2)$	$2C'_2$	$2C''_2$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	−1	−1	T_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	$(T_x, T_y), (R_x, R_y)$	(yz, zx)

The D_n Groups (continued)

D_5	E	$2C_5$	$2C_5^2$	$5C_2$		
A_1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	−1	T_z, R_z	
E_1	2	2 cos 72°	2 cos 144°	0	$(T_x, T_y), (R_x, R_y)$	(yz, zx)
E_2	2	2 cos 144°	2 cos 72°	0		(x^2-y^2, xy)

D_6	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$		
A_1	1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	1	−1	−1	T_z, R_z	
B_1	1	−1	1	−1	1	−1		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	$(T_x, T_y), (R_x, R_y)$	(yz, zx)
E_2	2	−1	−1	2	0	0		(x^2-y^2, xy)

The C_{nv} Groups

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	T_z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	T_x, R_y	zx
B_2	1	−1	−1	1	T_y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	T_z	x^2+y^2, z^2
A_2	1	1	−1	R_z	
E	2	−1	0	$(T_x, T_y), (R_x, R_y)$	$(x^2-y^2, xy), (yz, zx)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	T_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	$(T_x, T_y), (R_x, R_y)$	(yz, zx)

The C_{nv} Groups (continued)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	T_z	x^2+y^2, z^2
A_2	1	1	1	−1	R_z	
E_1	2	2 cos 72°	2 cos 144°	0	(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	2	2 cos 144°	2 cos 72°	0		(x^2-y^2, xy)

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	T_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		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	2	−1	−1	2	0	0		(x^2-y^2, xy)

The C_{nh} Groups

C_{2h}	E	C_2	i	σ_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	yz, zx
A_u	1	1	−1	−1	T_z,	
B_u	1	−1	−1	1	T_x, T_y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	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'	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\left.\begin{matrix}\epsilon^*\\\epsilon\end{matrix}\right\}$	(T_x, T_y)	(x^2-y^2, xy)
A''	1	1	1	−1	−1	−1	T_z	
E''	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$	$\begin{matrix}\epsilon^*\\\epsilon\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\begin{matrix}-\epsilon\\-\epsilon^*\end{matrix}$	$\left.\begin{matrix}-\epsilon^*\\-\epsilon\end{matrix}\right\}$	(R_x, R_y)	(yz, zx)

C_{4h}	E	C_4	C_2	C_4^3	i	S_4^3	σ_h	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	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}i\\-i\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\begin{matrix}-i\\i\end{matrix}$	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}i\\-i\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\left.\begin{matrix}-i\\i\end{matrix}\right\}$	(R_x, R_y)	(yz, zx)
A_u	1	1	1	1	−1	−1	−1	−1	T_z	
B_u	1	−1	1	−1	−1	1	−1	1		
E_u	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}i\\-i\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\begin{matrix}-i\\i\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\begin{matrix}-i\\i\end{matrix}$	$\begin{matrix}1\\1\end{matrix}$	$\left.\begin{matrix}i\\-i\end{matrix}\right\}$	(T_x, T_y)	

The C_{nh} Groups (continued)

C_{5h}	E	C_5	C_5^2	C_5^3	C_5^4	σ_h	S_5	S_5^7	S_5^3	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	ϵ^{2*}	ϵ^*	1	ϵ	ϵ^2	ϵ^{2*}	ϵ^*	(T_x, T_y)	
	1	ϵ^*	ϵ^{2*}	ϵ^2	ϵ	1	ϵ^*	ϵ^{2*}	ϵ^2	ϵ		
E_2'	1	ϵ^2	ϵ^*	ϵ	ϵ^{2*}	1	ϵ^2	ϵ^*	ϵ	ϵ^{2*}		(x^2-y^2, xy)
	1	ϵ^{2*}	ϵ	ϵ^*	ϵ^2	1	ϵ^{2*}	ϵ	ϵ^*	ϵ^2		
A″	1	1	1	1	1	−1	−1	−1	−1	−1	T_z	
E_1''	1	ϵ	ϵ^2	ϵ^{2*}	ϵ^*	−1	$-\epsilon$	$-\epsilon^2$	$-\epsilon^{2*}$	$-\epsilon^*$	(R_x, R_y)	(yz, zx)
	1	ϵ^*	ϵ^{2*}	ϵ^2	ϵ	−1	$-\epsilon^*$	$-\epsilon^{2*}$	$-\epsilon^2$	$-\epsilon$		
E_2''	1	ϵ^2	ϵ^*	ϵ	ϵ^{2*}	−1	$-\epsilon^2$	$-\epsilon^*$	$-\epsilon$	$-\epsilon^{2*}$		
	1	ϵ^{2*}	ϵ	ϵ^*	ϵ^2	−1	$-\epsilon^{2*}$	$-\epsilon$	$-\epsilon^*$	$-\epsilon^2$		

C_{6h}	E	C_6	C_3	C_2	C_3^2	C_6^5	i	S_3^5	S_6^5	σ_h	S_6	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	$-\epsilon^*$	−1	$-\epsilon$	ϵ^*	1	ϵ	$-\epsilon^*$	−1	$-\epsilon$	ϵ^*	(R_x, R_y)	(yz, zx)
	1	ϵ^*	$-\epsilon$	−1	$-\epsilon^*$	ϵ	1	ϵ^*	$-\epsilon$	−1	$-\epsilon^*$	ϵ		
E_{2g}	1	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$		(x^2-y^2, xy)
	1	$-\epsilon$	$-\epsilon^*$	1	$-\epsilon$	$-\epsilon^*$	1	$-\epsilon$	$-\epsilon^*$	1	$-\epsilon$	$-\epsilon^*$		
A_u	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	T_z	
B_u	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
E_{1u}	1	ϵ	$-\epsilon^*$	−1	$-\epsilon$	ϵ^*	−1	$-\epsilon$	ϵ^*	1	ϵ	$-\epsilon^*$	(T_x, T_y)	
	1	ϵ^*	$-\epsilon$	−1	$-\epsilon^*$	ϵ	−1	$-\epsilon^*$	ϵ	1	ϵ^*	$-\epsilon$		
E_{2u}	1	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$	−1	ϵ^*	ϵ	−1	ϵ^*	ϵ		
	1	$-\epsilon$	$-\epsilon^*$	1	$-\epsilon$	$-\epsilon^*$	−1	ϵ	ϵ^*	−1	ϵ	ϵ^*		

The D_{nh} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
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	zx
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	T_z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	T_y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	T_x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
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	$(T_x\ T_y)$	(x^2-y^2, xy)
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	T_z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(yz, zx)

The D_{nh} Groups (continued)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
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)	(yz, zx)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	T_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	(T_x, T_y)	

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
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	2 cos 72°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	(T_x, T_y)	
E_2'	2	2 cos 144°	2 cos 72°	0	2	2 cos 144°	2 cos 72°	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	T_z	
E_1''	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(R_x, R_y)	(yz, zx)
E_2''	2	2 cos 144°	2 cos 72°	0	−2	−2 cos 144°	−2 cos 72°	0		

The D_{nh} Groups (continued)

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
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)	(yz, zx)
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	T_z	
B_{1u}	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_{1u}	2	1	−1	−2	0	0	−2	−1	1	2	0	0	(T_x, T_y)	
E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0		

The D_{nd} Groups

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
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	T_z	xy
E	2	0	−2	0	0	$(T_x, T_y), (R_x, R_y)$	(yz, zx)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
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)	$(x^2-y^2, xy) (yz, zx)$
A_{1u}	1	1	1	−1	−1	−1		
A_{2u}	1	1	−1	−1	−1	1	T_z	
E_u	2	−1	0	−2	1	0	(T_x, T_y)	

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$		
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	T_z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(T_x, T_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)	(yz, zx)

The D_{nd} Groups (continued)

D_{5d}	E	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$		
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	2 cos 72°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	(R_x, R_y)	(yz, zx)
E_{2g}	2	2 cos 144°	2 cos 72°	0	2	2 cos 144°	2 cos 72°	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	T_z	
E_{1u}	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(T_x, T_y)	
E_{2u}	2	2 cos 144°	2 cos 72°	0	−2	−2 cos 144°	−2 cos 72°	0		

D_{6d}	E	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2S_{12}^5$	C_2	$6C_2'$	$6\sigma_d$		
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	T_z	
E_1	2	$\sqrt{3}$	1	0	−1	$-\sqrt{3}$	−2	0	0	(T_x, T_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)	(yz, zx)

The S_n Groups

S_4	E	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	x^2+y^2, z^2
B	1	−1	1	−1	T_z	x^2-y^2, xy
E	1	i	−1	−i	$(T_x, T_y), (R_x, R_y)$	(yz, zx)
	1	−i	−1	i		

S_6	E	C_3	C_3^2	i	S_6^5	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	ϵ^*	1	ϵ	ϵ^*	(R_x, R_y)	$(x^2-y^2, xy), (yz, zx)$
	1	ϵ^*	ϵ	1	ϵ^*	ϵ		
A_u	1	1	1	−1	−1	−1	T_z	
E_u	1	ϵ	ϵ^*	−1	$-\epsilon$	$-\epsilon^*$	(T_x, T_y)	
	1	ϵ^*	ϵ	−1	$-\epsilon^*$	$-\epsilon$		

S_8	E	S_8	C_4	S_8^3	C_2	S_8^5	C_4^3	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	T_z	
E_1	1	ϵ	i	$-\epsilon^*$	−1	$-\epsilon$	−i	ϵ^*	$(T_x, T_y), (R_x, R_y)$	
	1	ϵ^*	−i	$-\epsilon$	−1	$-\epsilon^*$	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	$-\epsilon^*$	−i	ϵ	−1	ϵ^*	i	$-\epsilon$		(yz, zx)
	1	$-\epsilon$	i	ϵ^*	−1	ϵ	−i	$-\epsilon^*$		

The Cubic Groups

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
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	(T_x, T_y, T_z)	(xy, yz, zx)

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
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		(xy, yz, zx)
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	(T_x, T_y, T_z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

The Groups $C_{\infty v}$ and $D_{\infty h}$ for Linear Molecules

$C_{\infty v}$	E	$2C_\infty^\Phi$	...	$\infty\sigma_v$		
$A_1 = \Sigma+$	1	1	...	1	T_z	x^2+y^2, z^2
$A_2 = \Sigma-$	1	1	...	-1	R_z	
$E_1 = \Pi$	2	$2\cos\ \Phi$	...	0	$(T_x, T_y), (R_x, R_y)$	(yz, zx)
$E_2 = \Delta$	2	$2\cos 2\Phi$	...	0		(x^2-y^2, xy)
$E_3 = \Phi$	2	$2\cos 3\Phi$	...	0		
...	...	...	...	...		

$D_{\infty h}$	E	$2C_\infty^\Phi$	...	$\infty\sigma_v$	i	$2S_\infty^\Phi$	...	∞C_2		
Σ_g+	1	1	...	1	1	1	...	1		x^2+y^2, z^2
Σ_g^-	1	1	...	-1	1	1	...	1	R_z	
Π_g	2	$2\cos\ \Phi$	...	0	2	$-2\cos\ \Phi$	...	0	(R_x, R_y)	(yz, zx)
Δ_g	2	$2\cos 2\Phi$	...	0	2	$2\cos 2\Phi$	...	0		(x^2-y^2, xy)
...	...	...	...	...	...	...	...	...		
Σ_u^+	1	1	...	1	-1	-1	...	-1	T_z	
Σ_u^-	1	1	...	-1	-1	-1	...	1		
Π_u	2	$2\cos\ \Phi$	...	0	-2	$2\cos\ \Phi$	...	0	(T_x, T_y)	
Δ_u	2	$2\cos 2\Phi$	...	0	-2	$-2\cos 2\Phi$	...	0		
...	...	...	...	...	...	...	...	...		

Reducing Formula

$\mathbf{a}_i = 1/h \sum \mathbf{X}^S{}_R \mathbf{X}^S{}_I \mathbf{N}^S$

h ; total number of operations in certain point group.

$\mathbf{X}^S{}_R$; Character (**X**) for reducible representation.

$\mathbf{X}^S{}_I$; Character (**X**) for reducible representation (from the character Table)

$\mathbf{N}^S$; Number of symmetry operation for each type or class of operation.

Contribution for the Character, $\chi(R)$, for each unshifted atom in Γ_{3N}

R	$\chi(R)$
E	+3
i	-3
σ	+1
C_2	-1
C_3^1, C_3^2	0
C_4^1, C_4^3	+1
C_6^1, C_6^5	+2
S_3^1, S_3^5	-2
S_4^1, S_4^3	-1
S_6^1, S_6^5	0

Notations of the Character Table

a	b		
f	c	d	e

a. Schoenflies symbols for point group

b. lists the symmetry operations (by classes) for that group

c. lists all the characters, for all irreducible representations, of each class of each operation

d. shows the irreducible representations for which the six vectors ,Tx, Ty, Tz, Rx, Ry, Rz, provide the bases

e. shows the funtions which are binary combinations of x, y, z (e.g. xy, z^2) provide bases for certain irreducible representations

f . lists conventional symbols for the irreducible representations called *Mulliken symbols.* All one –dimentional irreducible rep. Are labelled as A or B, all two-dimentional as E, all three-dimentional as T (in certain texts it is given the label F), four-dimentional as G and five-dimentional as H.

In addition to the letter, most Mulliken symbols possess certain subscripts and/or superscripts. For two- and higher – dimentional irreducible representations they can be regarded as lebels. For one-dimentional representations, they have the following specifications.

A : One-dimentional irreducible rep. if it is symmetry about Cn axis, i.e.($\chi = +1$)

B : ,, ,, ,, antisymm. ,, ($\chi = -1$)

Sub.$_1$: Irr. Rep is symmetry with respect to $C_2 \perp$ Cn (if no C_2), then Irr. Rep. Is symmetry with respect to σ_v

Sub.$_2$: Irr. Rep is antisymmetry under conditions as those in Sub$_1$ of above.

Sub.$_g$: (gerade) irr. rep. are symm. With respect to inversion at an i

Sub. $_u$: (ungerade) irr. rep. are antisymm. with respect to an i

` : irr. Rep are symm with respect to reflection in a σ_h

`` : irr. Rep. Are antisymm with respect to reflection in a σ_h