UNIVERSITI SAINS MALAYSIA

Final Examination
Academic Session 2008/2009

April 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 before you begin the examination.

Answer **FIVE** questions. You may answer **either** in Bahasa Malaysia or in 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 sebelum anda memulakan peperiksaan ini.*

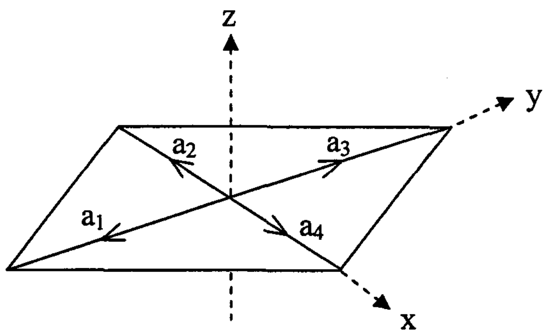
*Jawab **LIMA** soalan. Anda dibenarkan menjawab soalan **sama ada** dalam Bahasa Malaysia atau Bahasa Inggeris.*

Setiap jawapan mesti dijawab di dalam buku jawapan yang disediakan.

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

1. (a) Using vectors a_1, a_2, a_3, a_4 as the basis in the diagram below write down matrix and its character representing

Dengan menggunakan vektor a_1, a_2, a_3 dan a_4 dalam gambar rajah di bawah, tuliskan matriks dan karakternya yang mewakili



(i) C_4 rotation about the z-axis

Putaran C_4 pada paksi-z

(ii) C_2 rotation about the x-axis

Putaran C_2 pada paksi-x

(iii) Reflection in the xy-plane

Pantulan dalam satah-xy

[10 marks]

(b) Obtain the irreducible components of the following reducible representations.

Dapatkan komponen-komponen yang tidak terturunkan daripada perwakilan terturunkan berikut.

(i)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$
	5	2	3	-1	2	1

(ii)

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
	4	-1	1	2	0	-2

[10 marks]

...3/-

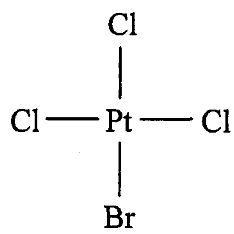
2. (a) For the $PtBrCl_3$ molecule,
Bagi molekul $PtBrCl_3$

(i) Identify its point group.
Tentukan kumpulan titiknya.

(ii) Produce the reducible representation (Γ) using unshifted atom method.
Dapatkan perwakilan terturunkan (Γ) dengan menggunakan kaedah atom tak bergerak.

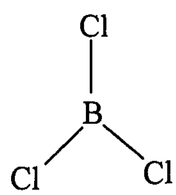
(iii) Reduce the reducible representation (Γ) to its irreducible representation.
Turunkan perwakilan terturunkan (Γ) kepada perwakilan tak terturunkan.

(iv) Predict the number of bands in the infrared and Raman spectra.
Ramalkan bilangan jalur dalam spektrum inframerah dan Raman.



[12 marks]

(b) Find the number and symmetry species of the infrared an Raman active vibrations of boron trichloride (D_{3h}).
Tentukan bilangan dan spesies simetri dalam getaran aktif inframerah dan Raman bagi boron triklorida (D_3h).



[8 marks]

...4/-

3. (a) Find the hybrid orbital of a central atom suitable for the formation of tetrahedral σ bonds like those in CH_4.

Tentukan orbital hibrid pada atom pusat yang sesuai untuk pembentukan ikatan σ tetrahedral seperti yang terdapat dalam molekul CH_4.

[6 marks]

(b) Starting from appropriate basis, predict the orbitals that are responsible for delocalized π-bonding in benzene, a D_{6h} molecule.

Bermula dengan asas yang bersesuaian, ramalkan orbital-orbital yang berperanan dalam pembentukan ikatan-π tak setempat dalam benzena, suatu molekul D_{6h}.

[7 marks]

(c) Using character table, draw the correlation diagram for the CCl_4 molecule.

Dengan menggunakan jadual karakter, lukis gambarajah korelasi untuk molekul CCl_4.

[7 marks]

4. Elaborate on two experimental results of the photoelectric effect that cannot be explained by wave theory of light. Interpret these experiment results in view of Einstein's hypothesis of the quantization of light.

Huraikan dua hasil eksperimen kesan fotoelektrik yang tidak dapat diterangkan oleh teori gelombang. Tafsirkan keputusan-keputusan ini dari pandangan hipotesis pengkuantuman cahaya Einstein.

[20 marks]

5. (a) Briefly discuss the postulates of quantum mechanics.

Bincangkan secara ringkas postulat-postulat mekanik kuantum.

[10 marks]

(b) The ground state wavefunction for a particle confined to a one-dimensional box of length $L = 10$ nm is

Fungsi gelombang keadaan asas untuk suatu zarah yg dihadkan pada kotak satu dimensi yang panjangnya $L = 10$ nm ialah

$$\psi = A\sin\left(\frac{\pi x}{L}\right)$$

(i) Calculate the normalization constant A.

Kira pemalar normalisasi A.

[6 marks]

...5/-

(ii) Calculate the probability that the particle is between x = 4.95 nm and 5.05 nm, and between x = 9.90 nm and 10.00 nm.

Kirakan kebarangkalian bahawa zarah itu berada di antara x = 4.95 nm dan 5.05 nm, dan antara x = 9.90 nm dan 10.00 nm.

[4 marks]

6. (a) Show that the eigenvalue for a Hermitian operator is always real.

Tunjukkan bahawa nilai eigen untuk suatu operator Hermitian adalah selalu sahih.

[10 marks]

(b) Get the eigenfunction $U_n(x)$, given that $\hat{A}U_n(x) = a_n U_n(x)$ where $\hat{A} = -i\dfrac{d}{dx}$.

If $U_n(x) = U_n(x+L)$, determine the value of a_n.

Dapatkan fungsi eigen $U_n(x)$, *diberi* $\hat{A}U_n(x) = a_n U_n(x)$ *dengan* $\hat{A} = -i\dfrac{d}{dx}$.

Jika $U_n(x) = U_n(x+L)$, *tentukan* a_n.

[10 marks]

- 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	$\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$				(T_x, T_y); (R_x, R_y)	(yz, zx)

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	$\begin{Bmatrix} 1 & \epsilon & \epsilon^2 & \epsilon^{2*} & \epsilon^* \\ 1 & \epsilon^* & \epsilon^{2*} & \epsilon^2 & \epsilon \end{Bmatrix}$					(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	$\begin{Bmatrix} 1 & \epsilon^2 & \epsilon^* & \epsilon & \epsilon^{2*} \\ 1 & \epsilon^{2*} & \epsilon & \epsilon^* & \epsilon^2 \end{Bmatrix}$						$(x^2-y^2$, xy)

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	$\begin{Bmatrix} 1 & \epsilon & -\epsilon^* & -1 & -\epsilon & \epsilon^* \\ 1 & \epsilon^* & -\epsilon & -1 & -\epsilon^* & \epsilon \end{Bmatrix}$						(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	$\begin{Bmatrix} 1 & -\epsilon^* & -\epsilon & 1 & -\epsilon^* & -\epsilon \\ 1 & -\epsilon & -\epsilon^* & 1 & -\epsilon & -\epsilon^* \end{Bmatrix}$							$(x^2-y^2$, xy)

APPENDIX

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	$\begin{cases}1\\1\end{cases}$	ϵ ϵ^*	ϵ^2 ϵ^{2*}	ϵ^3 ϵ^{3*}	ϵ^{3*} ϵ^3	ϵ^{2*} ϵ^2	ϵ^* ϵ	(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	$\begin{cases}1\\1\end{cases}$	ϵ^2 ϵ^{2*}	ϵ^{3*} ϵ^3	ϵ^* ϵ	ϵ ϵ^*	ϵ^3 ϵ^{3*}	ϵ^{2*} ϵ^2		(x^2-y^2, xy)
E_3	$\begin{cases}1\\1\end{cases}$	ϵ^3 ϵ^{3*}	ϵ^* ϵ	ϵ^2 ϵ^{2*}	ϵ^{2*} ϵ^2	ϵ ϵ^*	ϵ^{3*} 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	$\begin{cases}1\\1\end{cases}$	ϵ ϵ^*	i −i	−1 −1	−i i	$-\epsilon^*$ $-\epsilon$	$-\epsilon$ $-\epsilon^*$	ϵ^* ϵ	(T_x, T_y), (R_x, R_y)	(yz, zx)
E_2	$\begin{cases}1\\1\end{cases}$	i −i	−1 −1	1 1	−1 −1	−i i	i −i	−i i		(x^2-y^2, xy)
E_3	$\begin{cases}1\\1\end{cases}$	$-\epsilon$ $-\epsilon^*$	i −i	−1 −1	−i i	ϵ^* ϵ	ϵ ϵ^*	$-\epsilon^*$ $-\epsilon$		

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)

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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′	1	ϵ	ϵ^*	1	ϵ	ϵ^*	(T_x, T_y)	(x^2-y^2, xy)
	1	ϵ^*	ϵ	1	ϵ^*	ϵ		
A″	1	1	1	−1	−1	−1	T_z	
E″	1	ϵ	ϵ^*	−1	$-\epsilon$	$-\epsilon^*$	(R_x, R_y)	(yz, zx)
	1	ϵ^*	ϵ	−1	$-\epsilon^*$	$-\epsilon$		

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	1	i	−1	−i	1	i	−1	−i	(R_x, R_y)	(yz, zx)
	1	−i	−1	i	1	−i	−1	i		
A_u	1	1	1	1	−1	−1	−1	−1	T_z	
B_u	1	−1	1	−1	−1	1	−1	1		
E_u	1	i	−1	−i	−1	−i	1	i	(T_x, T_y)	
	1	−i	−1	i	−1	i	1	−i		

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		

APPENDIX

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 Φ	...	0	$(T_x, T_y), (R_x, R_y)$	(yz, zx)
$E_2 = \Delta$	2	2 cos 2Φ	...	0		(x^2-y^2, xy)
$E_3 = \Phi$	2	2 cos 3Φ	...	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 Φ	...	0	2	−2 cos Φ	...	0	(R_x, R_y)	(yz, zx)
Δ_g	2	2 cos 2Φ	...	0	2	2 cos 2Φ	...	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 Φ	...	0	−2	2 cos Φ	...	0	(T_x, T_y)	
Δ_u	2	2 cos 2Φ	...	0	−2	−2 cos 2Φ	...	0		
...	...	...	...	...	...	...	...	...		

Reducing Formula

$\mathbf{a_i} = 1/h\sum \mathbf{X^S{}_R X^S{}_1 N^S}$

h ; total number of operations in certain point group.

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

$\mathbf{X^S{}_1}$; 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

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