4

UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Kedua
Sidang Akademik 2003/2004

Februari/Mac 2004

KTE 211 - Teori Kumpulan Dan Spektroskopi

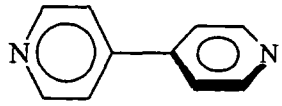
Masa : 2 jam

Sila pastikan bahawa kertas peperiksaan ini mengandungi TUJUH BELAS muka surat yang bercetak sebelum anda memulakan peperiksaan ini.

Jawab EMPAT soalan. Jika calon menjawab lebih daripada empat soalan hanya empat soalan pertama mengikut susunan dalam skrip jawapan akan diberi markah.

Jadual Karakter dilampirkan.

1. (a) Bagi molekul berikut:



(i) Nyatakan kumpulan titik.

(2 markah)

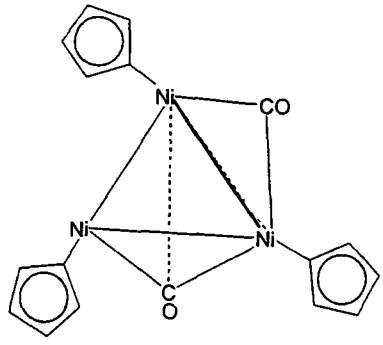
(ii) Gunakan matrik 2x2 untuk mewakili setiap operasi simetri bagi molekul tersebut.

(6 markah)

(iii) Nyatakan nilai karakter bagi setiap operasi simetri yang dijanakan dalam (ii).

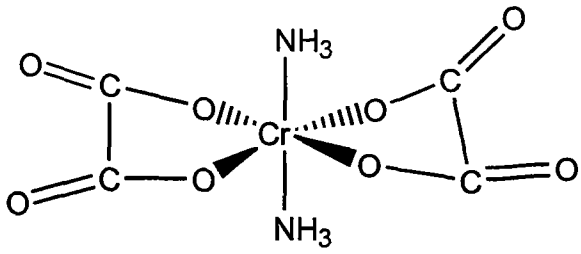
(4 markah)

(b) (i) Kompleks gugusan Ni, $[Ni_3(CO)_2(C_5H_5)_3]$, seperti berikut mempunyai struktur dengan kumpulan titik D_{3h}. Berikan penjelasan kenapa kompleks Ni berikut menunjukkan hanya satu jalur penyerapan untuk kumpulan karbonil dan satu jalur untuk kumpulan C_5H_5.



(6 markah)

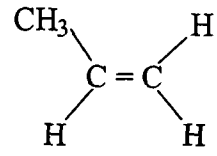
(ii) Nyatakan satu kaedah spektroskopi dan berikan dua alasan yang paling sesuai untuk pencirian kompleks berikut:



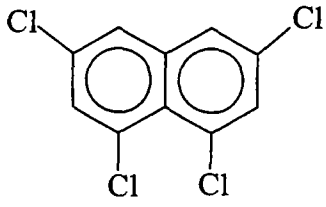
(7 markah)

2. (a) Nyatakan kumpulan titik bagi setiap molekul berikut:

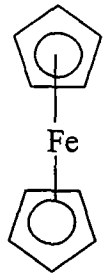
(i)



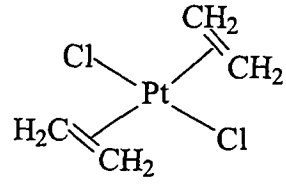
(ii)



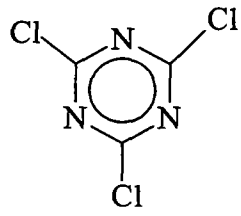
(iii)



(iv)



(v)

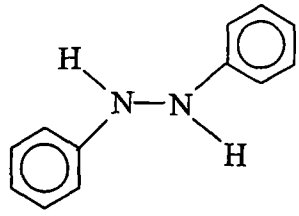


(10 markah)

(b) Dapatkan kumpulan titik bagi molekul *trans*-$PtCl_2Br_2$ dan binalah jadual pendaraban bagi operasi-operasi simetri yang boleh dijanakan atas molekul tersebut.

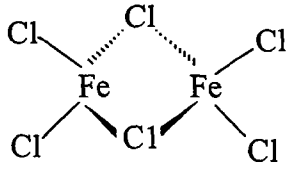
(5 markah)

(c) Dengan berdasarkan contoh molekul berikut, berikan ulasan mengenai perbezaan antara perwakilan degenerat dan perwakilan bukan degenerat.



(10 markah)

3. Bagi molekul berikut:



(a) Senaraikan unsur-unsur simetri yang mungkin.

(5 markah)

(b) Tentukan kumpulan titik.

(2 markah)

(c) Dengan berdasarkan ikatan Fe-Cl, dapatkan satu perwakilan terturunkan bagi kumpulan titik yang telah ditentukan dalam 3(ii).

(4 markah)

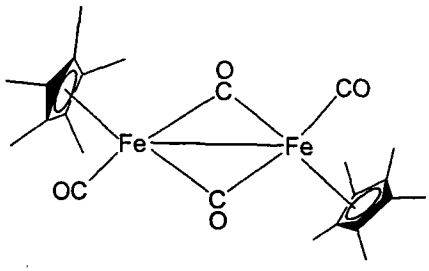
(d) Turunkan perwakilan terturunkan dalam 3(iii) kepada perwakilan tak terturunkan.

(8 markah)

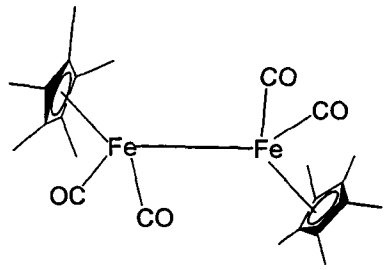
(e) Dapatkan bilangan dan spesies simetri bagi getaran yang aktif dalam Raman dan inframerah bagi molekul di atas.

(6 markah)

4. Kompleks $[\eta^5\text{-}C_5Me_5)_2Fe_2(CO)_4]$ mempamirkan dua jenis isomer iaitu Kompleks A dan Kompleks B seperti berikut:



Kompleks A



Kompleks B

(a) Berikan alasan bagaimana kaedah spektroskopi inframerah dan spektroskopi resonans magnetik nukleus (RMN), secara berasingan dapat membezakan kedua isomer tersebut.

(10 markah)

(b) Berikan penjelasan terhadap perbezaan nilai jalur penyerapan untuk kumpulan karbonil yang wujud dalam kedua kompleks tersebut.

(7 markah)

(c) Lakarkan spektrum IR untuk Kompleks A dan B serta nyatakan kumpulan berfungsi pada jalur yang diberikan.

(8 markah)

5. Tulis nota ringkas atau berikan penjelasan bagi setiap kenyataan berikut:

(a) Nyatakan perbezaan utama yang wujud dalam peralatan spektroskopi inframerah dan spektroskopi Raman.

(5 markah)

(b) Spektroskopi RMN ^{31}P tidak dapat digunakan untuk membezakan dua isomer yang wujud bagi kompleks $[PtCl_2(P(CH_3)_3)_2]$.

(5 markah)

(c) Satu sel unit bagi sesuatu hablur dicirikan mengikut parameter dengan simbol *a, b, c* dan α, β, γ. Perihalkan parameter yang digunakan.

(5 markah)

(d) Berikan penjelasan bagi turutan nilai ν seperti berikut:

$$\nu(C\text{-}H) > \nu(C{\equiv}O) > \nu(C{\equiv}Se) > \nu(Re{\equiv}Re) > \nu(Re\text{-}Re)$$

(5 markah)

(e) Lokasi puncak yang anjakan kimia dalam spektrum RMN dapat memperihalkan tenaga yang diperlukan untuk menghasilkan perubahan spin pada nukleus proton dalam sesuatu sebatian.

(5 markah)

-ooo O ooo-

LAMPIRAN

Character Tables

THE NONAXIAL GROUPS

C_1	E
A	1

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	−1	z, R_x, R_y	yz, xz

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_u	1	−1	x, y, z	

THE AXIAL GROUPS

▸ *The C_n Groups*

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	−1	x, y, R_x, R_y	yz, xz

C_3	E	C_3	C_3^2	$\varepsilon = \exp(2\pi i/3)$	
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$	$\begin{matrix} \varepsilon \\ \varepsilon^* \end{matrix}$	$\begin{matrix} \varepsilon^* \\ \varepsilon \end{matrix}\Big\}$	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (yz, xz)$

...8/-

C_4	E	C_4	C_2	C_4^3		
A	1	1	1	1	z, R_z	$x^2 + y^2$, z^2
B	1	−1	1	−1		$x^2 - y^2$, xy
E	$\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$				(x, y), (R_x, R_y)	(xz, yz)

C_5	E	C_5	C_5^2	C_5^3	C_5^4	$\varepsilon = \exp(2\pi i/5)$	
A	1	1	1	1	1	z, R_z	$x^2 + y^2$, z^2
E_1	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon \end{Bmatrix}$					(x, y), (R_x, R_y)	(yz, xz)
E_2	$\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 \end{Bmatrix}$						$(x^2 - y^2, xy)$

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5	$\varepsilon = \exp(2\pi i/6)$	
A	1	1	1	1	1	1	z, R_z	$x^2 + y^2$, z^2
B	1	−1	1	−1	1	−1		
E_1	$\begin{Bmatrix} 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon \end{Bmatrix}$						(x, y), (R_x, R_y)	(xz, yz)
E_2	$\begin{Bmatrix} 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon \\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* \end{Bmatrix}$							$(x^2 - y^2, xy)$

C_7	E	C_7	C_7^2	C_7^3	C_7^4	C_7^5	C_7^6	$\varepsilon = \exp(2\pi i/7)$	
A	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2$, z^2
E_1	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^3 & \varepsilon^{3*} & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^{3*} & \varepsilon^3 & \varepsilon^2 & \varepsilon \end{Bmatrix}$							(x, y), (R_x, R_y)	(xz, yz)
E_2	$\begin{Bmatrix} 1 & \varepsilon^2 & \varepsilon^{3*} & \varepsilon^* & \varepsilon & \varepsilon^3 & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon^3 & \varepsilon & \varepsilon^* & \varepsilon^{3*} & \varepsilon^2 \end{Bmatrix}$								$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix} 1 & \varepsilon^3 & \varepsilon^* & \varepsilon^2 & \varepsilon^{2*} & \varepsilon & \varepsilon^{3*} \\ 1 & \varepsilon^{3*} & \varepsilon & \varepsilon^{2*} & \varepsilon^2 & \varepsilon^* & \varepsilon^3 \end{Bmatrix}$								

C_8	E	C_8	C_4	C_2	C_4^3	C_8^3	C_8^5	C_8^7	$\varepsilon = \exp(2\pi i/8)$	
A	1	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2$, z^2
B	1	−1	1	1	1	−1	−1	−1		
E_1	$\begin{Bmatrix} 1 & \varepsilon & i & -1 & -i & -\varepsilon^* & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -i & -1 & i & -\varepsilon & -\varepsilon^* & \varepsilon \end{Bmatrix}$								(x, y), (R_x, R_y)	(xz, yz)
E_2	$\begin{Bmatrix} 1 & i & -1 & 1 & -1 & -i & i & -i \\ 1 & -i & -1 & 1 & -1 & i & -i & i \end{Bmatrix}$									$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix} 1 & -\varepsilon & i & -1 & -i & \varepsilon^* & \varepsilon & -\varepsilon^* \\ 1 & -\varepsilon^* & -i & -1 & i & \varepsilon & \varepsilon^* & -\varepsilon \end{Bmatrix}$									

.../-

▸ *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	z	$x^2 - y^2, xy$
E	$\begin{Bmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{Bmatrix}$				$(x, y), (R_x, R_y)$	(xz, yz)

S_6	E	C_3	C_3^2	i	S_6^5	S_6	$\varepsilon = \exp(2\pi i/3)$	
A_g	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_g	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon & 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$						(R_x, R_y)	$(x^2 - y^2, xy)$, (xy, yz)
A_u	1	1	1	−1	−1	−1	z	
E_u	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & -1 & -\varepsilon & -\varepsilon^* \\ 1 & \varepsilon^* & \varepsilon & -1 & -\varepsilon^* & -\varepsilon \end{Bmatrix}$						(x, y)	

S_8	E	S_8	C_4	S_8^3	C_2	S_8^5	C_4^3	S_8^7	$\varepsilon = \exp(2\pi i/8)$	
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	z	
E_1	$\begin{Bmatrix} 1 & \varepsilon & i & -\varepsilon^* & -1 & -\varepsilon & -i & \varepsilon^* \\ 1 & \varepsilon^* & -i & -\varepsilon & -1 & -\varepsilon^* & i & \varepsilon \end{Bmatrix}$								(x, y), (R_x, R_y)	
E_2	$\begin{Bmatrix} 1 & i & -1 & -i & 1 & i & -1 & -i \\ 1 & -i & -1 & i & 1 & -i & -1 & i \end{Bmatrix}$									$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix} 1 & -\varepsilon^* & -i & \varepsilon & -1 & \varepsilon^* & i & -\varepsilon \\ 1 & -\varepsilon & i & \varepsilon^* & -1 & \varepsilon & -i & -\varepsilon^* \end{Bmatrix}$									(xz, yz)

▸ *The* C_{nv} *Groups*

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

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

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	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	$(x, y), (R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	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	$(x, y), (R_x, R_y)$	(xz, yz)
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	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	$(x, y), (R_x, R_y)$	(xz, yz)
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	xz, yz
A_u	1	1	−1	−1	z	
B_u	1	−1	−1	1	x, y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5	$\varepsilon = \exp(2\pi i/3)$	
A'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E'	1	ε	ε^*	1	ε	ε^*	(x, y)	$(x^2 - y^2, xy)$
	1	ε^*	ε	1	ε^*	ε		
A''	1	1	1	−1	−1	−1	z	
E''	1	ε	ε^*	−1	$-\varepsilon$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)
	1	ε^*	ε	−1	$-\varepsilon^*$	$-\varepsilon$		

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)	(xz, yz)
	1	$-i$	−1	i	1	$-i$	−1	i		
A_u	1	1	1	1	−1	−1	−1	−1	z	
B_u	1	−1	1	−1	−1	1	−1	1		
E_u	1	i	−1	$-i$	−1	$-i$	1	i	(x, y)	
	1	$-i$	−1	i	−1	i	1	$-i$		

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	$\varepsilon = \exp(2\pi i/5)$	
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^*	(x, 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	z	
E_1''	1	ε	ε^2	ε^{2*}	ε^*	−1	$-\varepsilon$	$-\varepsilon^2$	$-\varepsilon^{2*}$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)
	1	ε^*	ε^{2*}	ε^2	ε	−1	$-\varepsilon^*$	$-\varepsilon^{2*}$	$-\varepsilon^2$	$-\varepsilon$		
E_2''	1	ε^2	ε^*	ε	ε^{2*}	−1	$-\varepsilon^2$	$-\varepsilon^*$	$-\varepsilon$	$-\varepsilon^{2*}$		
	1	ε^{2*}	ε	ε^*	ε^2	−1	$-\varepsilon^{2*}$	$-\varepsilon$	$-\varepsilon^*$	$-\varepsilon^2$		

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	$\varepsilon = \exp(2\pi i/6)$	
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	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	(R_x, R_y)	(xz, yz)
	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε		
E_{2g}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		$(x^2 - y^2, xy)$
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$		
A_u	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	z	
B_u	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
E_{1u}	1	ε	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	−1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	(x, y)	
	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε	−1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$		
E_{2u}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	−1	ε^*	ε	−1	ε^*	ε		
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	−1	ε	ε^*	−1	ε	ε^*		

.../12

THE DIHEDRAL GROUPS

▸ *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	z, R_z	xy
B_2	1	−1	1	−1	y, R_y	xz
B_3	1	−1	−1	1	x, R_x	yz

D_3	E	$2C_3$	$3C_2$	(x axis is coincident with C_2)	
A_1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	−1	z, R_z	
E	2	−1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

D_4	E	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$	(x axis coincident with C_2')	
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	−1	−1	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	$(x, y), (R_x, R_y)$	(xz, yz)

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

D_6	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	(x axis coincident with C_2')	
A_1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	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	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

► *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	xz
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	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	(x axis coincident with C_2)	
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	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	(x axis coincident with C_2')	
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)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	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	(x, y)	

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$	(x axis coincident with C_2)	
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	(x, 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	z	
E_1''	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(R_x, R_y)	(xz, yz)
E_2''	2	2 cos 144°	2 cos 72°	0	−2	−2 cos 144°	−2 cos 72°	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$	(x axis coincident with C_2')	
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)	(xz, yz)
E_{2g}	2	−1	−1	2	0	0	2	−1	−1	2	0	0		(x^2-y, 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	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	(x, y)	
E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0		

D_{4h}	E	$2C_4$	$2C_4^2$	$2C_4^3$	C_2	$4C_2'$	$4C_2''$	i	$2S_4^3$	$2S_4$	$2S_4^3$	σ_h	$4\sigma_v$	$4\sigma_d$	(x axis coincident with C_2')	
A_{1g}	1	1	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	−1	−1	R_z	
B_{1g}	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_{1g}	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	0	0	−2	2	0	0	2	0	0	−2	2	0	0		(x^2-y^2, xy)
E_{3g}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0		
A_{1u}	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	z	
B_{1u}	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_{1u}	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	−2	$-\sqrt{2}$	$\sqrt{2}$	0	2	0	0	(x, y)	
E_{2u}	2	0	0	−2	2	0	0	−2	0	0	2	−2	0	0		
E_{3u}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	−2	$\sqrt{2}$	$-\sqrt{2}$	0	2	0	0		

► *The D_{nd} Groups*

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$	(x axis coincident with C_2')	
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	z	xy
E	2	0	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$	(x axis coincident with C_2)	
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)	$(x^2-y^2, xy); (xz, yz)$
A_{1u}	1	1	1	−1	−1	−1		
A_{2u}	1	1	−1	−1	−1	1	z	
E_u	2	−1	0	−2	1	0	(x, y)	

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$	(x axis coincident with C_2')	
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	z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(x, 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)	(xz, yz)

D_{5d}	1	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$	(x axis coincident with C_2)	
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)	(xz, yz)
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	z	
E_{1u}	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(x, 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	$6C'_2$	$6\sigma_d$	(x axis coincident with C_2)	
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	z	
E_1	2	$\sqrt{3}$	1	0	−1	$-\sqrt{3}$	−2	0	0	(x, 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)	(xz, yz)

THE CUBIC GROUPS

▸ *Tetrahedral Groups*

T	E	$4C_3$	$4C_3^2$	$3C_2$	$\varepsilon = \exp(2\pi i/3)$	
A	1	1	1	1		$x^2 + y^2 + z^2$
E	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & 1 \\ 1 & \varepsilon^* & \varepsilon & 1 \end{Bmatrix}$					$(2z^2 - x^2 - y^2, x^2 - y^2)$
T	3	0	0	−1	$(R, R_y, R_z), (x, y, z)$	(xy, xz, yz)

T_h	E	$4C_3$	$4C_3^2$	$3C_2$	i	$4S_6$	$4S_6^5$	$3\sigma_h$	($\varepsilon = \exp(2\pi i/3)$	
A_g	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_u	1	1	1	1	−1	−1	−1	−1		
E_g	1	ε	ε^*	1	1	ε	ε^*	1		$(2z^2 - x^2 - y^2,$
	1	ε^*	ε	1	1	ε^*	ε	1		$x^2 - y^2)$
E_u	1	ε	ε^*	1	−1	$-\varepsilon$	$-\varepsilon^*$	−1		
	1	ε^*	ε	1	−1	$-\varepsilon^*$	$-\varepsilon$	−1		
T_g	3	0	0	−1	3	0	0	−1	(R_x, R_y, R_z)	(xz, yz, xy)
T_u	3	0	0	−1	−3	0	0	1	(x, y, z)	

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	(x, y, z)	(xy, xz, yz)

► *Octahedral Groups*

O	E	$6C_4$	$3C_2(=C_4^2)$	$8C_3$	$6C_2$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	−1	1	1	−1		
E	2	0	2	−1	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	1	−1	0	−1	$(R_x, R_y, R_z), (x, y, z)$	
T_2	3	−1	−1	0	1		(xy, xz, yz)

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		(xz, yz, xy)
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	(x, y, z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

Pemalar Asas dalam Kimia Fizik

Simbol	Keterangan	Nilai
N_A	Nombor Avogadro	6.022×10^{23} mol^{-1}
F	Pemalar Faraday	96,500 C mol^{-1}, atau coulomb per mol, elektron
e	Cas elektron	4.80×10^{-10} esu 1.60×10^{-19} C atau coulomb
m_e	Jisim elektron	9.11×10^{-28} g 9.11×10^{-31} kg
m_p	Jisim proton	1.67×10^{-24} g 1.67×10^{-27} kg
h	Pemalar Planck	6.626×10^{-27} erg s 6.626×10^{-34} J s
c	Halaju cahaya	3.0×10^{10} cm s^{-1} 3.0×10^{8}m s^{-1}
R	Pemalar gas	8.314×10^{7} erg K^{-1} mol^{-1} 8.314 J K^{-1} mol^{-1} 0.082 *l* atm K^{-1} mol^{-1} 1.987 cal K^{-1} mol^{-1}
k	Pemalar Boltzmann	1.380×10^{-16} erg K^{-1} molekul^{-1} 1.380×10^{-23} J K^{-1} molekul^{-1}
g		981 cm s^{-2} 9.81 m s^{-2}
1 atm		76 cmHg 1.013×10^{6} dyne cm^{-2} 101,325 N m^{-2}
$2.303 \frac{RT}{F}$		0.0591 V, atau volt, pada 25 °C

Berat Atom yang Berguna

H = 1.0	C = 12.0	I = 126.9	Fe = 55.8	As = 74.9
Br = 79.9	Cl = 35.5	Ag = 107.9	Pb = 207.0	Xe = 131.1
Na = 23.0	K = 39.1	N = 14.0	Cu = 63.5	F = 19.0
O = 16.0	S = 32.0	P = 31.0	Ca = 40.1	Mg = 24.0
Sn = 118.7	Cs = 132.9	Te = 128.0		