UNIVERSITI SAINS MALAYSIA

PEPERIKSAAN KURSUS SEMASA CUTI PANJANG
SIDANG AKADEMIK 2007/2008

JUN 2008

JIK 317 – KIMIA KUANTUM DAN TEORI KUMPULAN

MASA : 3 JAM

Sila pastikan bahawa kertas peperiksaan ini mengandungi **SEMBILAN** muka surat yang bercetak sebelum anda memulakan peperiksaan ini.

Jawab **SEMUA** soalan.

Setiap jawapan mesti dijawab di dalam buku jawapan yang disediakan.

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

1. Keadaan bagi suatu sistem kuantum diberikan oleh ungkapan

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

dengan

$$\begin{aligned} \widehat{H}\phi_1 &= \hbar\omega\phi_1 \\ \widehat{H}\phi_2 &= 2\hbar\omega\phi_2 \\ \widehat{H}\phi_3 &= 3\hbar\omega\phi_3 \\ \widehat{H}\phi_4 &= 4\hbar\omega\phi_4 \end{aligned}$$

$\widehat{H}$ adalah operator jumlah tenaga.

(a) Jika hanya satu pengukuran tenaga dilakukan pada sistem tersebut, berapakah kebarangkalian untuk mendapatkan setiap nilai eigen yang diberikan?

(10 markah)

(b) Dapatkan nilai jangkaan bagi pengukuran tenaga.

(10 markah)

2. Tunjukkan bahawa untuk suatu zarah berjisim m yang bergerak dalam kotak tiga dimensi, jika tenaga keupayaan V adalah sifar di kawasan $0 \le x \le a$, $0 \le y \le b$, $0 \le z \le c$, dan $V = \infty$ di kawasan lain, fungsi gelombang untuk zarah tersebut ialah

$$\psi(x,y,z) = \frac{2\sqrt{2}}{\sqrt{abc}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right) \sin\left(\frac{n_z \pi}{c} z\right)$$

dan tenaganya diberikan oleh

$$E_{n_x,n_y,n_z} = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right) \text{ dengan } n_x,\ n_y,\ n_z = 1,2,3,\ldots$$

(20 markah)

3. (a) Tunjukkan unsur-unsur simetri yang sepunya dan yang tidak sepunya bagi molekul BCl_3 dan PCl_3. Gunakan lakaran yang berlainan bagi setiap unsur simetri.

(12 markah)

(b) Tunjukkan bagaimana anda dapat menerbitkan kumpulan titik bagi molekul $POCl_3$.

(8 markah)

4. Senaraikan langkah-langkah yang mana Jadual Karakter boleh digunakan untuk menentukan orbital-orbital yang terlibat dalam pengikatan sigma dan pi bagi sesuatu molekul. Gunakan ion ClO_4^- sebagai contoh.

(20 markah)

5. Tunjukkan dengan jelas bagaimana spektroskopi IR dan Raman boleh digunakan untuk membezakenali antara bentuk satah dan piramid bagi molekul PF_3.

(20 markah)

Character tables

C_{2v}, $2mm$	E	C_2	σ_v	σ_v'	$h=4$	
A_1	1	1	1	1	z, z^2, x^2, y^2	
A_2	1	1	−1	−1	xy	R_z
B_1	1	−1	1	−1	x, xz	R_y
B_2	2	−1	−1	1	y, yz	R_x

C_{3v}, $3m$	E	$2C_3$	$3\sigma_v$	$h=6$	
A_1	1	1	1	z, z^2, x^2+y^2	
A_2	1	1	−1		R_z
E	2	−1	0	(x, y), (xy, x^2-y^2), (xz, yz)	(R_x, R_y)

C_{4v}, $4mm$	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$	$h=8$	
A_1	1	1	1	1	1	z, z^2, x^2+y^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	−2	0	0	0	(x, y), (xz, yz)	(R_x, R_y)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$	$h=10$, $\alpha=72°$	
A_1	1	1	1	1	z, z^2, x^2+y^2	
A_2	1	1	1	−1	-	R_z
E_1	2	$2\cos\alpha$	$2\cos 2\alpha$	0	(x, y), (xz, yz)	(R_x, R_y)
E_2	2	$2\cos 2\alpha$	$2\cos\alpha$	0	(xy, x^2-y^2)	

The groups C_1, C_s, C_i

C_1 (1)	E	$h = 1$
A	1	

$C_s = C_h$ (m)	E	σ_h	$h = 2$	
A′	1	1	x, y, R_z	x^2, y^2, z^2, xy
A″	1	−1	z, R_x, R_y	yz, zx

$C_i = S_2$ ($\bar{1}$)	E	i	$h = 2$	
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, zx, yz$
A_u	1	−1	x, y, z	

The groups C_n

C_2 (2)	E	C_2	$h = 2$	
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	−1	x, y, R_x, R_y	yz, zx

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

C_4 (4)	E	C_4	C_2	C_4^3	$h = 4$	
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	$\left\{\begin{matrix} 1 \\ 1 \end{matrix}\right.$	$\begin{matrix} i \\ -i \end{matrix}$	$\begin{matrix} -1 \\ 1 \end{matrix}$	$\left.\begin{matrix} -i \\ i \end{matrix}\right\}$	$(x, y)(R_x, R_y)$	(yz, zx)

The groups C_{nv}

C_{2v} (2*mm*)	E	C_2	$\sigma_v\,(xz)$	$\sigma'_v(yz)$	$h=4$	
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	zx
B_2	1	−1	−1	1	y, R_x	yz

C_{3v} (3*m*)	E	$2C_3$	$3\sigma_v$	$h=6$	
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)\ (R_x, R_y)$	$(x^2-y^2, xy)\ (zx, yz)$

C_{4v} (4*mm*)	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$	$h=8$	
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	$(x, y)\ (R_x, R_y)$	(zx, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$	$h=10,\ \alpha=72°$	
A_1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	−1	R_z	
E_1	2	$2\cos\alpha$	$2\cos 2\alpha$	0	$(x, y)(R_x, R_y)$	(zx, yz)
E_2	2	$2\cos 2\alpha$	$2\cos\alpha$	0		(x^2-y^2, xy)

C_{6v} (6*mm*)	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$	$h=12$	
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	$(x, y)\ (R_x, R_y)$	(zx, yz)
E_2	2	−1	−1	2	0	0		(x^2-y^2, xy)

$C_{\infty v}$	E	C_2	$2C_\phi$	$\infty\sigma_v$	$h=\infty$	
$A_1\ (\Sigma^+)$	1	1	1	1	z	x^2+y^2, z^2
$A_2\ (\Sigma^-)$	1	1	1	−1	R_z	
$E_1\ (\Pi)$	2	−2	$2\cos\phi$	0	$(x, y)\ (R_x, R_y)$	(zx, yz)
$E_2\ (\Delta)$	2	2	$2\cos 2\phi$	0		(xy, x^2-y^2)
⋮	⋮	⋮	⋮	⋮		

The groups D_n

D_2 (222)	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	$h=4$	
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	zx
B_3	1	−1	−1	1	x, R_x	yz

D_3 (32)	E	$2C_3$	$3C_2$	$h=6$	
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	−1	z, R_z	
E	2	−1	0	$(x, y)\ (R_x, R_y)$	$(x^2-y^2, xy)\ (zx, yz)$

The groups D_{nh}

D_{2h} (mmm)	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		$h=8$
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	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} ($\bar{6}m2$)	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		$h=12$
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)	(zx, yz)

D_{4h} ($4/mmm$)	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		$h=16$
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)	(zx, 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	$2S_5$	$2S_5^2$	$5\sigma_v$		$h=20$, $\alpha=72°$
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 α	2 cos 2α	0	2	2 cos α	2 cos 2α	0	(x, y)	
E_2'	2	2 cos 2α	2 cos α	0	2	2 cos 2α	2 cos α	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 α	2 cos 2α	0	−2	−2 cos α	−2 cos 2α	0	(R_x, R_y)	(zx, yz)
E_2''	2	2 cos 2α	2 cos α	0	−2	−2 cos 2α	−2 cos α	0		

The groups D_{nh} (continued)

D_{6h} (6/*mmm*)	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$	$h=24$	
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)	(zx, yz)
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	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		

$D_{\infty h}$	E	$\infty C_2'$	$2C_\phi$	i	$\infty\sigma_v$	$2S_\phi$	$h=\infty$	
$A_{1g}(\Sigma_g^+)$	1	1	1	1	1	1		z^2, x^2+y^2
$A_{1u}(\Sigma_u^-)$	1	−1	1	−1	1	−1	z	
$A_{2g}(\Sigma_g^-)$	1	−1	1	1	−1	1	R_z	
$A_{2u}(\Sigma_u^-)$	1	1	1	−1	−1	−1		
$E_{1g}(\Pi_g)$	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
$E_{1u}(\Pi_u)$	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
$E_{2g}(\Delta_g)$	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
$E_{2u}(\Delta_u)$	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

The groups D_{nd}

$D_{2d} = V_d$ ($\bar{4}2m$)	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$	$h=8$	
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)	(zx, yz)

D_{3d} ($\bar{3}m$)	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$	$h=12$	
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) (zx, 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)	

The groups D_{nd} (continued)

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$	$h=16$	
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)	(zx, yz)

The cubic groups

T_d ($\bar{4}3m$)	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	$h=24$	
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, yz, zx)

O_h ($m3m$)	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	$h=48$	
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	(x, y, z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

The icosahedral group

I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	$h=60$	
A_1	1	1	1	1	1		$x^2+y^2+z^2$
T_1	3	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	0	−1	(x, y, z) (R_x, R_y, R_z)	
T_2	3	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	0	−1		
G	4	−1	−1	1	0		
H	5	0	0	−1	1		$(2z^2-x^2-y^2, x^2-y^2, xy, yz, zx)$

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