UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Session 2008/2009

November 2008

ZAE 385/4 - Applied Spectroscopy
[Spektroskopi Gunaan]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains **ELEVEN** printed pages before you begin the examination.

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

Instruction: *Answer **FOUR (4)** questions. Answer **QUESTION 1** which is **compulsory** and **THREE (3)** other questions. Student are allowed to answer all questions in Bahasa Malaysia or in English.*

*[**Arahan**: Jawab **EMPAT (4)** soalan. Jawab **SOALAN 1** yang **diwajibkan** dan **TIGA (3)** soalan lain. Pelajar dibenarkan menjawab semua soalan sama ada dalam Bahasa Malaysia atau Bahasa Inggeris.]*

.../2-

1. (a) Define the following terms while giving an example for each:
[Takrifkan terma-terma berikut dengan memberi contoh bagi setiapnya :]

Raman spectroscopy (with equation), Infra Red Spectroscopy (with equation), stokes scattering (with energy diagram), anti stokes scattering (with energy diagram), Rayleigh Scattering (with energy diagram):
[Spektroskopi Raman (bersama persamaan), Spektroskopi Infra Merah (bersama persamaan), Serakan Stokes (bersama rajah tenaga), Serakan anti-Stokes (bersama rajah tenaga), Serakan Rayleigh (bersama rajah tenaga), momen dwikutub (bersama persamaan), keterkutuban (bersama persamaan), petua pemilihan.]

(35/200)

(b) Based upon the chloroform $CHCl_3$ Infra red transmission properties given on table (i) below, fill and complete the table (ii) below:
[Berdasarkan sifat-sifat transmisi infra-merah klorofom $CHCl_3$ yang diberi pada jadual (i) di bawah, isikan dan lengkapkan jadual (ii) di bawahnya :]

(35/200)

Table i
[Jadual i]

Fundamental Infra Red Frequencies of $CHCl_3$
[Frekuensi asas infra-merah bagi $CHCl_3$]

Frequency designation *[Gelaran frekuensi]*	**Frequency** *[Frekuensi]* (cm^{-1})	**Representation** *[Perwakilan]*
ν_1	**3025**	**A1**
ν_2	**668**	**A1**
ν_3	**373**	**A1**
ν_4	**1203**	**E**
ν_5	**773**	**E**
ν_6	**261**	**E**

...3/-

Table ii
[Jadual ii]

Overtones and combinations for $CHCl_3$
[Overtone dan kombinasi bagi $CHCl_3$]

Frequency *[Frekuensi]* (cm^{-1})	**Frequency Designation** *[Gelaran Frekuensi]*	**Representation** *[Representasi]*
2400	$?+\nu_4$	**$A1+A_2+E$**
1521	$?+\nu_5$	**$A1+A_2+E$**
1423	$?+\nu_2$	**E**
497	$\nu_5 - ?$	**A1+A2+E**
230	$\nu_5 - ?$	**A1+A2+3E**

(c) Based upon the table iii below , show and explain the interaction of :
[Berdasarkan kepada jadual iii berikut, tunjukkan dan jelaskan interaksi bagi :]

i) a degenerate mode E with itself.
[satu mod E degenerat dengannya sendiri]

ii) a breathing mode A1 with itself.
[satu mod bernafas A1 dengannya sendiri]

iii) a breathing mode with a degenerate mode
[satu mod bernafas dengan satu mod degenerat]

(30/200)

...4/-

Table iii
[Jadual iii]

	E	$2C_3$	$3\sigma v$
A1	1	1	1
E	2	-1	0

(d) (i) Derive the equation of selection rule for transitions between vibration levels.
[Terbitkan persamaan petua pemilihan bagi transisi-transisi antara paras-paras getaran.]

(50/200)

(e) Explain the following CHCl3 Infrared activity of the table below:
[Terangkan aktiviti infra-merah $CHCl_3$ di dalam jadual berikut :]

Representation *[Representasi]*	Infra Red Activity *[Aktiviti infra-merah]*
A1	Allowed
A2	Forbidden
E	Allowed
A1xA1	Allowed
A1xA2	Forbidden
A1xE	Allowed
A2xA2	Allowed
A2xE	Allowed
ExE	Allowed
$A1^n$	Allowed
(n even)$A2^n$	Allowed
(n odd)$A2^n$	Forbidden
E^n	Allowed

(50/200)

...5/-

2. (a) Diagonalize the following matrix M:
[Pepenjurukan matriks M berikut :]

$$\begin{pmatrix} 0 & 2 \\ 2 & 3 \end{pmatrix}$$

(32/100)

(b) Prove that the two vectors orthogonal.
[Buktikan bahawa kedua-dua vektor adalah ortogon]

(8/100)

(c) Fill the remaining terms on the cayley table below :
[Penuhkan baki terma-terma di dalam jadual Cayley berikut :]

(40/100)

	E	C_3	C_3^2	σ_v^a	σ_v^b	σ_v^c
E		C_3				
C_3			C_3			
C_3^2						
σ_v^a			σ_v^c			
σ_v^b		σ_v^c			E	C_3
σ_v^c	σ_v^c			C_3		

(d) Express the following terms while giving an example:
[Nyatakan maksud terma-terma berikut sambil memberi satu contoh pada setiapnya :]

reducible representation, irreducible representation.
[representasi terturunkan, representasi tak-terturunkan]

(20/100)

...6/-

3. (a) Derive Lagrange's equation (1 dimensional system) of a particle of mass m moving in Earth's gravitational field.
[Terbitkan persamaan Lagrange (sistem 1 dimensi) bagi satu zarah berjisim m yang bergerak di dalam medan graviti Bumi.]

(10/100)

(b) Figure 1 shows **three** equal masses connected by two identical springs and constrained to vibrate along the x-axis derive :
*[Rajah 1 menunjukkan **tiga** jisim sama yang bersambung dengan dua spring serba-sama dan terbendung untuk bergetar pada paksi-x. Terbitkan :]*

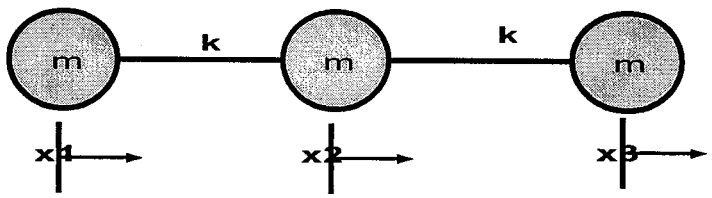

Figure 1

i) The potential energy
[Tenaga keupayaan]

ii) The kinetic energy
[Tenaga kinetik]

...7/-

iii) Solve the Lagrange equation of this system
[Selesaikan persamaan Lagrange bagi sistem ini]

iv) Calculate the oscillating modes of vibrations
[Hitungkan mod-mod osilasi getaran]

v) One of these modes will have a frequency equal to zero: what does this mode represent (explain in few words)?
[Salah satu dari mod-mod ini mempunyai frekuensi sama dengan sifar : Apakah yang diwakili oleh mod ini (terangkan dengan ringkas)?]

(65/100)

(c) $\mathbf{V}= a\mathbf{V}_1+b\mathbf{V}_2+c\mathbf{V}_3$, where $\mathbf{V}_1,\mathbf{V}_2$ and $\mathbf{V}_3$ are the eigenvectors of the **Symmetric** matrix **M** having an associated **non-degenerate** eigenvalues of λ_1, λ_2 *and* λ_3.
*[$V= aV_1+bV_2+cV_3$, di mana V_1, V_2 and V_3 adalah vektor-vektor eigen bagi satu matriks **bersimetri** M yang memiliki nilai eigen tak-degenerat yang berkaitan, iaitu λ_1, λ_2 and λ_3]*

If a projection operator is defined such as:
[Jika satu operator pengunjur ditakrifkan sebagai :]

$$\mathbf{P_1V}=a\mathbf{V_1},\quad \mathbf{P_2V}=b\mathbf{V_2},\quad \mathbf{P_3V}=c\mathbf{V_3}$$

Prove that:
[Buktikan bahawa :]

$$\mathbf{P_1}= [(\mathbf{M}-\lambda_2\mathbf{I})(\mathbf{M}-\lambda_3\mathbf{I})] / [(\lambda_1-\lambda_2)(\lambda_1-\lambda_3)]$$

(25/100)

...8/-

4. (a) Figure 2 shows a tri-atomic planar equilateral molecule having an equal stiffness constants between every 2 atoms. The normalized amplitude of the oscillating modes are listed on the table below :
[Rajah 2 menunjukkan satu molekul sama-sisi tri-atom menyatah yang memiliki nilai kakuan malar di antara setiap dua atom. Amplitud ternormal bagi mod-mod osilasi disenaraikan di dalam jadual berikut :]

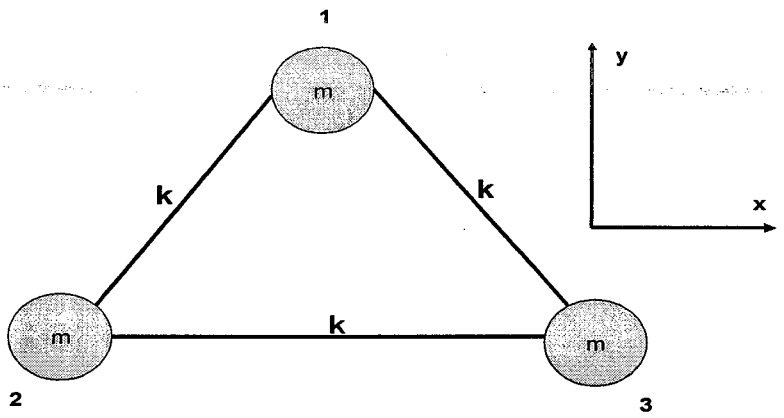

Figure number 2

λ	a1	a2	a3	a4	a5	a6
3	0	$1/\sqrt{3}$	-1/2	$-1/(2\sqrt{3})$	1/2	$-1/(2\sqrt{3})$
3/2	$1/\sqrt{3}$ 0	0 $1/\sqrt{3}$	$-1/(2\sqrt{3})$ 1/2	-1/2 $-1/(2\sqrt{3})$	$-1/(2\sqrt{3})$ -1/2	1/2 $-1/(2\sqrt{3})$
0	$1/\sqrt{3}$ 0 $1/\sqrt{3}$	0 $1/\sqrt{3}$ 0	$1/\sqrt{3}$ 0 $-1/(2\sqrt{3})$	0 $1/\sqrt{3}$ 1/2	$1/\sqrt{3}$ 0 $-1/(2\sqrt{3})$	0 $1/\sqrt{3}$ -1/2

...9/-

i) specify the degeneracy degree of every eigenvalue.
[tentukan darjah kedegeneratan bagi setiap nilai eigen.]

(15/100)

ii) Draw the oscillating modes based upon their normalized amplitudes.
[Lukiskan mod-mod osilasi berdasarkan amplitud-amplitud ternormal mereka.]

(60/100)

b) A degenerate matrix having three eigenvalues $\lambda_1, \lambda_2, \lambda_3$ with $\lambda_2=\lambda_3$. Prove that the projection matrix associated with the degenerate eigenvalues has the following form:
[Satu matriks degenerat mempunyai tiga nilai eigen $\lambda_1, \lambda_2, \lambda_3$ dengan $\lambda_2=\lambda_3$. Buktikan bahawa matriks unjuran berkaitan dengan nilai eigen degenerat tersebut memiliki bentuk :]

$$P_{22}= (M-\lambda_1 I)/(\lambda_2-\lambda_1).$$

(25/100)

5. Figure 3 shows a H_2O molecule that has many oscillation modes; these modes include rotational, vibration and translational. The vibration mode is divided into stretching and deflection.
[Rajah 3 menunjukkan satu molekul H_2O yang memiliki banyak mod osilasi; Mod-mod ini termasuk putaran, getaran dan translasi. Mod getaran terbahagi kepada regangan dan pesongan.]

...10/-

Hint : you may use the following formula to complete filling the table:
[Petua : anda mungkin boleh menggunakan rumus berikut untuk melengkapkan jadual tersebut.]

$$n_i = (1/h)\sum g_c \chi_i \chi_r$$

where:
[dimana]

n_i: the number of times the irreducible representation i occurs in the reducible representation.
[bilangan kali representasi i tak-terturunkan berlaku di dalam representasi terturunkan]

h: order of the group or total number of symmetry operations.
[tertib kumpulan atau jumlah bilangan operasi simetri]

g_c: number of symmetry operation in symmetry class.
[bilangan operasi simetri di dalam kelas simetri]

χ_i: character of the irreducible representation.
[ciri representasi tak-terturunkan.]

χ_r: character of the reducible representation.
[ciri representasi terturunkan.]

iii) Explain in few words the B_2 mode (row number 4) in the following table as well as the last 2 columns which column is raman active and which is infra red active.
[Terangkan dengan ringkas mod B_2 (baris nombor 4) di dalam jadual berikut bersama dengan 2 lajur terakhir, yang mana satu aktif roman dan yang mana aktif infra-merah.]

(30/100)

...12/-

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A1	1	1	1	1	z	x^2 y^2 z^2
A2	1	1	-1	-1	R_z	xy
B1	1	-1	1	-1	x, R_y	xz
B2	1	-1	-1	1	y,R_x	yz

iv) Deduce the Γtranslation , Γrotation and Γdeflection .
[Deduksikan Γtranslasi , Γputaran and Γpesongan]

Hint : Γtotal(3N) = Γtranslation + Γrotation + Γvibration.
[Petua : Γjumlah(3N) = Γtranslasi + Γputaran + Γgetaran]

(40/100)

- oooOooo -