



University of Technology
Department of Laser & Opto-electronic Engineering
Final Examination 2011-2012

Subject: Spectroscopy
Division: laser Engineering
Examiner: Dr. Fareed Rashid

Class: 3rd year
Time: 3 hours
Date: 5 / 6 / 2012



Answer five questions only

Q1) Find:

- (a) The transition energy levels of a non rigid molecule (in wavenumber), if the rotational constant is 10 cm^{-1} , the centrifugal distortion constant is $2.31 \times 10^{-3} \text{ cm}^{-1}$ and the rotational quantum number is 2.
- (b) The vibration energy levels (in wavenumber) of anharmonic oscillator, if an oscillation frequency is 1876.2 cm^{-1} , the anharmonicity constant is 0.016 and the vibration quantum number is 3.

Q2) Starting from the combined rotation-vibration energy prove that:

$$\dot{v}_{\text{spect}} = \dot{w}_0 + 2Bm - 4Dm^3 \quad \text{cm}^{-1} \quad (m = +1, +2, \dots)$$

Q3)

- (a) Find the population levels according to Boltzmann distribution if the rotational quantum number is 2, the rotational constant is 5 cm^{-1} .
- (b) Find the angular momentum of the rotator.
- (c) Find the maximum population.

Q4) a) In the photo –electric effect experiment, if the stopping potential ($v_0 = 4 \text{ volt}$) and the work function of the surface is ($\phi = 1.38 \text{ volts}$), find the wavelength of the emitted radiation.

b) State only 3 types of dispersers

Q5) a) Find the value of the energy difference between the $n=2$ and $n=3$ levels for lithium atom ($z=3$) in electron volts (ev), then convert it into (cm^{-1}).

b) Explain stark effect.

Q6) a) Find the frequency of radiation (using Balmer series) of the fourth level ($n=4$) if the Rydberg constant ($R = 1.966 \times 10^7 \text{ m}$).

b) What are the two corrections of central field model of atoms having more than one electron. (state them only).

Useful constants

$k = 1.381 \times 10^{-23} \text{ JK}^{-1}$; $T = 300 \text{ } ^\circ\text{K}$ (at room temperature); $h = 6.626 \times 10^{-34} \text{ Js}$;
 $c = 2.998 \times 10^8 \text{ ms}^{-1}$; atomic masses: $H = 1.673 \times 10^{-27} \text{ kg}$; $F = 31.55 \times 10^{-27} \text{ kg}$.

Charge of (e) 1.6×10^{-19}

Mass of (e)

$9.1 \times 10^{-31} \text{ kg}$

[Signature]

Q1. ~~Analytical expression~~

(a) The transition energy levels for a non rigid molecule (in wave number).

$$\begin{aligned}\epsilon_{J=2} &= B J(J+1) - D J^2(J+1)^2 \quad \text{cm}^{-1} \\ &= 10 \times 2(2+1) - [2.31 \times 10^{-3} \times (2)^2(2+1)^2] \\ &= 59.916 \quad \text{cm}^{-1}\end{aligned}$$

(b) The vibrational energy levels of harmonic oscillator (in wave number).

$$\begin{aligned}\epsilon_v &= \left(v + \frac{1}{2}\right) \bar{W}_e - \left(v + \frac{1}{2}\right)^2 \bar{W}_e x_e \quad \text{cm}^{-1} \\ \therefore \epsilon_{v=3} &= \left(3 + \frac{1}{2}\right) \times 1876.2 - \left(3 + \frac{1}{2}\right)^2 \times 1876.2 \times 0.016 \\ &= 6198.9648 \quad \text{cm}^{-1}\end{aligned}$$

Q.2

$$\bar{\nu}_{\text{spect.}} = \bar{\omega}_0 + 2Bm - 4Dm^3 \quad \text{cm}^{-1}, \quad (m = \pm 1, \pm 2, \dots)$$

The combined rotation-vibration energy.

$$E_{\text{total}} = E_{\text{rot.}} + E_{\text{vib}} \quad \text{joule}$$

$$\epsilon_{\text{total}} = \epsilon_{\text{rot.}} + \epsilon_{\text{vib.}} \quad \text{cm}^{-1}$$

$$\epsilon_{J,v} = \epsilon_J + \epsilon_v$$

$$\epsilon_J = BJ(J+1) - DJ^2(J+1)^2 + HJ^3(J+1)^3 + \dots \quad \text{cm}^{-1}$$

$$\epsilon_v = \left(\nu + \frac{1}{2}\right) \bar{\omega}_e - \left(\nu + \frac{1}{2}\right)^2 \bar{\omega}_e x_e \quad \text{cm}^{-1} \quad (\nu = 0, 1, 2, \dots)$$

$$\therefore \epsilon_{J,v} = \epsilon_J + \epsilon_v$$

$$= BJ(J+1) - DJ^2(J+1)^2 + HJ^3(J+1)^3 + \dots \\ + \left(\nu + \frac{1}{2}\right) \bar{\omega}_e - \left(\nu + \frac{1}{2}\right)^2 \bar{\omega}_e x_e \quad \text{cm}^{-1}$$

We ignore the small centrifugal distortion constant D, H , etc. then:

$$\epsilon_{\text{Total}} = \epsilon_{J,v} = BJ(J+1) + \left(\nu + \frac{1}{2}\right) \bar{\omega}_e - x_e \left(\nu + \frac{1}{2}\right)^2 \bar{\omega}_e$$

$$\text{We have } \Delta\nu = \pm 1, \pm 2, \dots \\ \Delta J = \pm 1$$

then the transition: (for $\nu=0 \rightarrow \nu=1$)

$$\Delta\epsilon_{J,v} = \epsilon_{J',\nu=1} - \epsilon_{J'',\nu=0} \\ = BJ'(J'+1) + \frac{1}{2} \bar{\omega}_e - \frac{1}{4} \bar{\omega}_e x_e - \left\{ BJ''(J''+1) + \frac{1}{2} \bar{\omega}_e - \frac{1}{4} \bar{\omega}_e x_e \right\} \\ = \bar{\omega}_0 + B(J' - J'')(J' + J'' + 1) \quad \text{cm}^{-1}$$

$$\text{and } \bar{\omega}_0 = \bar{\omega}_e(1 - 2x_e)$$

for $\Delta J = +1$, i.e. $J = J'' + 1$ or $J - J'' = +1$

$$\therefore \Delta \epsilon_{J,v} = \bar{W}_0 + 2B(J'' + 1) \quad \text{cm}^{-1} \quad \text{--- (1)} \quad (J'' = 0, 1, 2, \dots)$$

for $\Delta J = -1$, i.e. $J = J' + 1$ or $J' - J'' = -1$

$$\therefore \Delta \epsilon_{J,v} = \bar{W}_0 - 2B(J' + 1) \quad \text{cm}^{-1} \quad \text{--- (2)} \quad (J' = 0, 1, 2, \dots)$$

$$\therefore \Delta \epsilon_{J,v} = \bar{\nu}_{\text{spect.}} = \bar{W}_0 + 2Bm \quad \text{cm}^{-1}, \quad (m = \pm 1, \pm 2, \dots)$$

replacing m by $J'' + 1$ in eq. (1) and $J' + 1$ in eq. (2)

The inclusion of centrifugal distortion constant D leads to the following expression of the spectrum

$$\Delta \epsilon = \bar{\nu}_{\text{spect.}} = \bar{W}_0 + 2Bm - 4Dm^3 \quad \text{cm}^{-1}$$

$(m = \pm 1, \pm 2, \dots)$

Q3. (a) population levels

$$\begin{aligned}\frac{N_1}{N_0} &= \exp \left\{ -Bhc J(J+1) / kT \right\} \\ &= \exp \left\{ \frac{-5 \times 6.626 \times 10^{-34} \times 2.998 \times 10^8 \times 2(2+1)}{300 \times 1.38 \times 10^{-23}} \right\} \\ &= \exp (-1.4394 \times 10^3) \\ &= 0.99856\end{aligned}$$

(b) Angular momentum

$$\begin{aligned}P &= \sqrt{J(J+1)} \quad \text{units} \\ &= \sqrt{2(2+1)} \\ &= \sqrt{6}\end{aligned}$$

(c) Maximum Population

$$\begin{aligned}J &= \sqrt{\frac{kT}{2hcB}} - \frac{1}{2} \\ &= \sqrt{\frac{1.38 \times 10^{-23} \times 300}{2 \times 6.626 \times 10^{-34} \times 2.998 \times 10^8 \times 5}} - \frac{1}{2} \\ &= 4.515187721 - \frac{1}{2} \\ &= 4.0651\end{aligned}$$

Q.4 a/ $eV_0 = hf - \phi$

$\phi = 1.38 \text{ eV}$

$e = 1.6 \times 10^{-19} \text{ C}$

$V_0 = 4 \text{ volt}$

$f = ?$

$\therefore 1.6 \times 10^{-19} \times 4 = 6.63 \times 10^{-34} \times f - 1.38$

$\therefore f = \frac{6.4 \times 10^{-19} + 1.38 \times 10^{-19}}{6.63 \times 10^{-34}}$

$f = 0.97 \times 10^{15} \text{ hertz or } s^{-1}$

$f = \frac{c}{\lambda} \Rightarrow \lambda = \frac{c}{f}$

$= 3 \times 10^8$

$= \frac{3 \times 10^8}{0.97 \times 10^{15}}$

$= 3.96 \times 10^{-7} \text{ m}$

$= 396 \text{ nm}$

b/ 1. Prism

2. Diff. grating

3. Interferometer

$= \frac{3.96 \times 10^{-7}}{1.7} \times 10^7$
 $= 2.309 \text{ m}$
 $= 230.9 \text{ nm}$

Q.5 a/ $E_n = \frac{-13.6 Z^2}{n^2}$

for Li $\Rightarrow Z = 3$

$E_2 = \frac{-13.6 \times 9}{4} = -30.6 \text{ eV}$

$E_3 = \frac{-13.6 \times 9}{9} = -13.6 \text{ eV}$

$\Delta E = 17 \text{ eV}$

(5)

$$17 \text{ eV} \times 1.6 \times 10^{-19} = 27.2 \times 10^{-19} \text{ joule}$$

b/ Stark effect

is the splitting of energy levels due to the application of electric field

The Applied E-field distorts electron configuration so induce a dipole moment $\propto E$ where α is the polarizability

hence the interaction of the induced moment with the electric field yields $\propto E^2$

Q.6

a/ $\frac{1}{\lambda} = R \left(\frac{1}{2^2} - \frac{1}{n^2} \right)$

$$\frac{R}{\lambda} = 1.966 \times 10^7 \left(\frac{1}{4} - \frac{1}{16} \right)$$

$$f = 1.966 \times 10^7 \left(\frac{3}{16} \right) \times 3 \times 10^8$$

$$f = 1.1 \times 10^{15} \text{ s}^{-1}$$

b/ 1. Electrostatic interaction (L & S coupling)

2. Magnetic interaction (J coupling)