CHE-10

BACHELOR OF SCIENCE (B.Sc.)

Term-End Examination

December, 2005

CHE-10 : SPECTROSCOPY

Time : 2 hours *Maximum Marks : 50*

Note : *Attempt any **five** questions. All questions carry equal marks.*

$h = 6{\cdot}626 \times 10^{-34}$ Js
$c = 2{\cdot}998 \times 10^{8}$ ms^{-1}
$m_N = 14{\cdot}004$
$e = 1{\cdot}602 \times 10^{-19}$ C
$m_o = 15{\cdot}9994$
$m_p = 1{\cdot}672 \times 10^{-27}$ kg

1. (a) Explain the terms 'normal and anomalous Zeeman effect'. *2*

(b) What do you understand by the 'term symbol' in the context of atoms ? Derive it for the *P* and *D* states of the hydrogen atom. *3*

(c) What are symmetry elements and symmetry operations ? Identify symmetry elements in case of ammonia molecule. 3

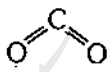
(d) How is molecular symmetry related to (i) dipole moment and (ii) optical activity ? 2

2. (a) Discuss briefly the factors affecting the intensities of rotational spectral lines. 2

(b) The rotational constant (B) for NO molecule is $1{\cdot}70\ cm^{-1}$. Calculate its bond length. 3

(c) Discuss the origin of P, Q, R branches in the IR spectrum of a vibrating rotator. 3

(d) Given below are two structures of CO_2 molecule :



O = C = O

How will you differentiate the two structures using IR and Raman spectra ? 2

3. (a) Write the energy expressions for (i) a harmonic oscillator and (ii) an anharmonic oscillator explaining various terms involved in them. What are the selection rules for these oscillators ? 4

(b) Explain Franck – Condon principle and discuss its use in explaining the intensities of spectral lines in electronic spectrum. 4

(c) The intensity of Stokes lines is generally greater than those of anti-Stokes lines. Explain. 2

4. (a) Calculate the stretching and bending modes of vibration for $CHCl_3$ and PF_3 molecules. 2

(b) Name the source of radiation and detectors for the following spectrometers : 3

(i) Microwave

(ii) IR

(iii) Raman

(c) Starting from the electronic configuration of the oxygen molecule, show that the complete term symbols for its ground state are $^3\Sigma_g^-$ and $^1\Sigma_g^+$. 3

(d) Distinguish between phosphorescence and fluorescence. 2

5. (a) Explain forbidden and allowed $d - d$ transitions with the help of examples. 2

(b) Calculate CFSE for Sc^{2+} ion. (At. No. of Sc is 21) 2

(c) Explain various terms involved in the expression for the magnetic moment of an electron. 2

(d) Write short notes on the following : 4

(i) Pascal triangle

(ii) α-cleavage

6. (a) Calculate the value of nuclear magneton for a proton. *2*

(b) Distinguish between chemical shift and coupling constant. *2*

(c) Make a rough sketch of high resolution ^{1}H-NMR spectrum of ethylene. *1*

(d) Discuss the ESR spectrum of methyl radical. *3*

(e) An M+2 peak of almost equal intensity as M^+ peak appears in the mass spectrum of bromoethane. Explain giving reason. *2*

7. (a) A compound with molecular formula C_8H_8O gives negative iodoform test and exhibits the following spectral data :

UV : λ_{max} 290 nm

IR : 3040, 2935, 2856, 2735, 1720, 1600, 1570 and 1460 cm^{-1}

NMR : (δ, $CDCl_3$) : 2·75 (*d*, 2H), 7·25 (*s*, 5H) and 9·72 (*t*, 1H)

Using the above spectral data, arrive at the structure of the compound. *4*

(b) Mercury (II) iodide is intensely coloured, though there is no possibility of $d - d$ transition in it. Explain. *2*

(c) Give one example each for the nuclei having $I = 0$, $\frac{1}{2}$ and 1. *1$\frac{1}{2}$*