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Chem(P)-IV

M.Sc. (Previous) Examination, 2019

CHEMISTRY

Paper - IV(CH-404)

(Spectroscopy)

Time Allowed : Three Hours

Maximum Marks : 75

Note: (i) No supplementary answer-book will be given to any candidate. Hence the candidates should write the answer directly in the main answer-book only.

(ii) All the parts of one question should be answered at one place in the answer book. One complete question should not be answered at different places in the answer book.

Attempt five questions in all, selecting at least one question from each Unit. All questions carry equal marks.

Unit-'I'

- 1 (a) Suppose for a rigid diatomic rotor, energy of 5th rotational energy level is 100 cm^{-1} , calculate energy gap between first excited state & second excited state in term of cm^{-1} 10

(1)

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(b) Write a short note on 'Intensity of Spectral Lines' 5

- 2 (a) The microwave spectrum of gaseous HCl consists of a series of equally spaced lines by 20.80 cm^{-1} . Calculate the internuclear distance of the molecule 7

(Given Plank's constant = $6.626 \times 10^{-34} \text{ Js}$,

Atomic mass of $^1\text{H} = 1.673 \times 10^{-27} \text{ Kg}$,

Atomic mass of $^{35}\text{Cl} = 58.06 \times 10^{-27} \text{ Kg}$)

- (b) Classify the following species as Linear rotor(s), Symmetric Top (s), Asymmetric Top (s) and Spherical Top (s). 8

PCl_3F_2 , O-Xylene, SF_4 , SO_2Cl_2 , C_3O_2 , BF_3 ,

N_2O , $\text{CH}_2 = \text{CHCl}$

Unit-'II'

- 3 (a) How would you distinguish in following pairs from IR Spectral data: 2×5

(i) Methanoic acid and Ethanoic acid

(ii) Ethyl nitrite and Nitroethane

(iii) Bromoform and Tetrachloromethane

(iv) Butanone and Ethanoyl Chloride

(v) Dimethyl amine and Trimethyl amine

- (b) Discuss metal ligand vibrations of metal carbonyls 5

- 4 (a) The vibrational levels NaI lie at the wave numbers 142.81, 427.31, 710.31, and 991.81 cm^{-1} . Show that they fit the expression
$$G(v) = \left(v + \frac{1}{2}\right) \bar{\nu} - \left(v + \frac{1}{2}\right)^2 \bar{\nu} x_e$$
 and deduce the zero point energy, and dissociation energy of the molecule. 5+5+5

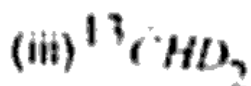
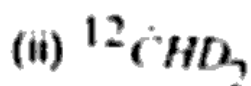
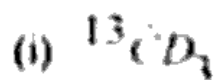
Unit-'III'

- 5 Write short notes on:
- (i) Vibrational progressions and geometry of the excited states 5
 - (ii) Spectra of alkali metal atoms 5
 - (iii) ESCA 5
- 6 (a) Using FEMO theory, estimate the wave number of the lowest energy transition in the 1,3,5-hexatriene. 6
- (b) Discuss Auger electron spectroscopy. 5
- (c) Write a short note on 'Frank-Condon Principle'. 4

Unit-'IV'

7. (a) Predict 'number of signals' in ^{13}C NMR spectra of following compounds: 1½×6
- (i) [14]-annulene
 - (ii) [18]-annulene
 - (iii) p-xylene
 - (iv) 1,3-dimethyl propadiene
 - (v) 1,4-diethyl-1-methyl cyclohexane
 - (vi) Ethanoic methanoic anhydride

(b) Predict the intensity ratio of peaks in ESR spectra of following species. 2×3



8. (a) Draw the following multiplets in ^1H NMR spectra:

(i) ddd (ii) ddt 5

(b) Discuss factors influencing coupling constant. 5

(c) Estimate the percentage of acetonitrile and benzene in a mixture, if both have same peak area in ^1H NMR spectra. 5

Unit-'V'

9. (a) Draw the following planes in cubical boxes have Miller indices as. 6

(i) $\bar{1}11$

(ii) $1\bar{1}1$

(iii) $11\bar{1}$

(b) Discuss 'Powder Method' of crystal structure analysis 5

(c) Discuss about the parameters of unit cell 4

10. (a) Differentiate between electron diffraction and neutron diffraction. 9

(b) Discuss absolute configuration of molecules with suitable examples 6

—x—

(4)

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