M. Sc. — Chem – IS (404)

5. (a) Discuss the classification of molecules in case of microwave spectroscopy. What is the difference between rigid rotator and non rigid rotator? Discuss the factors on which intensities of spectral line depends in case of microwave spectroscopy.

OR

- (b) Write the basic principle of photo electron spectroscopy. Discuss Koopman's thermo photo electron spectra of simple molecules.
- (a) Explain zero field splitting and Kramer's degeneracy in case of ESR spectroscopy. Discuss the applications of ESR spectroscopy.

OR

(b) Write the basic principle of Mossbauer spectroscopy. Discuss the applications to this technique to study the bonding and structure of iron compounds.



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2016 (January)

Time: 3 hours

Full Marks: 80

The figures in the right-hand margin indicate marks.

Answer from both the Sections as per direction.

(PHYSICAL SPECTROSCOPY)

Section - A

- Answer any four of the following: 4×4 = 16
 - (a) Calculate the first three lines in the absorption spectrum arising from 3S levels of hydrogen atom.
 - (b) Discuss the factors affecting the intensities of vibrational spectroscopy.
 - (c) Write note on ESCA.
 - (d) Discuss the important applications of photo electron spectroscopy.

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(Tum over)

- (e) Discuss the effect of isotopic substitution on spectral lines of a rotational spectra.
- (f) Draw the ESR spectrum of (i) methyl radical and (ii) triphenyl methyl radical. How do they arise?

OR

Answer all questions :

 $2 \times 8 = 16$

- (a) List all the electronic transitions in the molecule CH₃CHO and benzene.
- (b) What are hot bands?
- (c) Which of the following molecule will not show microwave rotational spectra and why ?
 - (i) H₂

(ii) HCI

(iii) H₂O

- (iv) CH₄
- (d) Write the rule of mutual exclusion principle.
- (e) The Mossbauer spectrum K₄[Fe(CN)₆] consists of one line whereas that of K₃[Fe(CN)₅NO] consists of two lines. Draw these spectra qualitatively and account for their appearance.
- (f) Draw the ESR spectra of triphenyl methyl radical and discuss its origin.

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(2)

Contd.

- (g) What is the difference between stokes line and anti-stokes line?
- (h) A molecule may possess zero vibrational energy. Comment.

Section - B

Answer all questions:

 $16 \times 4 = 64$

 (a) What is the difference between atomic spectra and moelcular spectra? Discuss the spectra of alkali metal atom.

OR

- (b) Discuss the Vibronic Transitions and Frank-Condon Principle in case of a molecule.
- (a) (i) Discuss the origin of P, Q, R lines.
 - (ii) The vibrational wave numbers of the following molecules in their v = 0 state are HCI 2885 cm⁻¹, DCI 1990 cm⁻¹, De 2990 cm⁻¹ and HD 3627 cm⁻¹. Calculate the energy change in KJ/mol of the reaction HCl + D₂ → DCl + HD.

OR

(b) Discuss the classical and quantum theory of origin of Raman lines. Explain how rule of

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(3)

(Turn over)