

M.Sc. CHEMISTRY
SECOND SEMESTER
MOLECULAR SPECTROSCOPY II
MSC – 205
[USE OMR FOR OBJECTIVE PART]

**SET
A**

Duration: 1:30 hrs.

Full Marks: 35

(Objective)

Time: 15 mins.

Marks: 10

Choose the correct answer from the following:

1×10=10

- Band head occur in the R branch of the rotational spectral line when
 - $r_e' > r_e''$
 - $r_e' < r_e''$
 - $r_e' = r_e''$
 - $r_e' \ll r_e''$
- 'Q' branch of rotational fine structure is present in the molecule
 - HCl
 - NO
 - N₂
 - CO
- The allowed transition is
 - $3\Sigma_g^- \leftrightarrow 3\Sigma_u^-$
 - $3\Sigma_g^- \leftrightarrow 1\Sigma_g^+$
 - $3\Sigma_u^- \leftrightarrow 1\Sigma_u^+$
 - $3\Sigma_g^+ \leftrightarrow 1\Sigma_u^+$
- The nucleus having nuclear spin $I=5/2$ is
 - ¹⁸O
 - ¹⁵N
 - ³⁵Cl
 - ¹⁷O
- The colour of which of the following species due to charge transfer transition (CT) is bright orange?
 - CrO₃
 - Cr₂O₃
 - Cu₂O
 - CuI
- The Mössbauer spectra of [Fe(CN)₆]²⁻ and [Fe(CN)₅NO]²⁻ consist of, respectively
 - 1 line each
 - 2 lines each
 - 1 and 2 lines
 - 2 and 4 lines
- The Mossbauer Spectroscopy uses _____ radiation
 - Microwave radiation
 - β radiation
 - γ radiation
 - Radio-frequency
- Which of the following will NOT show electron spin resonance?
 - Free electrons
 - Paramagnetic materials
 - Transition metals
 - Diamagnetic materials

9. A particular Mössbauer nucleus has spins of $5/2$ and $3/2$ in its excited and ground states respectively. The numbers of lines obtained in its γ -ray spectrum under the conditions of internal electric field gradient is
- | | |
|------|-------|
| a. 1 | b. 5 |
| c. 7 | d. 12 |
10. The ratio of peak splitting that can be observed with three equivalent protons will be
- | | |
|----------|------------|
| a. 1:1 | b. 1:2:1 |
| c. 1:3:1 | d. 1:3:3:1 |

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(Descriptive)

Time : 1 hr. 15 mins.

Marks:25

[Answer question no.1 & any two (2) from the rest]

1. a. Write the expressions for proton spin magnetic moment along Z direction. Show that the electron spin magnet is about 658 times stronger than the proton spin magnet. ($g_e = 2.0023$ and $g_p = 5.5857$). 3+2=5
b. In ^{57}Fe Mössbauer experiment source of 14.4 keV (equivalent to 3.5×10^{12} MHz) is moved towards absorbent at a velocity of 22 mms^{-1} . What is the shift in frequency of the source for this sample?

2. a. What do you mean by dissociation and dissociation energy of a diatomic molecule? Show that area under the curve $\Delta G_{v+1/2}$ versus v gives the dissociation energy measured from lowest vibrational state of the ground electronic state. [$\Delta G_{v+1/2} = G(v+1) - G(v)$; v is the vibrational quantum number]. 5+5=10
b. Show that the separation between the two spin states of a proton in a magnetic field is proportional to the magnetic field. State the condition of resonance of a free proton and protons in different chemical groups.

3. a. What are the three main types of intensity distribution of vibrational bands in electronic transitions? Explain the intensity distribution of the vibrational bands in the electronic transition of oxygen molecule with the help of Franck Condon principle. Define Franck Condon factor. 5+5=10
b. State the selection rule on the basis of symmetry property of the molecular electronic states. Write the expression of frequencies of P and R branch of rotational fine structure of vibrational bands in electronic transition. Why no spectral line is found in the P and R branch at the band origin?

4. a. What do you mean by Mössbauer effect and Doppler effect? 3+3+4
=10
- b. What do you mean by quadrupole effect? Explain it with the help of suitable example.
- c. What do you mean by isomer shift? Explain two factors that affect isomer shift.
5. a. What is the basic principle of ESR? 2+2+3+3
=10
- b. What is Drago's rule in ESR spectroscopy? How many hyperfine splitting lines will you observe in case of the complex $[\text{Ti}(\text{H}_2\text{O})_4(\text{NH}_3)_2]^{2+}$ (I for Ti is 3/2)?
- c. What do you mean by Hyperfine splitting in ESR? How many hyperfine splitting lines will you observe in the radicals HD, CD_2H , NH_2 , and CH_3CH_2 ?
- d. What are the requirements in Mössbauer spectroscopy? What is Mössbauer's contribution in this spectroscopy?

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