Enrollment No......................................

Faculty of Science

End Sem (Even) Examination May-2022
CH5CO08 Group Theory & Spectroscopy -II

Programme: M.Sc.   Branch/Specialisation: Chemistry

Duration: 3 Hrs.   **Maximum Marks: 60**

Note: All questions are compulsory. Internal choices, if any, are indicated. Answers of Q.1 (MCQs) should be written in full instead of only a, b, c or d.

Q.1   i.   TMS, used in NMR as a reference compound is: **1**
       (a) Trimethyl Silane   (b) Tetramethyl silane
       (c) Typical magnetic strength (d) Tetramethyl sulphur

   ii.   Number of signals observed in NMR spectra indicate: **1**
       (a) Electronic environment
       (b) Different types of protons
       (c) Number of equivalent protons
       (d) Intensities of protons

   iii.   Nuclear quadrupole moment is: **1**
       (a) e Q   (b) e / Q   (c) Q / e   (d) I

   iv.   Nuclear quadrupole moment is represented by: **1**
       (a) Magnetic moment   (b) Electric moment
       (c) Dipole moment   (d) None of these

   v.   Bohr magneton (β) for electron is: **1**
       (a) $m_e h/4\pi e$ (b) $e/4\pi m_e$ (c) $h/4\pi m_e$ (d) $eh/4\pi m_e$

   vi.   Selection rules for HFS of ESR spectra are: **1**
       (a) $\Delta m_s = \pm 1$, $\Delta m_I = 1$ (b) $\Delta m_s = \pm 1$, $\Delta m_I = 0$
       (c) $\Delta m_s = \pm 0$, $\Delta m_I = 1$ (d) $\Delta m_s = \pm 0$, $\Delta m_I = 0$

   vii.   Systematic study of X-ray was first made by: **1**
       (a) Mosley   (b) Rutherford
       (c) Bohr   (d) Bragg

   viii.   In X-ray diffraction the integrated reflection (R) is related with total **1** reflected energy (E), total incident radiation per c.c. (I) and uniform angular velocity ($\square$) as:
       (a) $R = E\square/I$ (b) $R = I/E\square$ (c) $R = E/I\square$ (d) $R = I\square/E$

ix. To be used in diffraction methods the wavelength of the particle has to be of the order: **1**
(a) 100Å   (b) 10Å   (c) 1Å   (d) 1000Å

x. The most suitable neutron for neutron diffraction analysis is: **1**
(a) Cold neutron   (b) Slow neutron
(c) High energy neutron   (d) Thermal neutron

Q.2   i. Discuss briefly about coupling constant 'J'. **2**
     ii. Discuss spin-spin interactions with suitable examples. **3**
     iii. Write a note on chemical shift and factors affecting chemical shift. **5**
OR   iv. Describe briefly about instrumentation of NMR spectrometer with suitable diagram. **5**

Q.3   i. Define quadrupole moment. **2**
     ii. Outline the principle of NQR spectroscopy. Show the splitting of quadrupole energy levels by diagram for a nucleus having nuclear spin 3/2 under spherical and axial symmetric field. **8**
OR   iii. Describe the applications of NQR spectroscopy in any two of followings with suitable examples: **8**
(a) Nature of Chemical bond
(b) Structural information
(c) Study of Charge transfer spectra

Q.4   i. Discuss principle of ESR spectroscopy. **3**
     ii. Discuss zero field splitting and Kramer's degeneracy? Explain hyperfine splitting pattern and multiplate spectra for 1,4-benzosemiquinone radical anion or methyl free radical. **7**
OR   iii. Write brief account on g- factor and g-value? Calculate the ESR frequency of an unpaired electron in a magnetic field of 0.33 Tesla. For free electron, g = 2.0023 and Bohr magneton, $\beta = 9.273 * 10^{-24}$ J/Tesla. **7**

Q.5   i. Write Bragg's equation. Discuss Bragg's condition for diffraction. **4**
     ii. Describe Debye Scherrer method of X-ray structural analysis of Crystals. **6**

OR   iii. (a) How X-ray intensities, structure factor and its relation to intensity and electron density? **6**
(b) Describe the procedure for an X-ray structure analysis, absolute configuration of molecules.

Q.6   Attempt any two:
     i. What is electron diffraction method? How is it superior to x-ray and neutron diffraction method? **5**
     ii. Discuss instrumentation for electron diffraction. Also describe any one important application of it. **5**
     iii. Discuss about neutron diffraction in brief. Discuss any one application of it. **5**

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Scheme of Marking

Note: The Paper Setter should provide the answer wise splitting of the marks in the scheme below.

Q.1　i.　TMS, used in NMR as a reference compound is:　　　　1
　　　　　(b) Tetramethyl silane

　　ii.　Number of signals observed in NMR spectra indicate:　　1
　　　　　(b) Different types of protons

　　iii.　Nuclear quadrupole moment is:　　　　　　　　　　1
　　　　　(a) e Q

　　iv.　Nuclear quadrupole moment is represented by:　　　1
　　　　　(b) Electric moment

　　v.　Bohr magneton (β) for electron is:　　　　　　　1
　　　　　(d) eh/4πm$_e$

　　vi　Selection rules for HFS of ESR spectra are:　　　　1
　　　　　(b) $\Delta ms = \pm 1$, $\Delta mI = 0$

　　vii.　Systematic study of X-ray was first made by:　　　1
　　　　　(a) Mosley

　　viii.　In X-ray diffraction the integrated reflection (R) is related with total　1
　　　　reflected energy (E), total incident radiation per c.c. (I) and uniform
　　　　angular velocity (ω) as:
　　　　　(a) $R = E\omega/I$

　　ix.　To be used in diffraction methods the wave length of the particle　1
　　　　has to be of the order:
　　　　　(c) 1Å

　　x.　The most suitable neutron for neutron diffraction analysis is:　　1
　　　　　(d) Thermal neutron

Q.2　i.　Discuss briefly about coupling constant 'J'.　　　　-2 marks　2

　　ii.　Discuss spin-spin interactions with suitable examples. - 3 marks　3

　　iii.　Write a note on Chemical shift　　　　　　　-3 marks　5
　　　　and factors affecting chemical shift.　　　　　-2 marks

OR　iv　Describe briefly about instrumentation of NMR spectrometer　5
　　　　　　　　　　　　　　　　　　　　　　　-3.5 marks

with suitable diagram.　　　　　　　　　　　　-1.5 marks

Q.3　i.　Define quadrupole moment.　　　　　　　　- 2 marks　2

　　ii.　Outline the principle of NQR spectroscopy.　　- 6 marks　8
　　　　Show the splitting of quadrupole energy levels by diagram for a
　　　　nucleus having nuclear spin 3/2 under spherical and axial
　　　　symmetric field.　　　　　　　　　　　　　- 2 marks

OR　iii.　Describe the applications of NQR spectroscopy in any two of　8
　　　　followings with suitable examples:
　　　　(a) Nature of Chemical bond　　　(b) Structural information
　　　　(c) Study of Charge transfer spectra　　　　- 4 + 4 marks

Q.4　i.　Discuss principle of ESR spectroscopy.　　　- 3 marks　3

　　ii.　Discuss zero field splitting and Kramer's degeneracy?　- 3 marks　7
　　　　Explain hyperfine splitting pattern and multiplate spectra for 1,4-
　　　　benzosemiquinone radical anion or methyl free radical.　- 4 marks

OR　iii.　Write brief account on g- factor and g-value?　　-4 marks　7
　　　　the ESR frequency of an unpaired electron in a magnetic field of
　　　　0.33 Tesla. For free electron g = 2.0023, Bohr magneton (β) = 9.273
　　　　x 10-24 J/Tesla　　　　　　　　　　　　　-3 marks

Q.5　i.　Write Bragg's equation.　　　　　　　　-1 mark　4
　　　　Discuss Braggs condition for diffraction.　　　-3 marks

　　ii.　Describe Debye Scherrer method of X-ray structural analysis of　6
　　　　Crystals.　　　　　　　　　　　　　　- 6 marks

OR　iii.　(a) How X-ray intensities, structure factor and its relation to　6
　　　　intensity and electron density?　　　　　　-2 marks
　　　　(b) Describe the procedure for an X-ray structure analysis, absolute
　　　　configuration of molecules.　　　　　　　- 3 marks

Q.6　　Attempt any two:

　　i.　What is electron diffraction method?　　　　-1.5 marks　5
　　　　How is it superior to x-ray and neutron diffraction method?
　　　　　　　　　　　　　　　　　　　　　　-3.5 marks

　　ii.　Discuss instrumentation for electron diffraction.　-3 marks　5
　　　　And describe any one important application of it.　-2 marks

　　iii.　Discuss about neutron diffraction in brief?　　-3 marks　5
　　　　Discuss any one application of it.　　　　　-2 marks

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