M.Sc. Examination, 2019

Semester-IV

Chemistry

Optional Course: CH-1022

(Physical Chemistry)

Time: Three Hours **Full Marks: 40**

Questions are of value as indicated in the margin.

Answer ***any four*** questions.

1. a) Write Maxwell's equation regarding electromagnetic radiation in free space. Prove that the electric field is perpendicular to the magnetic field and both are perpendicular to the propagation direction as well. 5
   b) Describe the principle for the determination of electron number density and drift speed of the charge carriers in a metallic conductor. 3+2

2. a) Discuss the effect of an electromagnetic field on a charged particle and show that the fundamental basis for spectroscopic transition is the interaction of the momenta of charged particle with the vector potential of radiation. 5
   b) Derive the resonance condition based on the elementary quantum mechanics for a spin system which is interacting with the applied time dependent magnetic field in the presence of a static magnetic field. What comment can you draw based on your result? Could you justify your comment based on classical mechanics? 2+1+2

3. a) Considering finite duration of the light pulse that excites absorption or emission, discuss the time-energy uncertainty principle. What gives the minimum line width for a spectroscopic transition? 2+1
   b) Monochromatic radiation is capable of pumping the final state – discuss. 2
   c) Derive expression for the expectation of components of magnetic dipole moment in the presence of a static magnetic field along z-direction. Using it for a two level spin system show that the expectation value of the magnetic dipolemoment exhibits precessional motion about the z-direction of a fixed angle with it. 2.5+2.5

4. a) Discuss Stark effect in linear and symmetric rotor molecules. Explain how a spherical rotor molecule like SiH_4 or CH_4 can be microwave active. 3+2
   b) Spins may only be found pointing either parallel or antiparallel to the quantizing field. Comment on the statement. 2
   c) Show that the equation of motion of the expectation value of the magnetic moment in the presence of a magnetic field exactly corresponds to the classical description. What comment can you draw here? 2+1

5. a) What is normal co-ordinates in vibrational spectroscopy? Derive the energy expression for diatomic harmonic oscillator type molecules. 1+4
   b) Show that an alternating magnetic field along x-direction can be split into two rotating magnetic field in the xy plane. 1
   c) Write the equation of motion for the magnetic moment in the presence of both static and a rotating magnetic fields. What would be it in a rotating co-ordinate system? Using it define 90° and 180° pulses. 1.5+1.5+1

6. a) Discuss the Born-Oppenheimer approximation in the vibrational problem of diatomic molecule and also mention its consequences. 5

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b) Write the Schrödinger equation in the laboratory co-ordinate system for the evolution of a magnetic moment in the presence of a magnetic field, $H = kH_0 + iH_1 \cos\omega_z t + jH_1 \sin\omega_z t$. What it would be in the rotating co-ordinate system? Solve the equation in the rotating co-ordinate system and using it at the resonance condition calculate component of the magnetic moment along the z-direction. What is the implication of your calculation? 1+1.5+0.5+2

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