



UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
End Semester Examination, December 2021

Course: Physical Chemistry V
Program: B.Sc. (Hons.) Chemistry
Course Code: CHEM 3002

Semester: V
Duration: 03 hrs.
Max. Marks: 100

Instructions: Read the instructions given below carefully:

1. All questions are compulsory.
2. Internal choice is given in question 4 of Section B and question 2 of section C.

SECTION A
(Scan and upload)

S. No.		Marks	CO
Q 1	What is the speed of an electron whose de Broglie wavelength is 0.1 nm?	4	CO1
Q 2	Explain the terms: Bathochromic, Hypsochromic, Hyperchromic and Hypochromic shift.	4	CO3
Q 3	For determining NMR, how many kinds of proton are there in the following compounds: a) CH ₃ CH ₃ b) CH ₃ CH ₂ CH ₃ c) (CH ₃) ₂ CHCH ₂ CH ₃ d) C ₆ H ₅ CH ₃	4	CO2
Q 4	A cricket ball weighing 100 g is to be located within 0.1 Å. What is the uncertainty in its velocity? Comment on your result. Mass of electron = 9.1x10 ⁻³¹ kg and Plank's constant = 6.626 x 10 ⁻³⁴ Js	4	CO1
Q 5	Discuss Born-Oppenheimer approximation.	4	CO1

SECTION B
(Scan and upload)

Q 1	Show that the average value of 1/r for an electron in the 1s-orbital of hydrogen atom is 1/a ₀ , where a ₀ is the Bohr radius; given that $\Psi = \frac{1}{\sqrt{\pi}a_0^{3/2}} e^{-r/a_0}$	10	CO2
Q 2	What are the main points of similarities and differences between VBT and MOT?	10	CO2
Q 3	Write the Schrodinger wave equation for a Simple Harmonic Oscillator explaining its potential energy curve.	10	CO1

Q 4	List all the electronic transitions possible for a) CH ₄ b) CH ₃ Cl c) H ₂ C=O <p style="text-align: center;">OR</p> Discuss in detail, how Stokes and Anti-Stokes lines appear in Raman spectroscopy. What is Raman shift?	10	CO3
SECTION-C (Scan and upload)			
Q 1	(a) An electron is confined to move in a one-dimensional box of 1 nm length. Calculate the probability of finding it in between $x = 0$ and $x = 0.2$ nm. (Given $\sin 0.4\pi = 0.9511$) (b) Apply quantum mechanical principles to calculate the coefficients of atomic orbitals in sp ² hybrid orbitals and write their wave functions.	20	CO2
Q 2	(a) Using the energy level expression and the selection rules, draw an energy level diagram and the spectral transitions for the microwave (pure rotational) spectrum of a rigid diatomic rotator. Also derive the expression for wavenumber (in cm ⁻¹) for P-Branch of spectra. <p style="text-align: center;">OR</p> With the help of a schematic diagram, explain briefly the Shielding and Deshielding of Protons in NMR studies. (b) A sample was excited by the 4358 Å line of mercury. A Raman line was observed at 4447 Å. Calculate the Raman shift in cm ⁻¹ . At what wavelength in Å would the anti-stokes line appear in the Raman spectrum of the sample. <p style="text-align: center;">OR</p> The pure rotational spectrum of gaseous HCl contains a series of equally spaced lines separated by 20.80 cm ⁻¹ . Calculate the internuclear distance of the molecule. The atomic masses of H and Cl are 1.673 x 10 ⁻²⁷ kg and 58.06 x 10 ⁻²⁷ kg respectively.	20	CO3