	Reg. No.:	
	Name :	

VIT BHOPAL
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TERM END EXAMINATIONS (TEE) –December 2021- January 2022.

Programme	:	**B.Tech (All Branches)**	Semester	:	**Fall 2021-2022**
Course	:	**Introduction to Computational Chemistry**	Code	:	**CHY1005**
Faculty	:	**Dr. Satyam Ravi**	Slot/Class No.	:	**B21+B22+B23/0328**
Time	:	**1½ hours**	Max. Marks	:	**50**

Answer ALL the Questions

Q. No.		Question Description	Marks
		PART - A (30 Marks)	
1	(a)	In a class of 50, 4 students were selected at random and their total marks in the final assessments are recorded, which are: 912, 936, 1082, 869. Find the standard deviation, absolute errors, relative error or percentage error of their marks.	10
		OR	
	(b)	Light of wavelength 8000 Å is incident on a Potassium surface for which the threshold wavelength of photo-electrons is 5420 Å. What is the work function of Potassium?	10
2	(a)	The temperature of 2.25 moles of an ideal gas increases from 30.2°C to 58.6°C as the gas is compressed adiabatically. Calculate q, w, ΔU and ΔH for this process, assuming that Cv = 5R/2; where R = 8.314 J/K.	10
		OR	
	(b)	Calculate the total number of bond distance, bond angles and dihedral angle in acetylene molecule. Write down the potential energy expressions as per the molecular mechanics approach.	10
3	(a)	Explain the different Intermolecular Forces with one examples each. Arrange ion-dipole, H-bond, London dispersion, ion-induced dipole and dipole induced dipole in relative strength of intermolecular forces.	10
		OR	
	(b)	To study the hydrophobic effect in a protein, what method you will choose – 1. Quantum mechanical 2. Molecular dynamics. Justify your answer from the perspective of computational cost.	10

PART - B (20 Marks)		
4	a. Write the Schrodinger Equation of the following system a. Particle in a box b. H atom b. Calculate the number of radial and angular nodes and the angular momentum of the following orbitals– 1. 4s 2. 3d	5+5
5	Draw the dissociation curve of H_2 molecule. Write down the expression for the Morse potential.	10