	Reg. No.:	
	Name :	

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Mid-Term Examinations – August 2021

Programme	:	**All B.Tech. and Integrated M.Tech. Courses**	Semester	:	**Fall 2021-22**
Course	:	**Introduction to Computational Chemistry**	Code	:	**CHY1005**
Faculty	:	**Dr. Satyam Ravi**	Slot/Class no.	:	**B21+B22+B23 / 0328**
Time	:	**90 Minutes**	Max. Marks	:	**50**

Answer all the Questions

Q.No.	Sub Sec.	Question Description	Marks
1	**(a)**	You're given the following information about the scores of different students in CHY-1005 subject. Calculate the standard deviation and the variance.	**7+3**

	Scores
1	30.0
2	32.0
3	34.2
4	35.6
5	42.5
6	43.2
7	12.0
8	45.9
9	36.8
10	33.3

	(b)	. In one observation, the time period of complex pendulum is given by $T = K(\frac{l}{g})^a$ If T is measured in sec then what should be the value of a in order to have correct dimension.	
2		The van der Waals equation of real gas is given by: $\left(P + \frac{a}{V^2}\right)(V - b) = RT$ Determine the units of *a*, *b* if P is the pressure, V is volume, R is the gas constant and T is the temperature. You can take the unit of pressure is atm, Volume is litter and T is in Kelvin?	**10**
3	**(a)**	Discuss the plum pudding model of the atomic structure and write its deficiency?	**5+5**
	(b)	It takes 285.5 kJ of energy to remove 1 mole of electrons from the atoms on the surface of rubidium metal. If rubidium metal is irradiated with 274-nm light, what is the maximum kinetic energy the released electrons can have?	
4	**(a)**	An electron in a one-dimensional box requires a wavelength of 100 pm to excite an electron from the n = 2 to the n = 3 energy level. Calculate the length of this box.	**5+5**
	(b)	Calculate the energy required to excite the hydrogen electron from level n = 2 to level n = 3, as per the quantum model of the hydrogen atom. Also calculate the wavelength of light that must be absorbed by a hydrogen atom in its 2^{nd} excited state to reach the third excited state.	
5		The temperature of 1.75 moles of an ideal gas increases from 10.2°C to 48.6°C as the gas is compressed adiabatically. Calculate q, w, ΔU and ΔH for this process, assuming that Cv = 3R/2; where R = 8.314 J/K.	**10**