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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.	: E21+E22+E23 / 0327
Time	: 90 Minutes	Max. Marks	: 50

Answer all the Questions

Q.No.	Sub Sec.	Question Description	Marks
1	(a)	In the last year, during the mid-semester the first five students of CHY-1005 scored the following numbers: 32, 29, 33, 33, 38, 40, 36, 38, 40 and 42. Calculate the <i>standard deviation and variance</i> for this data.	5+5
	(b)	Mr. X measures the period of oscillation of a simple pendulum. In successive measurements, the readings turn out to be 3.63 s, 4.56 s, 5.42 s, 4.71s and 1.80 s. Calculate the absolute errors, relative error and percentage error.	
2	(a)	The energy 'E' of a particle depends upon the time 't' and velocity 'v' according to the equation $E(t) = a(t) * v^2 + bt^3$ Determine the units of a, b. All have SI units.	6+4
	(b)	Each side of a cube is measured to be 5.32345 m. What are the total surface area and the volume of the cube to appropriate significant figures?	
3	(a)	Discuss the nuclear model of the atomic structure and write its deficiency?	5 + 5
	(b)	Light with a wavelength of 300. nm is incident on a potassium surface for which the work function is 2.26 eV. Calculate the kinetic energy and speed of the ejected electrons.	
4	(a)	Draw the wave function and probability distribution of a particle in 1D box for n = 10 and n =2. Please comment when n increases then how quantum mechanical results will change?	2

	(b)	Calculate the number of radial and angular nodes in the following orbitals – 1. 3s 2. 3f 3. 4p 4. 3d	8
5		2.50 mol of an ideal gas with $C_{v,m} = 12.47 \text{ J mol}^{-1} \text{ K}^{-1}$ is expanded adiabatically against a constant external pressure of 1.00 bar. The initial temperature and pressure of the gas are 325 K and 2.50 bar, respectively. The final pressure is 1.25 bar and final temperature is 268 K. Calculate the final q, w.	10