

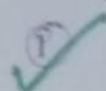


MID TERM EXAMINATIONS – April 2024

Programme	: B.Tech. and Int. M.Tech	Semester	: Winter 2023-24
Course Title/ Course Code	: Introduction to Computational Chemistry / CHY1005	Slot	: A11+A12+A13
Time	: 1 ½ hours	Max. Marks	: 50

Answer all the Questions

Q.No.	Sub. Sec.	Question Description	Marks
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Calculate the standard deviation of the marks scored in Chemistry subject of the selected seven students.

Students	Subject1
1	30.4
2	22.3
3	29.6
4	18.4
5	36.3
6	14.4
7	24.9

10



The time period (T) of a simple pendulum is proportional to the length of a string, and inversely proportional to the acceleration due to the gravity (g). Find out the expression of time period of simple pendulum based on dimensional analysis.

7

The measured value of the length of a simple pendulum is 20 cm with 2 mm accuracy. The time for 50 oscillations was measured to be 40 seconds with 1 second resolution. Find out the error in the measurement of acceleration due to gravity.

The velocity (V), time (T) and force (F) are chosen as the fundamental quantities. Express the dimension of the mass ([M]) in F, T and V.

3

The work function of palladium is 5.22 eV. What is the minimum frequency of light required to observe the photoelectric effect on Pd? If light with a 200 nm wavelength is absorbed by the surface, what is the velocity of the emitted electrons?

10

A student uses a trial wavefunction (ψ) for a particle in a box of length l which satisfy the boundary condition. The proposed wavefunction is as follows:

$$\Psi = A x (l - x)$$

10

Find out the normalization constant.

A sample consisting of 2.00 mol of He gas is expanded isothermally at 27°C from 20.0 dm³ to 30.0 dm³ (a) reversibly, (b) against a constant external pressure equal to the final pressure of the gas. Calculate q, w, ΔU for the two processes.
 (Hint: $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$)

10

