Reg. No.:

Name :

VIT BHOPAL
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TERM END EXAMINATIONS (TEE) – December 2021

Programme	**B.Tech. (All branches)**	**Semester**	**Fall 2021-22**
Course Name	**Introduction to Computational Chemistry**	**Course Code**	**CHY1005**
Faculty Name	**Dr. Sumit Mittal**	**Slot / Class No**	**A11+A12+A13/0324**
Time	**1½ hours**	**Max. Marks**	**50**

Answer ALL the Questions

Q. No.		Question Description	Marks
		PART - A – (3 x 10 = 30 Marks)	
1	(a)	Solve the following and report the result to the correct number of significant figures:	**10**
		(i) $\frac{4.625}{1.9} + \frac{1.72325}{0.125} + \frac{14.625}{0.235}$	
		(ii) $(0.152 \times 10^{-3}) + (5.14 \times 10^{-2}) + (4.090 \times 10^{-1})$	
		(iii) $(1.01 \times 10^{-3}) - (1.6 \times 10^{-5}) - (0.0412 \times 10^{-4})$	
		(iv) $2.13 \times 6.634 \times 10^{-34}$	
		OR	
	(b)	Considering all species in their first excited state, calculate the electronic energy for the following reaction: $\mathbf{He^{2+} + H \rightarrow He^{+} + H^{+}}$	**10**
2	(a)	Consider one mole of an ideal gas that occupies 2 L at 5 atm. This gas is transformed to a state where it occupies 6 L at 5 atm. The gas is further taken to a state where it occupies 6 L at 2 atm. Calculate the work involved in this two-step transformation.	**10**
		OR	
	(b)	"Hydrogen bond is a special type of dipole-dipole forces and are unusually strong". Justify the statement. Discuss the importance of hydrogen bonding for the structure of proteins.	**10**

3 (a) Discuss, in detail, the various terms that are included in a molecular mechanics based potential energy function. **10**

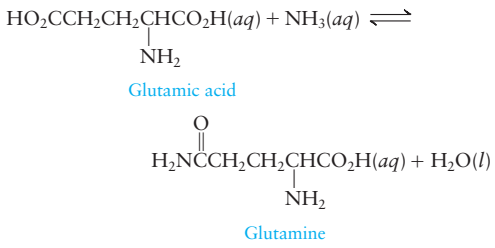
OR

(b) Enumerate the steps involved in performing molecular dynamics simulation of a chemical system. Discuss the factors that you need to keep in mind while setting up a simulation. **10**

Part - B – (2 x 10 = 20 Marks)

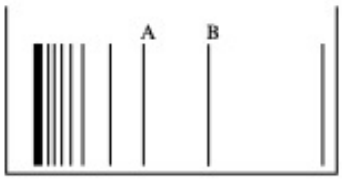
4 (i) ATP is the main source of energy for most cellular processes. When the cell needs energy, ATP undergoes hydrolysis to lose one phosphate and is converted into ADP. The ΔH^{o} for the hydrolysis is -24 kJ/mol and the ΔG^{o} is -30 kJ/mol. Calculate the ΔS^{o} and K for this reaction at 25 °C. **10**

(ii) When a human being eats chicken, glutamic acid present in chicken is metabolized to glutamine. The ΔH^{o} for this reaction is 17 kJ/mol and the ΔS^{o} is 10 J/K·mol. Calculate the ΔG^{o} and K for this reaction at 25 °C. Comment on the spontaneity of the reaction.



If nonspontaneous, suggest a method via which the cell can metabolize glutamic acid to generate fuel for different processes.

5 The emission spectrum for a hydrogen-like atom is shown below. The emission spectrum lines correspond to emission for the electron from an excited state to the n = 2 state. **10**



(i) Suggest the electronic transitions which correspond to lines A and B.

(ii) Given that the wavelength of line A is 150 nm, calculate the wavelength corresponding to line B.

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