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


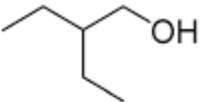
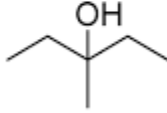
Programme	: B.Tech	Semester	: Fall 2021-2022
Course	: Introduction to Computational Chemistry	Code	: CHY1005
Faculty	: Dr. Satyam Ravi	Slot/Class No.	: E21+E22+E23/0327
Time	: 1½ hours	Max. Marks	: 50

Answer ALL the Questions

Q. No.	Question Description	Marks
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PART - A (30 Marks)

1	(a)	Evaluate as per correct number of significant figures: i) 100.32145/30001.1 ii) 12.4*32*14.11 iii) A milkman has 145 L of milk and Anjali takes 0.222 L of milk from him. How much milk is left with the milkman? iv) 88359 m ² / 3 m v) [(28.7 x 10 ⁵) ÷ 48.533] + 144.99	10
	OR		
	(b)	What were the key differences between Rutherford's and Bohr's model? What were the limitations of each of these models?	10
2	(a)	i) Assess the feasibility of the reaction: $\text{ClNO}_2(\text{g}) + \text{NO}(\text{g}) \rightarrow \text{NO}_2(\text{g}) + \text{ClNO}(\text{g})$ at 25 °C. ΔS° for $\text{ClNO}_2(\text{g})$ is 272.23 J/mol K, $\text{NO}(\text{g})$ is 210.8 J/mol K, $\text{NO}_2(\text{g})$ is 440.1 J/mol K, $\text{ClNO}(\text{g})$ is 261.58 J/mol K; ΔH_f° for $\text{ClNO}_2(\text{g})$ is 12.5 kJ/mol, $\text{NO}(\text{g})$ is 90.25 kJ/mol, $\text{NO}_2(\text{g})$ is 33.18 kJ/mol, $\text{ClNO}(\text{g})$ is 51.71 kJ/mol. ii) In a certain chemical process, a lab technician supplies 254 J of heat to a system. At the same time, 73 J of work is done on the system by its surroundings. What is the increase in the internal energy (in J) of the system?	10
	OR		
	(b)	Discuss the bond formation in H ₂ , NaCl using electronic configuration of each of the elements involved. How is this bonding different from that present in metallic Al? ii) Explain why once NaCl is formed, it does not dissociate back to form Na and Cl ₂ but in the presence of water, it dissociates into ions.	10

3	<p>(a) Arrange the following compounds in increasing order of their boiling point with proper reasoning:</p> <p>i) HF, HCl, HBr, HI i) HF, HCl, HBr, HI</p> <p>ii) NH₃ and PH₃</p> <p>iii) C₉H₉O⁻Na⁺, C₄H₉OH, C₄H₁₀O</p> <p>iv) CH₃CHO and CH₃CN</p> <p>v) 1-hexanol, 2-ethyl-1-butanol, 3-methyl-3-pentanol</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>1-hexanol</p> </div> <div style="text-align: center;">  <p>2-ethyl-1-butanol</p> </div> </div> <div style="text-align: center; margin-top: 20px;">  <p>3-methyl-3-pentanol</p> </div>	10
OR		
	(b) Write down the steps involved in the molecular dynamics simulation.	10
PART - B (20 Marks)		
4	<p>a) Calculate the probability of finding an electron in a state of $n=1$ between $x=0.25L$ to $0.75L$ in a conjugated molecule of length L.</p> <p>b) Draw the normalized wave function and probability density of the electron for states $n=2$ and $n=4$.</p>	10
5	Write down the expressions for the force field of the ethylene molecule.	10