2020

CHEMISTRY — HONOURS — PRACTICAL

Paper : DSE-A-1P

(Molecular Modelling and Drug Design)

Full Marks : 30

The figures in the margin indicate full marks.

All calculations can be done using calculator.

1. What is dihedral angle energy? The following table shows the variation of total energy of two carbon compounds A and B as a function of dihedral angle. Draw a plot of dihedral angle vs. total energy for both the compounds. Comment on the positions of the minima observed in the graph for both the compounds. Can you suggest the nature of A and B? Justify your answer. 5+10+8+2+5

Dihedral Angle (degrees)	Total Energy (A) (kcal/mol)	Total Energy (B) (kcal/mol)
0	3.5803	10.212
30	2.1934	6.9437
60	0.818	3.8231
90	2.1934	4.1762
120	3.5803	5.6321
150	2.1934	3.8969
180	0.818	2.1735
210	2.1934	3.8969
240	3.5803	5.6321
270	2.1934	4.1762
300	0.818	3.8231
330	2.1934	6.9437
360	3.5803	10.212

2020

CHEMISTRY — HONOURS — PRACTICAL

Paper : DSE-A-2P

(Application of Computers in Chemistry)

Full Marks : 30

The figures in the margin indicate full marks.

All calculation can be done using calculator.

Answer ***any one*** of the following.

1. Determine the Molar Enthalpy of Vaporization of water using Linear Least Square fit.

(a) Write down the theory using the following points :

(i) Clapeyron Equation and its derivation

(ii) Derivation of Clausius-Clapeyron Equation

(iii) Principle of Linear Least Square analysis and its implementation in Excel, determination of slope and intercept.

(b) Determine the Molar Enthalpy of Vaporization of water from the following temperature vs. pressure data using Linear Least Square fit. (using least square expressions for slope and intercept)

T/K	313.14	323.137	333.134	343.132	353.129
P/torr	55.364	92.592	149.51	233.847	355.343

(c) Write down the value of Molar Enthalpy of Vaporization from Linear Least Square fit along with proper unit. (3+5+7)+12+3

2. Determine the Michaelis-Menten constant (K_m) and the maximum rate (v_{max}) using linear least square analysis for the hydrolysis of carbobenzoxyglycyl – L – tryptophan (CBT) by the enzyme carboxypeptidase to give carbobenzoxyglycine (CB) and Tryptophan (T) according to

$$CBT + H_2O \rightarrow CB + T$$

(a) Write down the theory using the following points :

(i) Michaelis-Menten equation and it's derivation

(ii) Linewaver-Burk plot

(iii) Michaelis-Menten constant, its unit and significance

(iv) Principle of Linear Least Square analysis and its implementation in Excel, determination of slope and intercept.

(b) Determine the Michaelis-Menten constant (K_m) and the maximum rate (v_{max}) using the following data (using least square expressions for slope and intercept).

[CBT], mM	Rate, d[T]/dt, mM/s
1.00	0.0115
1.25	0.0139
1.50	0.0159
2.50	0.0240
5.00	0.0360
10.00	0.0532
15.00	0.0600
20.00	0.0640

(c) Write down the results, K_m and v_{max} for Least Square analysis. (4+1+3+7)+12+(1½×2)