

M.Sc. Examination 2019
Semester-IV
Chemistry
Course: CH-1020
(Optional: Physical Chemistry)

Time: Three Hours

Full Marks: 40

Questions are of equal value or as indicated in the margin.

Answer *any four* questions.

1. a) Discuss the different stages of light reactions in photosynthesis. 3
b) Give a sketch of Z-diagram for photosynthesis. Which serves as water oxidizing complex in photosynthesis? What is its function? 3+2
c) What is the function of the paraquat (PQ^{2+}) in the photolytic production of H_2 and O_2 from water using $Ru(bpy)_3^{2+}$ complex? 2
2. a) Sketch the band diagram of a (i) intrinsic semiconductor, (ii) n-type semiconductor, (iii) p-type semiconductor. 1.5
b) Show how band bending occurs in p-n junction and how it leads to charge separation upon irradiation of light on it. 2.5
c) With the help of a suitable diagram discuss the working principle of a Dye-sensitized solar cell (DSSC). 3
d) What criteria an electrolyte should fulfil to be used in DSSC. Give one example of such an electrolyte. 2
e) What is dark current? 1
3. a) The collision cross section is a measure of the size of the particle – Illustrate this idea. 2.5
b) Define impact parameter and centrifugal energy. 2
c) Using the law of conservation of energy find out an expression for collision energy and hence identify the centrifugal energy. 2.5
d) Write down the correlation between the reaction cross sections and the translational energy. 2
e) What is glory extrema? 1
4. a) The product angular distribution for rigid hard sphere potential is totally isotropic – Justify this. 3
b) The experimental measurement of velocity dependence of ' σ ', the reaction cross section, may give idea about the long range potential – Justify this giving proper reasons. 3
c) Draw the picture of product angular distribution of the following reactions:
(i) $CH_3 + K \rightarrow KI + CH_3$ (ii) $K + I_2 \rightarrow KI + I$.
How will you interpret the results? 2+2
5. a) The reaction cross sections for Alkali metal, halogen reactions are abnormally high – Comment on the statement. 2
b) What are the stationary points on potential energy surface (PES)? How will you distinguish between saddle point and a minimum of the PES? 2
c) Discuss the principle of geometry optimization by conjugate-gradient method. 3

P.T.O.

- d) If two HI molecules collide with translational energy, which is more than the twice the activation energy of the reaction, no reaction occurs. How will you account this observation? How the reaction between two HI molecules will be accomplished? 3
6. a) What do you mean by a quantum dot (QD)? The HOMO-LUMO gap of a QD increases with the decrease in size of the QD – Explain this in reference to particle in a 1-D box model. 1+2
- b) Using the assumption of the transition state theory, derive an expression for the rate constant in terms of partition function of the activated complex and the reactants. 7
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