M.Sc. Examination 2017

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) What is spectator model? What information one can obtain from such a model? 2
   b) Show that the beam flux is an exponentially decreasing function of the scattering length. 2.5
   c) The collision cross section (σ) for the interaction of CsCl with CH_2F_2 is greater than that for Ar – Justify the statement. 1.5
   d) Show that the collision cross section (σ) for the hard sphere collision is πd^2 where 'd' is the collision diameter. 2
   e) How the reaction cross section of a reaction depends on the translational energy of the colliding partners? 2

2. a) Using the idea of collision trajectories explain the term "rainbow" and "glory" impact parameters. 2
   b) One can obtain V(R), the intermolecular potential from the experimentally observed angular distribution – Justify this with proper reasons. 3
   c) What do you mean by stationary points on a potential energy surface? How to ascertain whether a particular stationary point is a saddle point or a minimum? 2
   d) Discuss in brief the salient features of any two semi-empirical potential energy surfaces for studying molecular reaction dynamics. 1.5+1.5

3. a) What do you mean by Direct reaction? Establish the concept of Direct reaction taking example of the following reactions:
   $CH_3I + K \rightarrow KI + CH_3$
   $K + I_2 \rightarrow KI + I$ 1+1+1
   b) How do you explain the extremely high reaction rates of $M + Br_2 \rightarrow MBr + Br$ (where M is an alkali metal atom) reaction? Draw the necessary potential energy diagram to model this reaction and hence explain the increase in reaction cross section for the sequence $Li \rightarrow Na \rightarrow K$. 1+1+2
   c) Establish a relation between the bulk rate constant $\langle k(v_r) \rangle$ and the reaction cross section (σ_R). Assuming the following model for σ_R;
   $\sigma_R = 0$ if $E_r < E_0$ and $\sigma_R = \pi d^2$ if $E_r \geq E_0$; (Symbols have their usual meaning), find out an expression for $\langle k(v_r) \rangle$. 1.5+1.5

4. a) What experimental results leads to the concept of photosystem in photosynthesis? What are the different components of the photosystem and mention their functions? 1+1
   b) How one ascertain that water oxidation is driven by 4 photon absorption? 1
   c) Discuss in brief the possible molecular mechanisms of water splitting in photosynthesis. 2+2

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d) Why $Ru(bpy)_3^{2+}$ is considered to be a good photocatalyst in artificial photosynthesis. 2

5. a) With a suitable diagram mention the different components in Dye-sensitized solar cell. What are their functions in solar cell operation? 1+2+2
   b) What are the different backward electron transfer processes and how those can be reduced? 1.5+1.5
   c) What are the different ways of expressing the photovoltaic efficiency of a solar cell? 2

6. a) Explain the working principle of Si p-n junction solar cell. 2
   b) Draw the energy level diagram of a p-n junction solar cell and find out an expression for the built-in voltage for this kind of solar cell. 1.2
   c) What role a nanoparticle can play in designing solar cell? 1
   d) What do you understand by type-I and type-II nanohybrids? Which one of these is better in solar cell application and why? 1+1+1
   e) What are advantages of dye sensitized solar cell over Si p-n junction solar cell? 1

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