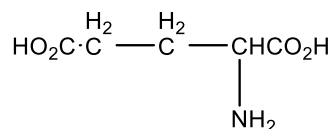


**CH1202: Physical Chemistry Laboratory**  
**Indian Institute of Science Education and Research Kolkata**  
**End-semester assignments**

**Full marks – 50**

**Date: 22/06/2020**

(1) The structure of glutamic acid is:



Write down its predominant forms in (a) strongly acidic and (b) strongly basic solutions, and (c) at its isoelectric point (pI = 3.2). 1+1+1

(2) Explain why is the isoelectric point of glutamine (pI = 5.7) found to be much higher than that of glycine. 2

(3) The  $\Delta G^0$  for decomposition of water:  $\text{H}_2\text{O}(\text{g}) \rightarrow \text{H}_2(\text{g}) + \frac{1}{2} \text{O}_2(\text{g})$  is  $+120 \text{ kJmol}^{-1}$  at 2500 K. Find out the degree of dissociation of  $\text{H}_2\text{O}$  at 2500 K and 1.00 bar pressure. (Given:  $R = 8.314 \text{ JK}^{-1}\text{mol}^{-1}$ ) 4

(4) What is the effect of adding 0.25 g-mole of  $\text{NH}_4\text{Cl}$  to a litre of 0.1 M  $\text{NH}_4\text{OH}$  solution on the degree of dissociation of the base?  $K_b = 1.8 \times 10^{-5}$ . 4

(5) In the reaction at equilibrium:  $\text{N}_2\text{O}_4(\text{g}) \rightleftharpoons 2\text{NO}_2(\text{g})$ , 18.46% of  $\text{N}_2\text{O}_4$  is dissociated at  $25^\circ\text{C}$  and 1.00 bar. Calculate (a) the equilibrium constant  $K$  at  $25^\circ\text{C}$  and (b)  $\Delta G^0$ . (Given:  $\Delta H^0 = +57.2 \text{ kJmol}^{-1}$  over the temperature range) 2+2

(6) Calculate the solubility product of silver chromate if its solubility be  $2.5 \times 10^{-2} \text{ g/L}$ . Also find the solubility in 0.001 M potassium chromate solution. The activity coefficients may be taken as unity. 3

(7) Assume that you are having a molecule that could be a potential pH indicator. Design a “complete” experimental procedure (required experimental steps in bullet points starting from the zero) to obtain the  $pK_{\text{In}}$  of the indicator. Note that it is totally a new molecule that you have synthesized. {Limit your answer to  $\frac{3}{4}$  of a page. Comprehensiveness need to be ensured / no need to elaborate the procedures} 6

(8) In the experiment to obtain the order of a chemical reaction, you have determined the initial rates of the reactions. What was the reason to focus on the initial rate? (Max. 5 lines) 3

(9) Consider the experiment no.7: Assume that you obtained the individual orders as 2 and 4 for  $\text{I}^-$  and  $\text{S}_2\text{O}_8^{2-}$  respectively. Construct a graph (time vs thiosulphate titration value) for the similar solutions (bottle 1-4) that you have performed in the experiment. {make a single plot with all the data and give a brief justification: Limit the whole answer with in  $\frac{3}{4}$  of a page} 6

(10) In experiment no. 4; if you had observed that these two species have considerable absorbance throughout the spectral range that you monitor, what would be the ways to proceed with the experiment using spectrophotometer? (max. ½ of a page) 5

(11) (a) In computational laboratory, you calculated the energies of a few small molecules. Which laws of mechanics are implemented in calculation of their energies?

(b) (i) If you are given a protein structure, which laws of mechanics are expected to be implemented in order to study the energies of its folded and unfolded conformations?

(ii) Justify the implementation of such mechanics in studying the above problem.

(c) Name two Computational Chemistry software used to study problems on protein structures.

(d) Explain the geometry optimization (OPT) and single point (SP) calculation methods implemented in Gaussian09 software. 1+1+1+1+1

(12) (a) Suppose two hydrogen atoms are separated by an interatomic distance 'r'. Qualitatively plot the potential energy of these atoms as a function of 'r'.

(b) From this plot indicate the bond length ('r<sub>e</sub>') of the hydrogen molecule.

(c) In the laboratory you noticed that the program gave an error while trying to keep them close to each other beyond a certain 'r'.

(i) What could be the reason behind such error?

(ii) Indicate the closest interatomic distance ('r<sub>0</sub>') for hydrogen molecules in the above potential energy plot.

(d) What is the unit of molecular energy that you calculated using Gaussian09? 1+1+1+1+1