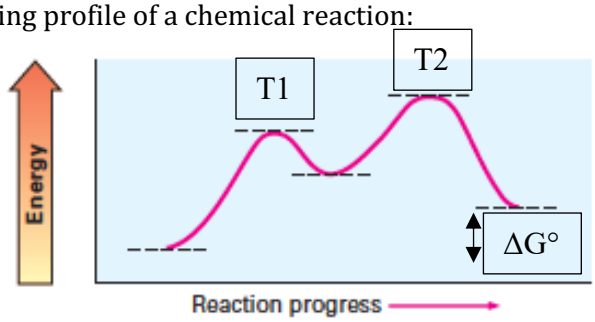
Organic Chemistry - Exercise 4

Distribution: October 10 2024
Help: October 17 2024
Return until: November 20 2024

1. Consider the following profile of a chemical reaction:



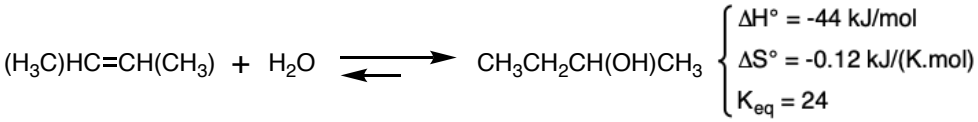
   a. Is ΔG° for the reaction positive or negative? Label it on the diagram.

      ΔG° is positive

   b. How many steps are involved in the reaction and how many transition states are there? Label the transition states on the diagram.

      2 steps and 2 transitions states are involved (cf. diagram)

2. Consider the following chemical reaction:



   a. Give the IUPAC names of the starting material and the products.

      But-2-ene, water, (R) or (S) butan-2-ol

   b. What is the reaction type?

      addition

   c. Is the reaction exothermic or endothermic?

      Exothermic since ΔH is negative

   d. Is the reaction favorable (spontaneous) or unfavorable (nonspontaneous) at room temperature (298 K)?

      ΔG=ΔH-TΔS=-8.24kJ/mol spontaneous

   e. what is the consequence of increasing the temperature at which the reaction is conducted?

      ΔS<0 so exotropic

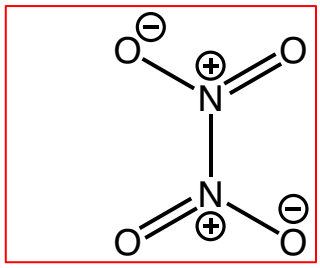
      It will increase ΔG even more and make the reaction less favorable

3. Consider the equilibrium of the following dimerization reaction:

$$2\,NO_2 \rightleftharpoons N_2O_4$$

NO_2 is a brown gas, whereas N_2O_4 is colorless. The Gibbs free energy of the dimerization reaction (left to right) is $\Delta G = -5.13$ kJ/mol at a temperature of 23 °C and $\Delta G = 8.41$ kJ/mol at a temperature of 100 °C.

a. Draw the correct structural formulae (Lewis structures) of N_2O_4.



b. What would you expect to observe with regard to color upon heating a sealed flask from room temperature to 100°C?

ΔG is positive for the forward reaction so the backward reaction is favored and therefore we will observe a brown color in the flask.

c. A sealed flask with a volume of V = 1 L is filled with 0.26 mol of pure NO_2. After a while the equilibrium is reached and a measurement shows that 0.08 mol N_2O_4 is present. Determine the equilibrium constant.

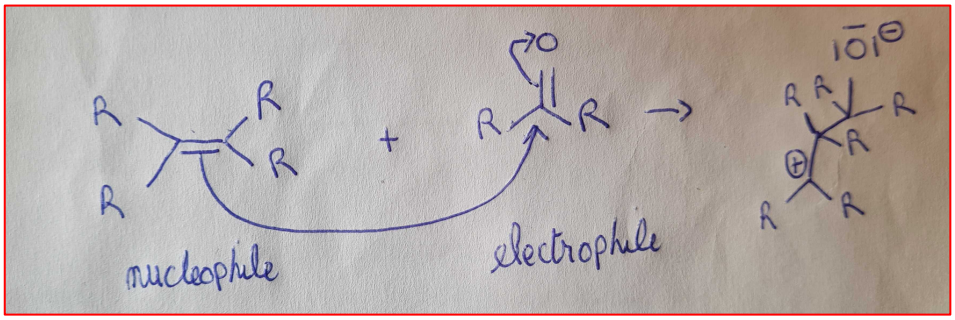
$[NO_2] = 0.10$mol/L ; $[N_2O_4] = 0.08$ mol/L ; $K = 0.08/[0.10]^2 = 8.0$ mol/L

4. Dibromine can participate both in polar reactions and in radical reactions. Discuss why this is favorably possible in each case.

Radical Reactions: Br_2 can undergo homolytic cleavage (breaking of the Br-Br bond with each bromine atom retaining one electron) when subjected to heat or light due to the low bond energy of the molecule. This results in the formation of two bromine radicals (Br•).

Polar Reactions: Despite being nonpolar, the dibromine molecule is highly polarizable due to its relatively large size. Therefore, the approach of a nucleophilic molecule can induce a dipole moment in bromine, resulting for example in the electrophilic addition of a bromine with an alkene.

5. An alkene $R_2C=CR_2$ and a ketone R2C=O can undergo a polar reaction together. Draw the reaction mechanism correctly (hint: electron pair pushing, formal charges), and describe the respective roles of the two molecules in this reaction..



Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 304–334.
Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**, pp. 152-161.
Chimie Organique: Les Grands Principes, John McMurry, *Dunod Editeur*, **2015**, pp. 95-98.
Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 407–441.
Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**, pp. 152-161 + 359-381.
Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2015**, pp. 103-125, 285-303, 327-351.