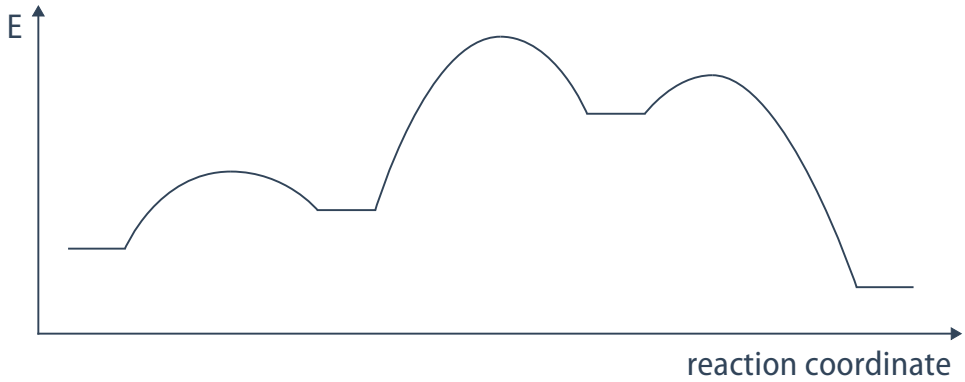
Organic Chemistry – Exercise 5

Distribution: October 30, 2025

Help: November 6, 2025

Return until: November 8, 2025

1. Consider the given profile of a chemical reaction.

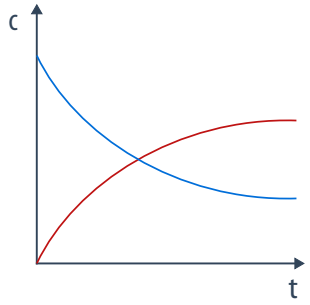


   a. Label ΔG° on the diagram. Is its value positive or negative for this reaction? Is the reaction spontaneous or not?

   b. How many elementary steps are there in the mechanism of this reaction? Label all the transition states on the diagram.

   c. Which step is the rate determining step? Explain why.

d. The concentration of one of the reactants and one of the products were followed over a period of time. The following dependences of species concentration on time were observed. Which curve corresponds to the concentration of the reactant and which one corresponds to the concentration of the product? Sketch the concentration dependence for the same reaction if a catalyst is introduced in the system.



2. Consider the given chemical reaction.

a. Give the IUPAC names of the reactants and the product. Include stereochemical information.

b. What is the reaction type?

The standard enthalpy and entropy of this reaction are, respectively, $\Delta H° = -44$ kJ mol^{-1} and $\Delta S° = -120$ J K^{-1} mol^{-1}.

c. Is this reaction endothermic or exothermic?

d. Is this reaction spontaneous at room temperature?

e. Calculate the equilibrium constant for this reaction at room temperature.

f. What is the highest temperature at which this reaction can be carried out?

3. Ammonia is industrially synthesized through the Haber-Bosch process. The reaction enthalpy is $\Delta H° = -92.3$ kJ mol^{-1} and the reaction entropy is $\Delta S° = -198.5$ J K^{-1} mol^{-1}.

This process is carried out in the presence of a solid catalyst, containing wüstite, aluminium oxide, potassium oxide, calcium oxide, magnesium oxide and molybdenum, under high pressure (60–180 bar) and at elevated temperature (300–500 °C).

a. Calculate the equilibrium constant at 400 °C.

b. **Bonus question:** Even though the reaction is exothermic, it is performed at elevated temperatures. What could be the reason for this?

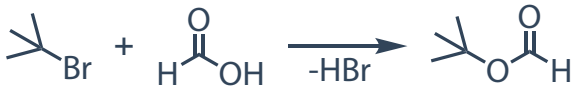
c. If a reactor with the volume of $V = 1\ dm^3$ is loaded with 50 mol of N_2, 50 mol of H_2 and 50 mol of NH_3, will the reaction proceed in the direction of ammonia production or consumption? Consider the temperature to be 400 °C.

d. If the system described in the previous point is allowed to reach equilibrium, calculate the equilibrium concentrations of nitrogen, hydrogen and ammonia. *Hint*: if you are not familiar with numerical solving of equations, you can use online solvers to solve the polynomial equation that you will get.

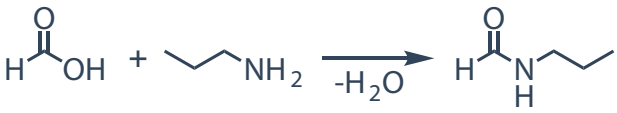
4. Formic acid (methanoic acid) can act as both a nucleophile and an electrophile.
    a. Show three resonance structures of formic acid.

    b. Based on its structure, explain why formic acid can act as both a nucleophile and an electrophile.

    c. This is a reaction between *tert*-butyl bromide and formic acid. What is the reaction type? Is formic acid acting as a nucleophile or an electrophile in this reaction?



    d. This is a reaction between formic acid and propan-1-amine. What is the reaction type? Is formic acid acting as a nucleophile or an electrophile in this reaction?



5. In acidic medium, 4-hydroxybutanal forms a cyclic hemiacetal. The reaction is shown below.

   a. What is the reaction type? Which group is acting as a nucleophile and which is acting as an electrophile?

   b. Label all chiral centers in the starting compound and the product with an asterisk.

Reading Suggestions:

Clayden, Greeves, Warren, *Oxford University Press*, **2012**.

Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**.

Chimie Organique, Les Grands Principes, John McMurry, *Dunod Editeur*, **2009**.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**.