THE EQUILIBRIUM CONSTANT OF THE FORMATION REACTION OF A COMPLEX

1. PURPOSE OF THE WORK

Determining the equilibrium constant of the complex ($[Fe(NCS)]^{2+}$).

2. THEORETICAL NOTIONS

For a reversible reaction in homogeneous systems:

$$\nu_A A + \nu_B B \rightleftharpoons \nu_C C + \nu_D D \qquad (1)$$

the equilibrium constant is given by the expression:

$$K_C = \frac{C_C^{\nu_C} \cdot C_D^{\nu_D}}{C_A^{\nu_A} \cdot C_B^{\nu_B}} \qquad (2)$$

The equilibrium constant, using the standard reaction isotherm:

$$\Delta G_T^0 = -RT \ln K_c \qquad (3)$$

In this work will be determined the equilibrium constant for the reaction:

$$Fe^{2+} + SCN^- \rightleftharpoons [Fe(NCS)]^{2+} \qquad (4)$$

	Fe^{2+}	SCN^-	$[Fe(NCS)]^{2+}$
Initial:	*a*	*b*	0
Equilibrium:	*a-x*	*b-x*	*x*

The equilibrium concentration of colored complex ion $[Fe(NCS)]^{2+}$ will be determined using the spectrophotometer “SP-850”, based on the Lambert-Beer law:

$$E = \varepsilon \cdot c \cdot l \qquad (5)$$

where: E - extinction measured experimentally (absorbance);

ε - extinction molar coefficient;

c - concentration of solution (mol / L);

l - the thickness of the bowl (1 cm).

3. THE EXPERIMENTAL PART

3.1. APPARATUS AND SUBSTANCES

- Spectrophotometer SP-850
- Iron sulphate solution (III) 10^{-1} M
- Iron sulphate solution (III) $3 \cdot 10^{-3}$ M
- Potassium sulfocyanide solution $3 \cdot 10^{-3}$ M
- 4 x 5 mL graduated pipettes
- Cuvettes for spectrophotometer
- Pump for pipettes

Fig. 1. The experimental installation

3.2. PROCEDURE

3.2.1. The control sample (vial 1) is prepared by mixing 1 mL of 10^{-1} M iron (III) sulfate solution and 5 mL of distilled water in a vial. Then sample 2 is prepared by mixing 1 mL of 10^{-1} M iron (III) sulphate solution, $3 \cdot 10^{-3}$ M potassium sulfocyanide and 4 mL of distilled water in another vial.

3.2.2. From the solutions of iron sulphate (III) $3 \cdot 10^{-3}$ M and potassium sulphocyanide $3 \cdot 10^{-3}$ M, six further samples in further six vials are prepared successively, the compositions of which are given in the following table:

Nr. crt.	**Fe^{3+}**		**SCN^-**		**V_{apa}, [mL]**
	V, [mL]	**$a \cdot 10^3$, [ion g/L]**	**V, [mL]**	**$b \cdot 10^3$, [ion g/L]**	
3	3,0	1,50	0	0	3,0
4	3,0	1,50	3,0	1,50	0
5	3,5	1,75	2,5	1,25	0
6	2,5	1,25	3,0	1,50	0,5
7	3,0	1,50	2,5	1,25	0,5
8	3,0	1,50	2,0	1,00	1,0

3.2.3. The absorption spectrum for sample 2 is recorded by measuring the extinction at different wavelengths, in the range 430 nm-670 nm, using the spectrophotometer "SP-850". For this purpose, the device is supplied to the 220 V grid and started up. Allow 20 minutes for the lamp to enter in operating mode. The wavelength is fixed by handling the micrometric drum from the right side to the wavelength, $\lambda = 430$ nm. After switching to absorbance mode (by pressing the A key), the vessel with the control sample is inserted into the place and calibrated by pressing the 100% T key. After zero is shown, the vial with control is replaced with the sample vial and the absorbance value of the sample is read. The recording of the spectrum in the range 450-670 nm is continued using a step of 20 nm. Before each reading, at each wavelength the device will be calibrated with the control sample.

ATTENTION: In the 430-470 nm range, work on filter 2, and in the 490-670 nm range, work will be done on filter 3. The filter is set by rotating the drum found in the cuvette device.

3.2.4. The graphs show the extinctions obtained according to the wavelength E = f (λ). Considering that sample 2 contains a large excess of Fe^{3+} ions, it can be assumed that in the equilibrium mixture all the amount of SCN^- ions is bound in complex combination. Consequently, the spectrum of sample 2 represents the characteristic spectrum of the complex ion $[Fe(NCS)]^{2+}$ concentration $c = 5.00 \cdot 10^{-4}$ gram ion/L. From this graph it can be determined based on the Lambert-Beer law (5) the extinction molar coefficient, absorb, of the complex combination at the wavelength corresponding to the maximum absorption. The optical path is 1 cm.

3.2.5. Attach the micrometric drum to the wavelength corresponding to the maximum absorption in the sample spectrum 1, calibrate again using sample 2 as the control sample and determine the extinctions corresponding to mixtures 4-8.

4. EXPERIMENTAL DATA PROCESSING

4.1. The molar extinction coefficient (ε) from the data recorded for sample 2 is determined:

$$\varepsilon = \frac{E_{max, sample 2}}{c \cdot l} \quad \text{where}$$

$E_{max,\ sample2}$ is read from the graph $E = f(\lambda)$ previously constructed, the concentration $c = 5.00 \cdot 10^{-4}$ ion gram/L and $l = 1$ cm.

4.2. Using the molar extinction coefficient (ε) previously determined, calculate the corresponding equilibrium concentrations (x) for the complex ion $[Fe(NCS)]^{2+}$:

$$x = c = \frac{E_{sample}}{\varepsilon \cdot l}$$ for samples 4 – 8.

4.3. Calculate the equilibrium constant for samples 4-8, using the relation (2) customized for this reaction.

4.4. The standard free reaction enthalpy ΔG_T^o is calculated, using the relation (3), where K_c is the average of the equilibrium constants obtained in point 4.3.

5. QUESTIONS

5.1. Write the formula for equilibrium constant for the studied reaction.

5.2. What is the significance of the equilibrium constant?

5.3. How does the equilibrium constant vary with the concentration?

5.4. Interpret the value of the standard free enthalpy calculated for the studied reaction.