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SPECTROPHOTOMETRIC DETERMINATION OF ACTIVATION PARAMETERS FOR THE EXTRACTION PROCESS OF THIONIN-THIOCYANATE IONIC PAIR

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Different activation parameters for the of tionin-thiocyanate ionic pair extraction process: enthalpy (ΔH), entropy (ΔS), Gibbs energy (ΔG) changes; activation energy have been determined by means of spectrophotometric method (E_a).

***Keywords*:** thionine, thiocyanate, spectrophotometry, activation factor.

Introduction. Activation parameters of the reaction, between thionin and thiocyanate by means of spectrophotometric method through spectrophotometric method were studied in the present article. Thionine has maximum wave length absorption at 600 *nm*. This reaction has been studied spectrophotometrically by monitoring the absorbance of thionine at 600 *nm*. In all phases of the study the optimized conditions were used (Tab. 1).

Table 1

Optimized condition

Thionine concentration	$1.566 \cdot 10^{-4}$ *mol/L*
pH	6–7
Solvent	isobutyl keton
Temperature	30^0C
Time	240 *s*

Partial order of the reaction was used in Table 2.

Table 2

Partial and total order of the reaction

The parameter under study	Order
Thionine, *n*	0.890
Thiocyanate, *n*'	1.074
H^+, *n*"	–0.072
General	1.892

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Thus, the equation rate is: $W = k[\text{thionine}]^{n} \cdot [\text{tiocyanate}^{-}]^{n'} \cdot [\text{H}]^{n''}$ (k) is the rate constant for the reaction respectively n, n', n'' are partial orders of the reaction with respect to different reactants in the reaction.

Determination of ε.

In order to determine ε in the reaction, the concentration of thionine limitation $17.4 \cdot 10^{-6}$ until $1.566 \cdot 10^{-4}$ *mol*/*L* was used. Absorption was recorded. The finally result appears in Tab. 3.

Table 3

Thionine concentration effect

[thionin] $\cdot 10^5$, *mol*/*L*	*A*
1.74	0.041
3.48	0.080
5.22	0.121
6.96	0.174
8.7	0.219
10.44	0.270
12.18	0.301
13.92	0.342
15.66	0.398

The Bear low $A = \varepsilon bc$, $b = 1cm$. After drawing the absorption according to the concentration, we can find: $\varepsilon = 2559.633\ M^{-1} \cdot cm^{-1}$, $W = 0.999\ M/s$.

Determination of activation parameter.

To determine activation energy in the reaction to the temperature, limitation of $5°C$ until $30°C$ was used.

The values of all factors used in the optimal concentration and absorption conditions were recorded in two time parameters 60 *s* (τ_1) and 180 *s* (τ_2) as we can see in Tab. 4.

Table 4

Temperature effect

T, °*C*	*T*, *K*	$1/T$, K^{-1}	$\Delta A = A(\tau_2) - A(\tau_1)$	*k*	ln *k*
5	279.15	0.00358	0.202	28.107	3.336
10	283.15	0.00353	0.218	30.333	3.412
15	288.15	0.00347	0.238	33.111	3.500
20	293.15	0.00341	0.254	35.338	3.565
25	298.15	0.00335	0.280	38.962	3.663
30	303.15	0.00330	0.289	41.453	3.725

The Arrhenius equation: $\ln k = \ln A - E_a/RT$. After, drawing the $\ln k$ according to $1/T$, we can find $E_a = 11.594\ kJ/mol$, $W = -1.0\ M/s$, $A = 4149.116$. By using the Eyring theory of transition state, the activation parameter ΔG, ΔH and ΔS were also calculated for the reaction.

Table 5

Activation parameter

ε	2559.633 $M^{-1} \cdot cm^{-1}$
E_a	11.594 *kJ/mol*
A	4149.116
ΔH	9.074 *kJ/mol*
ΔS	0.1267 *kJ/mol*
ΔG	–29.335 *kJ/mol*

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