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СОЛЬВАТАЦИЯ 1-МЕТИЛ-2-МЕРКАПТОИМИДАЗОЛА И ЕЕ СОЛЬВАТАЦИОННЫЙ ВКЛАД В КОМПЛЕКСООБРАЗОВАНИЕ С ИОНОМ СЕРЕБРА (I) В ВОДНО-ЭТАНОЛЬНЫХ РАСТВОРИТЕЛЯХ

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Влияние растворителей на сольватацию биолигандов, содержащих N- и S-донорные атомы, представляет исключительный интерес для фармацевтики и медицины. Изучение термодинамики реакций сольватации и комплексообразования этих молекул актуально. В данной работе методом изотермической калориметрии при T=298,15 K были определены тепловые эффекты растворения 1-метил-2-меркаптоимидазола (1M2MI) в воде и водно-этанольных растворителях переменного состава с содержанием 0,2, 0,4, 0,6 и 0,9 мольных долей этанола. Из термохимических данных были рассчитаны стандартные значения энтальпий растворения 1M2MI в воде и в водном растворе этанола и энтальпии переноса 1M2MI из воды в водно-этанольные растворители. Методом бомбовой калориметрии были определены теплоты сгорания 1M2MI и рассчитана энтальпия образования 1M2MI. Полученные энтальпийные характеристики 1M2MI представляют научный интерес как индивидуальные термодинамические параметры 1M2MI, а также важны для анализа влияния энтальпии растворения реагентов на изменение энтальпий реакций комплексообразования с участием 1M2MI. В качестве примера был проведен анализ соотношений энтальпийных характеристик реагентов и их влияния на энтальпию реакции образования его комплекса с серебром (I) [Ag 1M2MI]$^+$. Результаты исследования показывают, что соотношение энтальпийных сольватационных вкладов 1M2MI и Ag^+ в изменение энтальпии комплексообразования [Ag 1M2MI]$^+$ отличается от соотношений их сольватационных вкладов в изменение энергии Гиббса комплексообразования. Изменения энтальпии переноса 1M2MI незначительны по сравнению с изменением энтальпии переноса иона серебра (I) и, вероятно, не оказывают существенного влияния на изменение энтальпии реакции при переносе из воды в водно-этанольные растворители.

Ключевые слова: 1–метил-2-меркаптоимидазол, сольватация, комплексообразование, водно-этанольные растворители, энтальпия сольватации, термодинамические параметры сольватации и комплексообразования, ион серебра (I)

SOLVATION OF 1-METHYL-2-MERCAPTOIMIDAZOLE AND ITS SOLVATION CONTRIBUTION TO COMPLEXATION WITH SILVER (I) ION IN WATER-ETHANOL SOLVENTS

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The influence of solvents on the solvation of bioligands containing N- and S- donor atoms are of exceptional interest for pharmaceuticals and medicine. The study of the thermodynamics of solvation reactions and complexation of these molecules is relevant. The solution calorimetry method was used to determine the heat effects of dissolution of 1-methyl-2-mercaptoimidazole (1M2MI) in water and in water-ethanol solvents of 0.2, 0.4, 0.6 and 0.9 mole fractions of ethanol at T=298.15 K. From the thermochemical data, the standard enthalpies of dissolution of 1M2MI and the changes in the enthalpy of transfer of 1M2MI from water to water-ethanol solvents were calculated. In addition, a combustion calorimeter was applied to determine heat of 1M2MI combustion and the enthalpy of 1M2MI formation was calculated. The obtained enthalpy characteristics of 1M2MI are of scientific interest as individual thermodynamic parameters of 1M2MI, and are also important for the analysis of enthalpy solvation contributions of reagents to the change in the enthalpies of complexation reactions involving 1M2MI. As an example, the analysis of the ratios of the enthalpy resolvation characteristics of the reagents and their influence on the reaction enthalpy of [Ag 1M2MI]$^+$ complex formation was done. The results of this study show that the enthalpy solvation ratio between 1M2MI and Ag$^+$ is different from that for their Gibbs energy solvation characteristics. The changes in the enthalpy of transfer of 1M2MI are insignificant compared to the change in the enthalpy of transfer of the silver ion (I) and probably will not have a significant effect on the change in the enthalpy of the reaction when changing the composition of the water-ethanol solvents.

Keywords: 1–methyl-2-mercaptoimidazole, solvation, complex formation, aqueous-ethanol solvents, enthalpy of solvation, thermodynamic parameters of solvation and complex formation, silver (I) ion

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INTRODUCTION

Most biologically significant reactions occur in solutions. The study of the thermodynamics of solvation reactions and complexation of reagents is very relevant. The study of the role of the solvent is also very important [1-3]. Since ions exist in solutions precisely in the form of solvate complexes, during complex formation, the solvent molecules are replaced by a ligand in the internal coordination sphere of the central ion. A significant difference in the concentration of the solvent and ligand levels out the difference in their donor capacity. Thus, the solvent is both a medium and a direct participant in the chemical process [3].

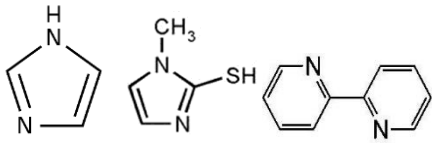
Previously studies of the solvent effect on the thermodynamics of complexation of *d*-metal ions with N- or O- donor amine and carboxylate ligands [4-6] as well as on the thermodynamics of complexation between crown-ethers and amino acids [7-8] are revealed a number of regularities in the change in the solvate state of the reagents and the thermodynamics of complex formation reactions. The data obtained turned out to be necessary to find a shift in the equilibria of complexation during the transition from water to water-organic solvents.

Our choice of imidazole as an object of research is due to its exceptional importance for pharmacy and therapeutic practice. This has been noted by a number of authors who have devoted their research to its anticonvulsant [9], antimicrobial [9-11], antitumor [11-14], anti-inflammatory [9, 12, 15], antitumor [9, 16], antiviral [11-12], and antibacterial properties. [10, 12, 17, 18] and antifungal [19-20] properties.

One of the mercapto-derivatives of imidazole is 1-methyl-2-mercaptoimidazole (1M2MI). 1M2MI is the active component of the pharmaceutical drug methimazole, also known under the trade name thiothiazole, which belongs to the group of imidazole antithyroid drugs [21-23]. These drugs act by inhibiting the peroxidase system, blocking the synthesis of the hormones thyroxine and triiodothyronine.

The introduction of a mercapto group into the imidazole molecule leads to a decrease in its basic properties, which is determined by the thione-thiol rearrangement of the 1M2MI molecule. This is due, first of all, to the presence of a sulfur atom, an active reaction center with variable valence, as well as the high lability of the S-H bond, the cleavage of which, depending on the conditions, can lead to the generation of thiyl radicals, thiolate anions, and sulfenyl cations, which are relatively stable and highly reactive intermediates [24-25].

Due to the presence of N- and S- donor atoms in the molecule, 1-methyl-2-mercaptoimidazole exhibits high reactivity in complexation with metal ions [25, 26]. In order to evaluate the reactivity of 1M2MI with biometal ions, in this study the heat effects of 1M2MI dissolution in water-ethanol mixed solvents were determined, and the enthalpy characteristics of 1M2MI solvation in water-ethanol solvents were calculated. The obtained results were compared with literature data on the effect of water-ethanol solvent on enthalpy changes during the transfer of imidazole and 2,2-dipyridyl from water to water-ethanol solvents. The structural formulas of the amino ligands imidazole, 1-methyl-2-mercaptoimidazole and 2,2-dipyridyl are shown in Fig. 1. The influence of 1M2MI solvation on the thermodynamics of the reaction of formation of a silver(I) monocomplex with 1M2MI in water-ethanol solvents of variable composition of EtOH was analyzed.



a b c

Fig. 1. Structural formulas: a - imidazole, b - 1-methyl-2-mercaptoimidazole, c - 2,2'-dipyridyl
Рис. 1. Структурные формулы: a - имидазол, b - 1-метил-2-меркаптоимидазол, c - 2,2'-дипиридил

MATERIALS AND METHODS

1M2MI (98.5% by weight) from «Alfa Aesar. Shore Road. Heysham. LA3, England» was used without additional purification. Rectified ethyl alcohol was purified by distillation at atmospheric pressure before use. The residual amount of water in ethanol (no more than 5% by weight) was determined by density (by weighing a calibrated pycnometer with ethanol on a Shimadzu AUX220D analytical balance) and taken into account when preparing water-ethanol solvents. Mixed water-ethanol solvents were prepared using bidistilled water by the gravimetric method. Determination of the heat effects of dissolution of 1M2MI in water and in water-ethanol solvents of composition 0.2, 0.4, 0.6 and 0.9 mole fractions of ethanol (mol. fr.) was carried out at T = 298.15 K on an ampule solution calorimetric with an isothermal shell. The design of the calorimetric cell is similar to those described previously [27]. The chemical calibration of the calorimeter was made by the enthalpy of dissolution of crystalline potassium chloride in water. The value obtained was $\Delta_{sol}H^0$(KCl, ∞H_2O, 298.15 K) = 17.22 ± 0.04 kJ·mol^{-1} and it is satisfactorily coincides with the most reliable literary value 17.243 ± 0.018 kJ·mol^{-1} [28].

Based on calorimetric data, the enthalpies of dissolution of 1M2MI in water and in water-ethanol solvents at 0.2, 0.4, 0.6 and 0.9 mol. fr. of ethanol at T = 298.15 K were calculated.

The heat of combustion of 1M2MI was measured in the IKA C6000 isoperibol calorimeter. The compounds were stored in a vacuum desiccator over phosphorus pentoxide.

RESULTS AND DISCUSSION

The concentration conditions of the experiments, molar and standard enthalpies of dissolution of 1M2MI in water-ethanol solvents are given in Table 1. The absence of a concentration dependence of the heat effects of dissolution of 1M2MI and the low concentrations of 1M2MI, close to the state of an infinitely dilute solution, made it possible to accept the average values of the molar enthalpies of dissolution as the standard.

The enthalpies of 1M2MI dissolution in water and in water-ethanol solvents are endothermic. When moving from water to water-ethanol solvents with a high ethanol content, a slight decrease in the endothermicity of dissolution of 1M2MI is observed compared to water. However, the change in the endothermicity of 1M2MI is not monotonous, and in a solvent with a composition of 0.2 mol. fr. ethanol, its local maximum is observed.

Table 1

Concentration conditions of the experiments, molar enthalpies of dissolution ($\Delta_{sol}H_m$) and standard enthalpies of dissolution ($\Delta_{sol}H^0$) and enthalpies of transfer ($\Delta_{tr}H^0$) of 1-methyl-2-mercaptoimidazole in water-ethanol solvents, T = 298.15 K

Таблица 1. **Концентрационные условия экспериментов, молярные энтальпии растворения ($\Delta_{sol}H_m$), стандартные энтальпии растворения ($\Delta_{sol}H^0$) и энтальпии переноса ($\Delta_{tr}H^0$) 1-метил-2-меркаптоимидазола в водно-этанольных растворителях, T = 298,15 K**

X_{EtOH}, mol.fr.	C_{1M2MI}, mol·L^{-1}·10^{-3}	$\Delta_{sol}H^m$, kJ·mol^{-1}	$\Delta_{sol}H^0$, kJ·mol^{-1}	$\Delta_{tr}H^0$, kJ·mol^{-1}
0.0	1.95	6.32	6.50±0.15	0
	1.95	6.22		
	1.95	6.24		
	2.12	6.43		
	2.14	6.49		
	2.76	6.62		
	2.96	6.40		
	4.53	6.81		
	7.46	6.94		
0.2	13.77	8.46	8.26±0.43	1.76
	15.08	8.15		
	20.34	8.17		
0.4	6.20	6.72	6.73±0.39	0.23
	7.10	6.38		
	7.27	6.89		
	7.48	6.92		
0.6	5.19	5.47	5.67±0.23	-0.83
	5.69	5.77		
	6.85	5.78		
	7.27	5.66		
0.9	5.33	6.22	5.91±1.3	-0.69
	5.64	5.52		
	6.59	5.99		

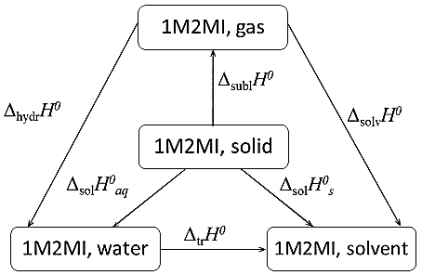


Fig. 2. Thermodynamic cycle for calculating the enthalpy of solvation: $\Delta_{sol}H^0_{aq}$; $\Delta_{sol}H^0_s$; $\Delta_{hydr}H^0$; $\Delta_{solv}H^0$; $\Delta_{subl}H^0$; $\Delta_{tr}H^0$; - Enthalpies of dissolution in water and in a mixed solvent; hydration, solvation, sublimation and transfer of 1-methyl-2-mercaptoimidazole from water to a mixed solvent, respectively

Рис. 2. Термодинамический цикл для расчета энтальпии сольватации: $\Delta_{sol}H^0_{aq}$; $\Delta_{sol}H^0_s$; $\Delta_{hydr}H^0$; $\Delta_{solv}H^0$; $\Delta_{subl}H^0$; $\Delta_{tr}H^0$; - Энтальпии растворения в воде и в смешанном растворителе; энтальпии гидратации, сольватации, сублимации и переноса 1-метил-2-меркаптоимидазола из воды в смешанный растворитель, соответственно

According to the solvation-thermodynamic approach [2], enthalpies of transfer term quantitatively reflect the influence of the solvent on changes in the enthalpy of solvation the reagents. The enthalpies of transfer of 1-methyl-2-mercaptoimidazole from water to binary solvents were calculated based on the thermodynamic cycle (Fig. 2).

Based on the experimental heats of 1M2MI dissolution in mixed water-ethanol solvents, the enthalpies of transfer of 1M2MI from water to water-ethanol solvents were calculated as:

$$\Delta_{tr}H^0 = \Delta_{sol}H^0{}_s - \Delta_{sol}H^0{}_{aq}, \quad (1)$$

where $\Delta_{sol}H^0{}_s$ and $\Delta_{sol}H^0{}_{aq}$ – standard molar enthalpies of solution in a mixed water-ethanol solvent (S) and in water (aq).

The calculated $\Delta_{tr}H^0$(1M2MI) values are reported in the Table 1. The enthalpy of transfer from water to water-ethanol mixtures for ammonia and amines that have cyclic substituents and functional groups of different nature in their structure 2,2'-dipyridyl, 1-methyl-2-mercaptoimidazole and imidazole are plotted against water-ethanol solvent composition in the Fig. 3.

Despite the differences in the structure of amines, the range of compositions of water-ethanol solvent 0.1-0.2 mol. fr. for all amines shows a maxima of endothermicity of the enthalpy of transfer. The introduction of methyl and mercapto groups into the imidazole molecule significantly reduces the maximum of endothermicity for 1M2MI compared to imidazole. For 2,2'-dipyridyl, the endothermic extremum is maximal compared to other amines. For ammonia, the endothermicity of the transfer increases significantly when moving from water to a solvent of 0.2 mol % ethanol and is comparable in $\Delta_{tr}H^0$ value to imidazole in this region of solvent compositions. Subsequent additions of cosolvent to water lead to a further smooth increase in the positive $\Delta_{tr}H^0$ values of ammonia. The endothermic extremes of $\Delta_{tr}H^0$ of amines upon the first additions of ethanol are explained by the effect of hydrophobic hydration and weakening of the solvation of amino groups of non-electrolytes. Hydrophobic hydration characterizes the strengthening of interactions between distant water molecules under the action of particles of the dissolved substance. Hydrophobic effects are a specific property of solvents that have a spatial network of hydrogen bonds. Arnet et al. [30] showed that the endothermic maxima on the dependences of the enthalpies of dissolution of non-electrolytes on the composition of the water-ethanol solvent increase with increasing size of the non-electrolyte molecules. There is an opinion [30] that the increase in the endothermicity of dissolution of non-electrolytes is due to an increase in the endo effect of cavity formation in a highly structured solvent. Consequently, the significantly larger value of the $\Delta_{tr}H^0$ extremum for 2,2'-Dipy compared to ammonia and imidazole can be explained by different energies of cavity formation during the solvation of amine molecules of different molecular volumes. However, it should be taken into account that the contribution from the resolvation of nitrogen atoms to the enthalpy of transfer of an organic molecule is quite large, since the nitrogen heteroatom is the most reactive fragment of these molecules.

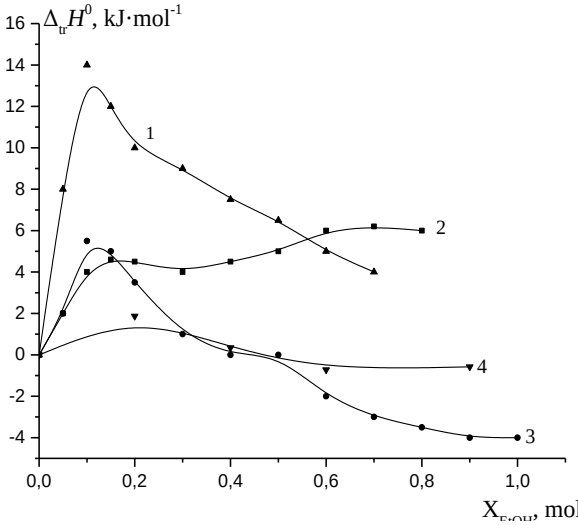


Fig. 3. Enthalpies of transfer from water to water-ethanol solvents of 1–2,2'-dipyridyl [29], 2–ammonia, 3–imidazole [29], 4 – 1-methyl-2-mercaptoimidazole

Рис. 3. Энтальпии переноса из воды в водно-этанольные растворители 1-2,2'-дипиридила [29], 2–аммиака, 3–имидазола [29], 4 – 1-метил-2-меркаптоимидазола

Previously, changes in the Gibbs energy of 1M2MI transfer from water to water-ethanol solvents were determined in [31]. Also the dependence $\Delta_{tr}G^0$ (1M2MI) = $F(X_{EtOH})$ has an endothermic maximum in the range of 0.2 mol.fr. of EtOH. Subsequent additions of ethanol lead to a decrease in the endothermicity of 1M2MI solvation with a transition from positive values of $\Delta_{tr}G^0$ to negative values at $X_{EtOH} \approx 0.45$ mol.fr. In solvents of the composition $X_{EtOH} > 0.6$ mol.fr. the values of $\Delta_{tr}G^0$(1M2MI) remain constant. This indicates that the changes of the 1M2MI solvation state are completed at $X_{EtOH} \approx 0.6$ mol.fr.

Using the enthalpy characteristics of 1M2MI obtained in this study and the $\Delta_{tr}G^0$(1M2MI) values from [31], the entropic contributions to the change in transfer Gibbs energy from water to aqueous-ethanol solvents were estimated in accordance with the equation:

$$\Delta_{tr}G^0 = \Delta_{tr}H^0 - T\Delta_{tr}S^0. \quad (2)$$

The dynamics of changes in the thermodynamic characteristics of 1M2MI solvation in aqueous-ethanol solvents is shown in Fig. 4.

The change in the Gibbs energy of 1M2MI resolvation is determined by its enthalpy component up to $X_{EtOH} \approx 0.45$ mol.fr. The entropic solvation contribution prevails with subsequent ethanol additions and leads to hardening of the solvate shell of 1M2MI.

On the other hand, the process of dissolution of $C_4H_6N_2S$ in water can be represented by the scheme:

$$C_4H_6N_2S\,(cr) + nH_2O = C_4H_6N_2S{\cdot}nH_2O\,(sol). \quad (3)$$

Standard enthalpies of formation of 1M2MI solution at infinite dilutions were calculated using the equation:

$$\Delta_f H^0(C_4H_6N_2S_{\,sol,nH_2O,\,298.15\,K}) = \Delta_f H^0(C_4H_6N_2S,_{\,cr,\,298.15\,K}) + \\ + \Delta_{sol}H(C_4H_6N_2S,_{\,cr.,\,298.15\,K}), \quad (4)$$

where $\Delta_f H^0(C_4H_6N_2S,_{\,cr.,\,298.15\,K})$ – standard enthalpy of formation of crystalline 1M2MI; $\Delta_{sol}H(C_4H_6N_2S,_{\,cr.,\,298.15\,K})$ – heat of solution of 1M2MI in water (Table 2).

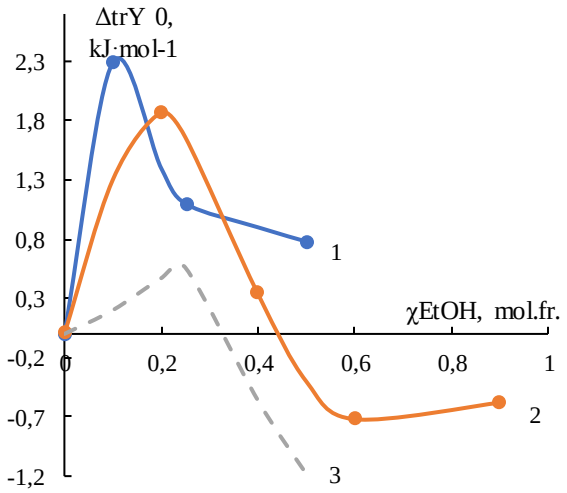


Fig. 4. Thermodynamics of 1-M2MI solvation in aqueous ethanol solvents: 1 - $\Delta_{tr}G^0$ [31], 2- $\Delta_{tr}H^0$, 3 - $T\Delta_{tr}S^0$

Рис. 4. Термодинамика сольватации 1-М2МИ в водно-этанольных растворителях: 1 - $\Delta_{tr}G^0$ [31], 2- $\Delta_{tr}H^0$, 3 - $T\Delta_{tr}S^0$

Table 2

Enthalpy of dissolution of $C_4H_6N_2S$ in water at 298.15 K

***Таблица 2.* Энтальпии растворения $C_4H_6N_2S$ в воде при 298,15 К**

m, g	$m{\cdot}10^3$, mol $C_4H_6N_2S$ /1000 g H_2O	n, mol H_2O/mol $C_4H_6N_2S$	$\Delta_{sol}H^m$, kJ·mol^{-1}	$\Delta_f H^0(C_4H_6N_2S_{\,sol,nH2O,\,298.15\,K})$, kJ·mol^{-1}
0.01101	2.288	24272	6.32	-11033.0
0.01103	2.286	24272	6.22	-11032.9
0.01104	2.286	24272	6.24	-11032.9
0.01200	2.494	22250	6.43	-11033.1
0.01213	2.827	19632	6.49	-11033.2
0.01562	3.492	15893	6.62	-11033.3
0.01673	3.534	15706	6.40	-11033.1
0.02561	5.324	10425	6.81	-11033.5
0.04223	8.779	6322	6.94	-11033.6

To calculate the enthalpies of formation of 1M2MI, experimental data are required on the heat of dissolution of 1M2MI in water (Tables 1 and 2) at infinite dilution and the heat of formation of crystalline 1M2MI.

The integral enthalpy during the dissolution of 1M2MI with infinite dilution was determined by extrapolating the linear dependence of $_{sol}H_m$ on $m^{1/2}$ to the zero value of molality (m). The experimental points within the margin of error are placed on a straight line. The segments cut off in straight lines when extrapolated to the ordinate axis give the thermal effect of dissolution at zero ionic ion strength and the resulting value refers to a hypothetical solution. They are key quantities in the thermochemistry of a compound, and open up the possibility of conducting rigorous thermodynamic calculations in systems with 1M2MI.

The heat of formation of crystalline 1M2MI was obtained from combustion calorimetry results using IKA C6000 isoperibol calorimeter.

The standard enthalpy of combustion ($\Delta_c H^0$) of compounds can be calculated as:

$$\Delta_c H^0 = \Delta_c U^0 + \Delta nRT, \quad (5)$$

where Δn is the change in the number of moles of gas in the chemical equation for the combustion process of substances.

The value $\Delta_c U^B_{(cr.,298\,K)}$, obtained by us experimentally for 1M2MI ($C_4H_6N_2S$), refers to the combustion reaction:

$$C_4H_6N_2S_{(cr.)} + 6.5O_{2(g.)} = \\ = 4CO_{2(g.)} + SO_{2(g.)} + 3H_2O_{(liq.)} + N_{2(g.)}. \quad (6)$$

The value of $\Delta_c U^B$ obtained as a result of the experiment refers to the isothermal combustion reaction of the 1M2MI under real conditions of the process.

Errors in determining the values of heat of combustion were calculated similarly to the error of the energy equivalent of the calorimeter with a confidence level of 0.95.

For sulfur-containing compounds, the equation for calculating the heat of formation is:

$$\Delta_f H^0 = (C_mH_nN_pS_{j\ cr.,\ 298\ K}) = m\Delta_f H^0(CO_{2,\ g,\ 298\ K}) + n/2\ \Delta_f H^0(H_2O_{,\ liq,\ 298\ K}) + j\Delta_f H^0(SO_{2\ g.,\ 298\ K}) - \Delta_c H^0(C_mH_nN_pS_{j\ cr.,\ 298\ K}). \quad (7)$$

The value of $\Delta_c H^0$ obtained for 1M2MI from equation (5) is 13745.8 kJ·mol^{-1} and was used to calculate the enthalpy of formation of crystalline $C_4H_6N_2S$:

$$\Delta_f H^0(C_4H_6N_2S_{,\ cr.,\ 298.15\ K}) = 4\Delta_f H^0(CO_{2,\ g,\ 298.15\ K}) + 3\Delta_f H^0(H_2O_{,\ liq.,\ 298.15\ K}) + \Delta_f H^0(SO_{2,\ g,\ 298,15\ K}) - \Delta_c H^0(C_4H_6N_2S_{,\ cr.,\ 298.15\ K}). \quad (8)$$

Standard enthalpies of formation $\Delta_f H^0(CO_{2,\ g,\ 298.15\ K})$ = -393.51 ± 0.04 kJ·mol^{-1}, $\Delta_f H^0(H_2O_{,\ liq.,\ 298.15\ K})$ = -285.81 ± 0.04 kJ·mol^{-1}, $\Delta_f H^0(SO_{2,\ g.,\ 298.15\ K})$ = -296.9 ± 0.05 kJ·mol^{-1} [32]. As a result, the calculated average value $\Delta_f H^0(C_4H_6N_2S_{\ cr.,\ 298.15\ K})$ = −11026.4 ± 0.05 kJ·mol^{-1} was accepted as standard.

The obtained enthalpy characteristics of 1M2MI are necessary for the analysis of the contributions of enthalpic solvation of reagents to the change in the enthalpies of complexation reactions involving 1M2MI. One of such processes is the reaction of formation of 1M2MI complexes with silver ion (I) in water-ethanol solvents. It was previously established that the coordination of the silver (I) ion with thia derivatives of imidazole occurs via the sulfur atom and mono-, bis-, and tris-substituted complexes of the silver (I) ion with 1M2MI are possible [33]. The stability constants of the silver (I) complexes with 1M2MI were determined and an analysis of the solvation contributions to the change in the Gibbs energy of complex formation was performed [31]. It was found that the stability of all complex forms is minimal in a solvent of 0.1 mol. fr. ethanol. Subsequent additions of ethanol to water cause a monotonic increase in the stability of complex particles. The increase in the solvation of the monocomplex particle determines the strengthening of the silver monocomplex due to the compensation of the solvation contributions of the central ion and ligand when moving from water to the water-ethanol solvent.

The available literature data on the change in the enthalpy of transfer of silver ion from water to water-ethanol solvents [35] and the enthalpy characteristics of 1M2MI obtained in this work allow to make a conclusion about the ratios of the enthalpy resolvation characteristics of the reagents and their influence on

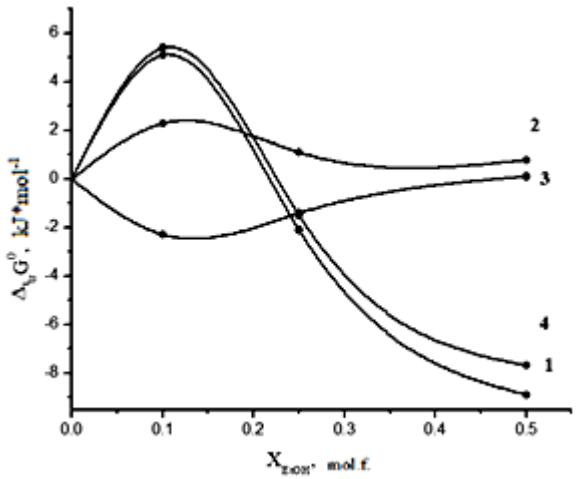


Fig. 5. The effect of water-ethanol solvent on the Gibbs energies of transfer of the reaction of formation of a monocomplex of silver (I) ion with 1M2MI, reagents and reaction products: 1-$\Delta_{tr}G^0_{r1}$ [31]; 2-$\Delta_{tr}G^0$(1M2MI) [34]; 3-$\Delta_{tr}G^0(Ag^+)$ [34]; 4-$\Delta_{tr}G^0$[Ag(1M2MI)]$^+$ [31]

Рис. 5. Влияние водно-этанольного растворителя на энергии Гиббса переноса реакции образования монокомплекса иона серебра (I) с 1М2МИ, реагентов и продуктов реакции: 1-$\Delta_{tr}G^0_{r1}$ [31]; 2-$\Delta_{tr}G^0$(1М2МИ) [34]; 3-$\Delta_{tr}G^0(Ag^+)$ [34]; 4-$\Delta_{tr}G^0$[Ag(1М2МИ)]$^+$ [31]

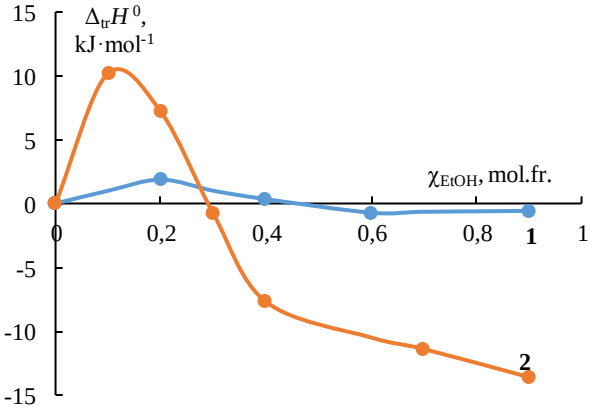


Fig. 6. Changes in the enthalpies of solvation of 1M2MI (1) and Ag^+ (2) [35] in water-ethanol solvents

Рис. 6. Изменения энтальпий сольватации 1М2МИ (1) и Ag^+ (2) [35] в водно-этанольных растворителях

the reaction enthalpy of [Ag 1M2MI]$^+$ complex formation. Currently, there is no information in the literature on the enthalpy of [Ag 1M2MI]$^+$ complexation in water-ethanol solvents.However, the results of this study show that the enthalpy solvation ratio between 1M2MI and Ag^+ is different from that for their Gibbs energy solvation characteristics (Fig. 5,6). The changes in the enthalpy of transfer of 1M2MI are insignificant compared to the change in the enthalpy of transfer of the silver ion (I) and probably will not have a significant effect on the change in the enthalpy of the reaction when changing the composition of the water-ethanol solvent.

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CONFLICTS OF INTERESTA

Авторы заявляют об отсутствии конфликта интересов, требующего раскрытия в данной статье.

The authors declare the absence of a conflict of interest warranting disclosure in this article.

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