ELECTROCHEMICAL PROPERTIES OF AQUEOUS SOLUTIONS OF SODIUM AMINOMETHANESULFONATES

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The pH and conductometric study of the electrochemical properties of aqueous solutions ($1 \cdot 10^{-4} \div 9 \cdot 10^{-3}$ M) $\text{YNHCH}_2\text{SO}_3\text{Na}$ ($\text{Y} = \text{H}, \text{CH}_3, \text{HOCH}_2\text{CH}_2, (\text{CH}_3)_3\text{C}$ and $\text{C}_6\text{H}_5\text{CH}_2$) was carried out. The values of the limiting electrical conductivity were calculated by extrapolation according to Shidlovsky. The activation parameters of the electrical conductivity of the systems “sodium aminomethanesulfonate – H_2O ” at 293–313 K were obtained.

Key words: aminomethanesulfonic acids, aqueous solutions, hydrolysis, conductivity.

INTRODUCTION. The theoretical interest in aminomethanesulfonic acid and its N-alkylated derivatives is explained by their specific physicochemical properties and a wide spectrum of biological activity [1–5]. Under physiological conditions ($\text{pH} = 6.8 - 7.8$), the degree of dissociation of the sulfo group, in contrast to α -aminocarboxylic acids, is 100%, and the pK_a values of the amino group are in the range of physiological pH values [6–9]. The sulfo group can act as an anionic fragment and a hydrogen bond acceptor when interacting with a potential biological target [10].

Solubility and permeability are two biopharmaceutical parameters responsible for effective bioavailability and good correlation between *in vitro* and *in vivo* studies [11]. The improvement of solubility and dissolution rate,

as well as bioavailability of amino acids, continues to be a challenge for pharmaceutical technologists. The hydrotropic action of sulfonates and amino acids is considered as one of the important methods of solubilization [12, 13]. Conductometric studies of aminomethanesulfonates at a definite and infinite dilution in a solvent system provide valuable information about ion-ion (complexation, association) and ion-solvent (solvation) interactions.

Therefore, the determination of the temperature and concentration dependences of the molar electrical conductivity of aqueous solutions of sodium aminomethanesulfonates and monoethanolammonium is, of course, an actual task. To determine the factors affecting the electrical conductivity of aqueous solutions of sodium aminomethanesulfonates,

a pH and conductometric study of their behavior was carried out in the temperature range of 293–313 K.

EXPERIMENTAL PART. The studies used AMSA, its N-methyl (**MeAMSA**), N-(2-hydroxyethyl) (**HEAMSA**), N-*tert*-butyl (**t-BuAMSA**) and N-benzyl (**BzAMSA**) derivatives synthesized according to original methods [3, 14]. Aqueous solutions of sodium salts $\text{YNHCH}_2\text{SO}_3\text{Na}$ ($\text{Y} = \text{H}$ (**AMSNa**), CH_3 (**MeAMSNa**), HOCH_2CH_2 (**HEAMSNa**), $(\text{CH}_3)_3\text{C}$ (**t-BuAMSNa**) and $\text{C}_6\text{H}_5\text{CH}_2$ (**BzAMSNa**)) were prepared by NaOH reacting with the corresponding acids in equimolar amounts.

Potentiometric measurements were carried out using a universal EB-74 ionomer and a pH-meter of the pH-150M type. The pH measurement accuracy was ± 0.05 units (EB-74) and ± 0.02 units (pH-150M), and for the redox potential ± 1 mV (EB-74). Conductometric measurements were performed on an Expert-002 conductometer (the relative error was $\leq 0.5\%$).

Electrochemical properties of aqueous solutions of sodium aminomethanesulfonates

Fig. 1–5 show the results of pH and conductometric studies of aqueous solutions ($1 \cdot 10^{-4} \div 1 \cdot 10^{-2}$ M) AMSNa, MeAMSNa, HEAMSNa, *t*-BuAMSNa and BzAMSNa in the temperature range $293 \div 313$ K. Judging by the results of conductometric study of the systems AMSNa – H_2O (Fig. 1b) and YAMSNa – H_2O (Fig. 2b – 5b), an increase in temperature from 293 to 313 K is accompanied by an increase in the electrical conductivity of the systems (similar to aqueous solutions of AMSA [15], YAMSA [16] and glycine [11]) due to an increase in the degree of dissociation of electrolytes and (or) the mobility of the resulting ions. In this case,

for all the systems under study, acidic properties decrease with an increase in temperature from 293 to 308 K (Fig. 1a – 5a).

Aminosulfonic acids, like amino-carboxylic acids, belong to the class of organic ampholytes and in solution can be in several ionic forms. The qualitative and quantitative composition of amino acid forms depends on the type of amino acid and the pH of the solution [6, 10, 11, 15].

Fig. 1. pH (a) and molar conductivity (b) of aqueous solutions of AMSNa. T (K): 293–1; 298–2; 303–3; 308–4; 313–5.

Even in the simplest case of an aqueous solution of an individual amino acid, a complex mixture is formed, consisting of zwitter-

ions, amino acid cations and anions, protons, and hydroxyl anions. The mutual influence of all components of the system on each other determines the complexity in the study of the electrochemical behavior of solutions of amino acids and their salts.

$$K_h = \frac{[\text{YN}^+\text{H}_2\text{CH}_2\text{SO}_3^-] \cdot [\text{OH}^-]}{[\text{YNHCH}_2\text{SO}_3^-]} \quad (2)$$

Fig. 2. pH (a) and molar conductivity (b) of aqueous solutions of MeAMSN a. T (K): 293–1; 298–2; 303–3; 308–4; 313–5.

In aqueous solutions of YAMSN a pH > 7.0 is due to hydrolysis of aminomethanesulfonate ions (reaction 1) with the formation of zwitterions:

Fig. 3. pH (a) and molar conductivity (b) of aqueous solutions of HeAMSN a. T (K): 293–1; 298–2; 303–3; 308–4; 313–5.

With equations (1), (3), we have a system of equations that take into account the law of effective masses (2), material balance according to YAMSA (4) and the condition of electroneutrality (5).

$$Q_{\text{YAMSNa}} =$$

$$= [\text{Y}\overset{+}{\text{N}}\text{H}_2\text{CH}_2\text{SO}_3^-] + [\text{YNHCH}_2\text{SO}_3^-]$$

$$[\text{YNHCH}_2\text{SO}_3^-] + [\text{OH}^-] = [\text{H}^+] + [\text{Na}^+]$$

(3)

(4)

(5)

tion by reaction (6) [17]. At pH < 7.0, in aqueous solutions of YAMSNa (Y – CH₃, HOCH₂CH₂, (CH₃)₃C and C₆H₅CH₂), unlike AMSNa, hydrolytic decomposition of N-alkylaminomethanesulfonate ions occurs with the formation of alkylaminomethanol and hydrosulfite ions:

Fig. 4. pH (a) and molar conductivity (b) of aqueous solutions of *t*-BuAMSNa. T (K): 293–1; 298–2; 303–3; 308–4; 313–5.

N-alkylation of aminomethanesulfonate anions promotes hydrolytic decomposi-

Fig. 5. pH (a) and molar conductivity (b) of aqueous solutions of BzAMSNa. T (K): 293–1; 298–2; 303–3; 308–4; 313–5.

Along with this, dissociation (7) of HSO_3^- occurs, as well as protonation (8) and (9) at the nitrogen atoms of N-alkylaminomethanesulfonate ions and alkyl-aminomethanol, respectively:

In this case, the material balance according to YAMSN_a takes the form (10), and the condition of electroneutrality - (11). In addition, equation (12) must be taken into account.

$$\begin{aligned} Q_{\text{YAMSA}} = & [\text{YNHCH}_2\text{SO}_3^-] + \\ & + [\text{YNHCH}_2\text{OH}] + [\text{Y}\overset{+}{\text{N}}\text{H}_2\text{CH}_2\text{SO}_3^-] + \\ & + [\text{Y}\overset{+}{\text{N}}\text{HCH}_2\text{OH}] \end{aligned} \quad (10)$$

$$\begin{aligned} & [\text{YNHCH}_2\text{SO}_3^-] + [\text{OH}^-] + [\text{HSO}_3^-] + \\ & + 2[\text{SO}_3^{2-}] = [\text{H}^+] + [\text{Na}^+] + [\text{Y}\overset{+}{\text{N}}\text{HCH}_2\text{OH}] \end{aligned} \quad (11)$$

$$\begin{aligned} & [\text{YNHCH}_2\text{OH}] + [\text{Y}\overset{+}{\text{N}}\text{HCH}_2\text{OH}] = \\ & = [\text{HSO}_3^-] + [\text{SO}_3^{2-}] \end{aligned} \quad (12)$$

Due to the lack of data on equilibrium (9), we calculated, similarly to [6, 8], the ion-molecular composition of aqueous solutions of YAMSN_a only at pH > 7.0 on the basis of pH-metric data (Fig. 1a-5a).

The ionic strength of sodium aminomethane sulfonate solutions at pH > 7.0 is determined by the following expression:

$$\begin{aligned} \mu = & \frac{1}{2} \cdot ([\text{YNHCH}_2\text{SO}_3^-] \cdot (-1)^2 + \\ & + [\text{OH}^-] \cdot (-1)^2 + [\text{H}^+] \cdot (-1)^2 + [\text{Na}^+] \cdot (-1)^2 + \\ & + [\text{Y}\overset{+}{\text{N}}\text{H}_2\text{CH}_2\text{SO}_3^-] \cdot 2^2) \end{aligned} \quad (13)$$

Due to the fact that the degree of hydrolysis of aminomethanesulfonate anions and N-alkylaminomethanesulfonate anions by reaction (1) does not exceed 2.0 %, then μ is practically equal to C_{YAMSN_a} for all studied sodium aminomethanesulfonates in the region $C_{\text{YAMSN}_a} = (2.0 \div 10 \cdot 10^{-3} \text{ mol} \cdot \text{l}^{-1})$ in the investigated temperature range.

Using the obtained data, the constants of hydrolysis (2) of aminomethanesulfonate and N-alkylaminomethanesulfonate anions were calculated.

$$\text{p}K_h = -\lg K_h \quad (14)$$

Dependences of $\text{p}K_h = f(\mu)$ are described by the equation (15), coefficients of which are in the Table 1.

$$\text{p}K_h = A_i + B_i \cdot \sqrt{\mu} + C_i \cdot \mu \quad (15)$$

Analyzing the data in the table. 1, it should be noted that for the studied acids the constants of equation (15) are related to each other by directly proportional dependences (16) - (19).

$$\begin{aligned} B_{\text{AMS}} = & -731.2 + 157.6 \cdot A_{\text{AMS}} - \\ & - 8.148 \cdot (A_{\text{AMS}})^2; R^2 = 0.9985 \end{aligned} \quad (16)$$

$$\begin{aligned} C_{\text{AMS}} = & 4902 + 1039 \cdot A_{\text{AMS}} + \\ & + 53.66 \cdot (A_{\text{AMS}})^2; R^2 = 0.9980 \end{aligned} \quad (17)$$

$$\begin{aligned} B_{\text{BzAMS}} = & -165.3 + 45.31 \cdot A_{\text{BzAMS}} - \\ & - 2.550 \cdot (A_{\text{BzAMS}})^2; R^2 = 0.9879 \end{aligned} \quad (18)$$

$$\begin{aligned} C_{\text{BzAMS}} = & 1129 + 292.5 \cdot A_{\text{BzAMS}} + \\ & + 16.60 \cdot (A_{\text{BzAMS}})^2; R^2 = 0.9846 \end{aligned} \quad (19)$$

According to the definition [18], the coefficient A_i in equation (15) is the negative decimal logarithm of the thermodynamic hydrolysis constant K_h . The $\text{p}K_h = f(T)$ dependences are shown in Fig. 6.

The observed straight-line dependences (Fig. 7) of the thermodynamic constants of hydrolysis of N-methyl, N-*tert*-butyl and N-benzyl-aminomethanesulfonate anions on the thermodynamic constants of hydrolysis of aminomethanesulfonate anions are described

by the equation (20), the parameters of which are given in the Table 2, and testify to the similarity in these processes.

$$pK_h^T(YNHCH_2SO_3^-) = A_i + B_i \cdot pK_h^T(NH_2CH_2SO_3^-) \quad (20)$$

Table 1

The values of the coefficients in equation (15) for aqueous solutions of YAMSNa.

$$C_{YAMSNa} = (0.1 \div 10.0) \cdot 10^{-3} \text{ mol} \cdot \text{l}^{-1}; n = 9$$

T, K	A_i	B_i	C_i	R^2
$NH_2CH_2SO_3^-$				
293	10.63	23.06	-76.68	0.9999
298	10.31	27.03	-102.4	0.9997
303	10.04	29.59	-119.1	0.9992
308	9.87	30.18	-122.8	0.9991
313	9.71	30.49	-124.6	0.9991
$H_3CNHCH_2SO_3^-$				
298	10.72	16.66	-39.07	0.9992
303	10.52	17.35	-42.37	0.9999
308	10.27	19.63	-56.03	0.9998
313	10.15	19.10	-52.63	0.9997
$HOCH_2CH_2NHCH_2SO_3^-$				
293	10.74	20.05	-57.10	0.9998
298	10.40	24.28	-83.49	0.9999
303	10.20	24.97	-87.45	0.9997
308	10.38	17.04	-40.03	0.9999
313	10.14	19.16	-51.87	0.9999
$(CH_3)_3CNHCH_2SO_3^-$				
298	10.19	29.48	-116.9	0.9992
303	10.15	26.04	-94.36	0.9999
308	9.91	28.34	-109.6	0.9996
313	9.75	28.63	-111.5	0.9993
$C_6H_5CH_2NHCH_2SO_3^-$				
293	10.36	29.78	-119.5	0.9994
298	10.13	31.45	-130.9	0.9995
303	9.94	32.25	-136.3	0.9995
308	9.74	33.73	-147.1	0.9992
313	9.58	33.99	-148.6	0.9991

Thus, the molar electrical conductivity of aqueous solutions of sodium aminomethanesulfonates is determined by the equation (21):

$$\lambda = \lambda_{\text{Na}^+}^0 \cdot a_{\text{Na}^+} + \lambda_{\text{OH}^-}^0 \cdot a_{\text{OH}^-} + \lambda_{\text{YNHCH}_2\text{SO}_3^-}^0 \cdot a_{\text{YNHCH}_2\text{SO}_3^-} + \lambda_{\text{YNH}_2\text{CH}_2\text{SO}_3^+}^0 \cdot a_{\text{YNH}_2\text{CH}_2\text{SO}_3^+} \quad (21)$$

Fig. 6. Temperature dependence of thermodynamic hydrolysis constants of $\text{YNHCH}_2\text{SO}_3^-$.

Y – H (1), CH_3 (2), HOCH_2CH_2 (3), $(\text{CH}_3)_3\text{C}$ (4) and $\text{C}_6\text{H}_5\text{CH}_2$ (5).

Table 2

Coefficient values in the equation (20)

Y	A_i	B_i	R^2
CH_3	0.5854	0.9847	0.9804
$(\text{CH}_3)_3\text{C}$	2.6621	0.7332	0.9571
$\text{C}_6\text{H}_5\text{CH}_2$	1.4430	0.8413	0.9883

R-squared values ($R^2 \geq 0.98$) indicate a satisfactory nature of the correlation according to equation (22), and the values of the limiting electrical conductivity (λ_0) are numerically equal to the coefficients B_0 . Thus, the experimental values of the limiting molar electrical

Data on the electrical conductivity of aqueous solutions of sodium aminomethanesulfonates given in the Table 3, represent the result of a correlation analysis of the dependence of λ ($\text{Ohm}^{-1}\cdot\text{sm}^2\cdot\text{mol}^{-1}$) on the molar concentration of YAMSNa in a four-parameter dependence according to Shidlovsky (22), which describes the behavior of solutions of weak 1:1 electrolytes at a concentrations more than $10^{-3} \text{ mol}\cdot\text{l}^{-1}$ [19].

$$\lambda = B_0 + B_1 \cdot C^{0.5} + B_2 \cdot C + B_3 \cdot C^{1.5} \quad (22)$$

Fig. 7. Mutual dependences of thermodynamic hydrolysis constants of $\text{YNHCH}_2\text{SO}_3^-$.

conductivity of aqueous solutions of sodium aminomethanesulfonates obtained by extrapolation according to Shidlovsky, like λ_0 of aqueous solutions of N-derivatives of amino-methanesulfonic acid [16], increase with increasing temperature.

According to Kohlrausch's law for weak electrolytes [20], the limiting electrical conductivity of aqueous solutions of sodium aminomethanesulfonates is determined by expression (23).

$$\lambda_{\text{YNHCH}_2\text{SO}_3\text{Na}}^0 = \lambda_{\text{Na}^+}^0 + h^0(\lambda_{\text{OH}^-}^0 + \lambda_{\text{YNH}_2\text{CH}_2\text{SO}_3^+}^0) + (1 - h^0)\lambda_{\text{YNHCH}_2\text{SO}_3^-}^0 \quad (23)$$

where h^0 – the degree of hydrolysis of aminomethanesulfonate ions at infinite dilution.

In infinitely dilute solutions of hydrolyzed $\text{YNHCH}_2\text{SO}_3\text{Na}$, hydrolysis occurs at the anion (1). The degree of hydrolysis will be determined, like [20], by the following equation:

$$h^0 = \frac{\sqrt{K_w}}{K_h^\tau + \sqrt{K_w}}. \quad (24)$$

Then the limiting molar electrical conductivity of sodium aminomethanesulfonates is:

$$\lambda_{\text{YNHCH}_2\text{SO}_3\text{Na}}^0 = \lambda_{\text{Na}^+}^0 + \frac{\sqrt{K_w}}{K_h^\tau + \sqrt{K_w}} (\lambda_{\text{OH}^-}^0 + \lambda_{\text{YNH}_2\text{CH}_2\text{SO}_3^-}^0) + (1 - \frac{\sqrt{K_w}}{K_h^\tau + \sqrt{K_w}}) \lambda_{\text{YNHCH}_2\text{SO}_3}^0, \quad (25)$$

Table 3

Parameters of Shidlovsky equation (22) for aqueous solutions

YAMSNa. $C_{\text{YAMSNa}} = (1.0 \div 10.0) \cdot 10^{-3} \text{ mol} \cdot \text{l}^{-1}$; $n = 15$

T, K	B_0	$-B_1$	$B_2 \cdot 10^{-5}$	$-B_3 \cdot 10^{-5}$	R^2
AMSNa					
293	1364	54663	7.8136	40.00	0.9789
298	1384	54526	7.7048	40.00	0.9814
303	1447	56444	7.9312	40.00	0.9841
308	1546	60086	8.4271	40.00	0.9841
313	1759	70660	100.00	50.00	0.9805
MeAMSNa					
298	131.5	1757	0.2402	1.160	0.9783
303	174.7	2021	0.1345	0.160	0.9912
308	296.5	8141	1.1200	5.110	0.9965
313	295.4	7788	1.0800	5.010	0.9936
HEAMSNa					
293	183.5	2524	0.0826	0.517	0.9802
298	235.0	4356	0.3286	0.606	0.9874
303	242.5	4991	0.2946	0.445	0.9879
308	264.2	4595	0.4183	1.440	0.994
313	309.4	5860	0.5500	1.730	0.9937
t-BuAMSNa					
298	105.5	1410	0.0200	1.000	0.9393
303	136.4	2602	0.3833	1.890	0.9798
308	171.9	3859	0.5636	2.770	0.9940
313	201.3	4456	0.5930	2.650	0.9740
BzAMSNa					
293	112.1	2192	0.2724	1.220	0.9947
298	125.0	2443	0.2951	1.310	0.9951
303	123.9	2232	0.2709	1.220	0.9918
308	149.2	3154	0.3921	1.750	0.9907
313	147.3	2696	0.0309	1.330	0.9910

The observed linear dependences (Fig. 8) of the limiting molar electrical conductivity of aqueous solutions of N-methyl, N-2-hydroxyethyl, N-*tert*-butyl and N-benzyl-aminomethanesodium sulfonates on the limiting molar conductivity of aqueous solutions of sodium aminomethanesulfonate are described by equation (26), the parameters of which are given in the Table 4, and testify to the similarity in these processes.

$$\lambda_{\text{YNH}_2\text{CH}_2\text{SO}_3\text{Na}}^0 = A_i + B_i \cdot \lambda_{\text{NH}_2\text{CH}_2\text{SO}_3\text{Na}}^0 \quad (26)$$

Judging by the data in the Table 3, N-alkylation of sodium aminomethanesulfonate leads to a decrease in the values of the limiting molar electrical conductivity of its aqueous solutions. This fact is indicated by negative values of the coefficient A_i in equation (26) (Table 4).

Considering the fact that the limiting mobility of hydroxide ions and Na^+ at 298 K are respectively equal to $199.2 \text{ Ohm}^{-1}\cdot\text{sm}^2\cdot\text{mol}^{-1}$ and $50.1 \text{ Ohm}^{-1}\cdot\text{sm}^2\cdot\text{mol}^{-1}$ [21], then

$$\begin{aligned} \lambda^0(\text{AMSNa}) &> \lambda^0(\text{HEMSNa}) > \lambda^0(\text{OH}^-) > \\ &> \lambda^0(\text{MeAMSNa}) \approx \lambda^0(\text{BzAMSNa}) > \\ &> \lambda^0(t\text{BuAMSNa}) > \lambda^0(\text{Na}^+) \text{ and} \\ \lambda^0(\text{AMSNa}) &> \lambda^0(\text{OH}^-) + \lambda^0(\text{Na}^+) > \\ &> \lambda^0(\text{HEMSNa}) > \lambda^0(\text{MeAMSNa}) \approx \\ &\approx \lambda^0(\text{BzAMSNa}) > \lambda^0(t\text{BuAMSNa}). \end{aligned}$$

The latter, obviously, indicates a decrease in the mobility of hydroxide ions in solutions of MeAMSNa, HEAMSNa, *t*-BuAMSNa, BzAMSNa, compared with the value of mobility during the transfer along the chains of water H-bonds. A similar situation occurs with the mobility of hydroxonium ions in aqueous solutions of MeAMSA, HEAMSA, *t*-BuAMSNa [16] and aspartic acid [22], as well as with the mobility of hydroxyl ions in HEAMSA solutions [16].

Fig. 8. Mutual dependences of the limiting molar electrical conductivity of aqueous solutions $\text{YNHCH}_2\text{SO}_3\text{Na}$. Y – CH_3 (2), HOCH_2CH_2 (3), $(\text{CH}_3)_3\text{C}$ (4) and $\text{C}_6\text{H}_5\text{CH}_2$ (5).

Table 4

Coefficient values in the equation (26)

Y	A_i	B_i	R^2
CH_3	-48.623	7.3949	0.9964
HOCH_2CH_2	-3.0572	1.1761	0.9948
$(\text{CH}_3)_3\text{C}$	-26.707	4.3399	0.9798
$\text{C}_6\text{H}_5\text{CH}_2$	-9.4619	1.9683	0.8684

Activation parameters of electrical conductivity of aqueous solutions of sodium aminomethane sulfonates

The dependences of $\ln\lambda$ on $1/T$ are linear, which makes it possible to determine the effective activation energies of electrical conductivity [19] (Table 5). Transferring the analogy between the Arrhenius equations (27) and Eyring (28) from kinetics to electrical conductivity, we calculated the activation enthalpy of electrical conductivity using equation (29) and the activation entropy using equation (30) [19], the values of which are given in the Table 5.

$$k = A \cdot e^{-\frac{E_a}{RT}} \quad (27)$$

$$\lambda = A \cdot e^{-\frac{E_a}{RT}} \quad (28)$$

$$\Delta H^\# = E_a - RT \quad (29)$$

$$\Delta S^\# = -205.8 + 19.15 \cdot \lg \lambda / T + E_a / T \quad (30)$$

The processes of formation of activated complexes $0.001 \leq Q_{YAMSA} \leq 0.009$ M are endothermic (Table 5). Negative values of $\Delta S^\#$ indicate that atoms in activated complexes are located more “compactly” than in initial systems [23], that is, during the formation of activated complexes, the number of rotational and vibrational degrees of freedom decreases. For the reactions of association and dimerization, the activation entropies have large numerical values [24]. The same is observed for the molar

electrical conductivity of aqueous solutions of N-alkylaminomethanesulfonic acids [16].

The entropic and enthalpy components of the studied processes mutually compensate each other (Table 5). The compensatory effect is expressed by equation (31), the parameters of which are given in the Table 6, which corresponds to the presence of a compensation effect similar to the usual kinetic effect with the temperature $T_{i\lambda}$ similar to the isokinetic one.

$$\Delta H^\# = \alpha_i + T_{i\lambda} \cdot \Delta S^\# \quad (31)$$

In the case of the parameters of equation (30), a compensation effect is also observed [25] (Table 5), expressed by equation (32), the parameters of which are given in the Table 7.

$$\ln(A) = \alpha_i + E_a / (R \cdot T_{i\lambda}) \quad (32)$$

Table 5

Activation parameters of electrical conductivity of YAMSNa water solutions according to Eyring. T=298 K

$C_{YAMSNa} \cdot 10^{-3}, M$	$E_a, kJ \cdot mol^{-1}$	$\ln(A)$	R^2	$\Delta H^\#, kJ \cdot mol^{-1}$	$\Delta S^\#, J \cdot mol^{-1} \cdot K^{-1}$
AMSNa					
0.5	10.6	10.52	0.9647	8.14	-170
0.6	9.82	10.05	0.9918	7.34	-173
0.7	9.60	9.84	0.9939	7.13	-173
0.8	9.73	9.78	0.9760	7.26	-173
0.9	9.89	9.77	0.9996	7.41	-172
1.0	9.14	9.58	0.9954	6.67	-175
2.0	10.9	9.56	0.9701	8.43	-169
3.0	11.0	9.36	0.9846	8.54	-169
4.0	10.2	8.87	0.998	7.74	-171
5.0	10.5	8.87	0.9919	8.03	-170
6.0	10.6	8.83	0.9929	8.09	-170
7.0	10.0	8.53	0.9897	7.51	-172
8.0	9.67	8.34	0.9939	7.19	-173
9.0	10.0	8.43	0.9279	7.55	-172

Table 5 continuation

MeAMSNa					
2.0	13.2	9.85	0.9973	10.7	-161
3.0	10.3	8.67	0.9990	7.85	-171
4.0	12.1	9.34	0.9996	9.66	-165
5.0	12.7	9.59	0.9919	10.2	-163
6.0	12.4	9.44	0.9975	9.88	-164
7.0	11.7	8.53	0.9897	9.23	-166
8.0	12.5	9.45	0.9995	10.0	-164
9.0	11.3	8.96	0.9916	8.78	-168
HEAMSNa					
1.0	13.8	10.5	0.9947	11.4	-159
2.0	19.9	12.6	0.9702	17.4	-139
3.0	20.1	12.6	0.9502	17.6	-138
4.0	21.6	13.1	0.9617	19.2	-133
5.0	20.0	12.4	0.9513	17.5	-139
6.0	23.1	13.6	0.9534	20.6	-128
7.0	17.8	11.4	0.9365	15.3	-146
8.0	20.0	12.3	0.9528	17.5	-139
9.0	21.6	12.9	0.9325	19.1	-133
<i>t</i> -BuAMSNa					
1.0	17.2	11.3	0.9716	14.8	-148
2.0	12.1	9.21	0.9904	9.66	-165
3.0	20.1	12.6	0.9502	9.69	-165
4.0	12.3	9.24	0.9933	9.84	-164
5.0	12.9	9.44	0.9973	10.4	-163
6.0	12.7	9.36	0.9934	10.2	-163
7.0	13.0	9.50	0.9974	10.6	-162
8.0	12.8	9.39	0.9815	10.4	-163
9.0	12.9	9.40	0.9691	10.4	-162
BzAMSNa					
1.0	10.2	8.36	0.9894	7.73	-171
2.0	11.4	8.74	0.9955	8.88	-168
4.0	9.71	7.94	0.9954	7.23	-173
5.0	8.90	7.58	0.9876	6.43	-176
6.0	9.68	7.86	0.9826	7.20	-173
7.0	8.29	7.26	0.9790	5.81	-178
8.0	8.49	7.32	0.9934	6.01	-177
9.0	8.68	7.37	0.9755	6.21	-177

Table 6

Values of parameters of equation (31) and physicochemical properties of sodium aminomethanesulfonates

Acid	α_p , kJ·mol ⁻¹	T _{il}	R ²	MR, Å [7]	lgP _{ow} [7]	V, Å ³ [7]
MeMSNa	58.81	298.0	0.999	24.15	-0.27	506.8(3)
HEAMSNa	58.85	298.0	0.999	30.44	-0.71	637.32(8)
<i>t</i> -BuAMSNa	58.81	298.0	0.999	37.95	0.57	825.9(5)
BzAMSNa	58.88	298.0	0.999	48.76	1.51	946.93(17)

Keys: R² – approximation confidence value; MR – molar refraction; P_{ow} – partition coefficient in the octanol – water system; V – molar volume.

Table 7

Values of parameters of equation (32)

Salt	α_p , kJ·mol ⁻¹	T _{il}	R ²
MeAMSNa	-1.444	310.9	0.999
HEAMSNa	-1.860	343.0	0.974
<i>t</i> -BuAMSNa	-1.177	288.4	0.999
BzAMSNa	-0.750	242.2	0.998

Thus, by processing the data of conductometric studies, the activation parameters of the electrical conductivity of the systems “sodium aminomethanesulfonate – water” at 293–313 K were obtained. The obtained data on the acid-base and electrochemical properties of the YAMSNa – H₂O systems are recommended for use in chemical analysis, microbiological and biochemical studies, as well as in the simulation of chemisorption processes of capturing acid gases (CO₂ and SO₂).

Acknowledgement. The work was carried out with financial support from the Ministry of Education and Science of Ukraine.

ЕЛЕКТРОХІМІЧНІ ВЛАСТИВОСТІ ВОДНИХ РОЗЧИНІВ АМІНОМЕТАНСУЛЬФОНАТІВ НАТРІЮ

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Здійснено рН- і кондуктометричне дослідження електрохімічних властивостей водних розчинів (1·10⁻⁴ ÷ 9·10⁻³ М) YNHCH₂SO₃Na (Y = Н (AMSNa), CH₃ (MeAMSNa), HOCH₂CH₂ (HEAMSNa), (CH₃)₃C (*t*-BuAMSNa) и C₆H₅CH₂ (BzAMSNa)) в області температур 293–313 К. За результатами кондуктометричного дослідження систем YNHCH₂SO₃Na – H₂O збільшення температури від 293 до

313 K супроводжується підвищенням молярної електропровідності систем внаслідок зростання ступеня дисоціації електролітів і/або рухливості утворених іонів. При цьому для всіх досліджуваних систем кислотні властивості з ростом температури від 293 до 308 K знижуються. Оцінено концентраційні та температурні залежності констант гідролізу амінометансульфонату та N-алкіламінометансульфонатів (алкіл: метил, 2-гідроксиетил, *трет*-бутил і бензил). Спостережувані прямолінійні залежності термодинамічних констант гідролізу N-метил, N-*трет*-бутил і N-бензил-амінометансульфонат аніонів від термодинамічних констант гідролізу амінометансульфонат аніонів свідчать про подібність в зазначених процесах. Розраховано значення граничної молярної електропровідності шляхом екстраполяції за Шидловським. З урахуванням літературних даних встановлено, що граничні рухливості зменшуються в рядах: $\lambda^0(\text{AMSNa}) > \lambda^0(\text{HEMSNa}) > \lambda^0(\text{OH}^-) > \lambda^0(\text{MeAMSNa}) \approx \lambda^0(\text{BzAMSNa}) > \lambda^0(t\text{BuAMSNa}) > \lambda^0(\text{Na}^+)$ та $\lambda^0(\text{AMSNa}) > \lambda^0(\text{OH}^-) + \lambda^0(\text{Na}^+) > \lambda^0(\text{HEMSNa}) > \lambda^0(\text{MeAMSNa}) \approx \lambda^0(\text{BzAMSNa}) > \lambda^0(t\text{-BuAMSNa})$. Відзначено відносне зниження рухливості іонів водню в розчинах MeAMSNa, HEMS, *t*-BuAMSNa та BzAMSNa порівняно з величиною рухливості при перенесенні по ланцюгах H-зв'язків води. Виявлено компенсаційні ефекти в активісційних параметрах молярної електропровідності системи амінометансульфонат натрію – вода в області температур 293–313 K.

Ключові слова: амінометансульфокислоти, водні розчини, гідроліз, електропровідність.

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Стаття надійшла 26.11.2020.