THERMODYNAMIC CHARACTERISTICS OF AMMONIUM ION SOLVATION IN N-METHYLPYRROLIDONE–WATER SOLUTIONS

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Based on the standard values of the heat capacity $\overline{C^{\circ}_{p,i}}$ of an ammonium ion, the values of the change in heat capacity during the solvation $\Delta_{\text{solv.}}C^{\circ}_{p,i}$ of an ammonium ion in a mixed solvent N-methylpyrrolidone **(**MP)-water at 298.15 K are determined. The magnitude of the ammonium ion is represented as the sum of four contributions: electrostatic $\Delta_{\text{el.}}C^{\circ}_{p,i}$, cavity formation $\Delta_{\text{cav.}}C^{\circ}_{p,i}$, structural changes in the solvent $\Delta_{\text{str.}}C^{\circ}_{p,i}$, and specific ion-solvent interactions $\Delta_{\text{sp.int.}}C^{\circ}_{p,i}$. The values of the contributions are calculated based on experimental data and model representations. The calculation results are presented in the table.

The change in heat capacity during solvation $\Delta_{\text{solv.}}C^{\circ}_{p,i}$ of an ammonium ion in a mixed solvent MP – water, MP and water at 298.15 K and contributions to this value caused by specific interactions, electrostatic interactions, cavity formation, and changes in the solvent structure

J/mol·K	X_{MP}						
	0,00	0,10	0,33	0,50	0,75	0,90	1,00
$\Delta_{\text{solv.}}C^{\circ}_{p,i}$	-62	-78	-80	-41	-17	7	12
$\Delta_{\text{sp.int.}}C^{\circ}_{p,i}$	30	4	2	-7	-5	-8	-9
$\Delta_{\text{el.}}C^{\circ}_{p,i}$	-218	-225	-236	-319	-310	-285	-295
$\Delta_{\text{cav.}}C^{\circ}_{p,i}$	41	82	97	92	109	116	134
$\Delta_{\text{str.}}C^{\circ}_{p,i}$	85	60	57	193	189	170	155

The dependences of the obtained values on the composition of the mixture are discussed in connection with the structure of the mixed solvent.

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