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**POLYTHERMAL SOLUBILITY AND PHASE EQUILIBRIA IN THE ACETATE
CARBAMIDE–MONOETHANOLAMINE–WATER SYSTEM FOR THE
DEVELOPMENT OF AGROCHEMICAL DEFOLIANT COMPONENTS**

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Abstract: This study investigates the polythermal solubility and phase equilibria of the acetate carbamide–monoethanolamine–water system within the temperature range of $-53\text{ }^{\circ}\text{C}$ to $+20\text{ }^{\circ}\text{C}$. Using the polythermal solubility method, the crystallization regions, eutectic compositions, and invariant points of the ternary system were determined. The solubility diagram revealed the coexistence of multiple solid phases, including ice, acetate carbamide, monoethanolamine hydrates, and a newly formed compound—acetate carbamide–monoethanolammonium. The phase boundaries and isotherms constructed for each $10\text{ }^{\circ}\text{C}$ interval describe the physicochemical behavior of the system with high accuracy. The obtained results provide a theoretical and practical basis for the synthesis of efficient agrochemical defoliant components and physiologically active fertilizer additives derived from aminoalcohol and amide–acid systems.

Key words: polythermal solubility, acetate carbamide, monoethanolamine, ternary system, phase equilibrium, eutectic point, agrochemical defoliant.

INTRODUCTION

The study of solubility and phase equilibria in multicomponent systems containing organic compounds is of great importance in modern solution chemistry, chemical technology, and agrochemical synthesis. Understanding the behavior of such systems provides the foundation for designing new physiologically active substances, fertilizers, and defoliants with improved efficiency and environmental compatibility. Amino alcohols, carbamides, and carboxylic acids form a wide class of compounds that exhibit high reactivity due to the presence of multiple functional groups such as $-\text{OH}$, $-\text{NH}_2$, and $-\text{CONH}_2$. Among them, monoethanolamine and urea (carbamide) are particularly significant because of their strong hydrogen-bonding capability and ability to form complex associative structures in aqueous media. These properties play a decisive role in regulating solubility, crystallization, and the formation of new compounds in multicomponent systems.

Acetate carbamide, a reaction product of acetic acid and urea, demonstrates unique physicochemical properties and serves as an effective donor of nitrogen and carbon in agrochemical formulations. Its combination with monoethanolamine provides an opportunity to obtain new coordination and associative compounds possessing both nutritional and

physiological activity for plants. The mutual interaction of these components can influence oxidation–reduction processes, protein metabolism, and enzymatic activity in plant cells, making such systems promising for the synthesis of multifunctional agrochemical agents, particularly defoliant and growth regulators.

Despite the growing interest in organic–inorganic hybrid systems, limited data are available on the solubility behavior and crystallization characteristics of the acetate carbamide–monoethanolamine–water system. Previous studies have mainly focused on binary systems such as acetate carbamide–water or monoethanolamine–water, leaving the ternary system insufficiently explored. Therefore, it is essential to investigate its phase equilibria using precise physicochemical methods to understand the complex interactions between the components and their temperature-dependent solubility.

The present research aims to construct the polythermal solubility diagram of the $\text{CH}_3\text{COOH}\cdot\text{CO}(\text{NH}_2)_2 - \text{NH}_2\text{C}_2\text{H}_4\text{OH} - \text{H}_2\text{O}$ system, to determine the boundaries of crystallization fields, eutectic points, and invariant equilibria, and to identify new solid phases formed within the studied temperature range ($-53\text{ }^\circ\text{C}$ to $+20\text{ }^\circ\text{C}$). The results of this investigation are expected to provide new insights into the thermodynamic stability and phase relationships of the system, contributing to the rational design of eco-friendly and highly effective agrochemical defoliant compositions. By clarifying the physicochemical interactions between acetate carbamide and monoethanolamine in aqueous solutions, this work lays the groundwork for future development of advanced formulations used in agriculture and related chemical industries.

MATERIAL AND METHODS

The investigation of the polythermal solubility and phase equilibria in the acetate carbamide–monoethanolamine–water system was carried out using classical physicochemical methods combined with precise temperature–concentration control. The study covered a temperature range from $-53\text{ }^\circ\text{C}$ to $+20\text{ }^\circ\text{C}$, which allowed the identification of low-temperature crystallization fields and eutectic regions.

Materials. Chemically pure reagents were used in all experiments. Acetic acid (CH_3COOH), urea ($\text{CO}(\text{NH}_2)_2$), and monoethanolamine ($\text{NH}_2\text{C}_2\text{H}_4\text{OH}$) were used to prepare the ternary system. Acetate carbamide was synthesized by slowly adding concentrated acetic acid to a 50% aqueous solution of urea under continuous stirring, following the procedure described in previous studies. The resulting product was crystallized, dried in a desiccator, and stored in tightly closed containers to prevent moisture absorption. Deionized water was used as the solvent throughout all experiments to ensure the purity of the system.

Experimental procedure. The solubility of the components was determined by the polythermal method, which involves preparing a series of mixtures with accurately measured mass ratios of components and equilibrating them at specific temperatures until phase separation occurred. The mixtures were placed in sealed glass ampoules to prevent evaporation and contamination. Each ampoule was maintained at a constant temperature for several hours in a cryostat or thermostatic bath, depending on the temperature range. After equilibrium was reached, the solid and liquid phases were separated by rapid filtration at the corresponding temperature.

Analytical methods. The concentration of components in the liquid phase was determined by chemical titration and gravimetric analysis, depending on the chemical nature of the component. The composition of the solid phases was identified using differential thermal analysis (DTA) and X-ray diffraction (XRD) when necessary, while the freezing points and crystallization intervals were established by visual thermal observation and temperature recording techniques.

Construction of diagrams. The obtained solubility data were plotted as polythermal solubility diagrams, where isothermal lines were drawn for every $10\text{ }^\circ\text{C}$ interval. The regions corresponding to ice, acetate carbamide, monoethanolamine hydrates, and the newly formed

acetate carbamide–monoethanolammonium compound were clearly delineated. The triple and eutectic points were determined from the intersection of solubility curves, allowing for the precise definition of equilibrium relationships within the ternary system.

This methodological approach ensured high reproducibility and accuracy in determining the phase composition and temperature boundaries of the studied system, forming a reliable basis for interpreting its physicochemical behavior and constructing the complete phase diagram.

RESULTS AND DISCUSSION

Amino alcohols, carboxylic acids, ethanolamines, and the compounds derived from them exhibit high physiological activity. In particular, ethanolamines possess high reactivity and show chemical activity through both their amino and hydroxyl functional groups. Ethanolamines and their salts formed with acids are known to enhance oxidation–reduction processes in plants, stimulate protein metabolism, and increase the activity of enzymatic systems.

The simultaneous synthesis of physiologically active and effective nutrient preparations, along with the study of the physicochemical properties of system components and their application in chlorate-containing defoliant compositions, is considered to be of great practical importance.

Initially, acetate carbamide was synthesized by slowly adding concentrated acetic acid to a 50% aqueous solution of urea under continuous stirring. The obtained product was then used to study its interaction with monoethanolamine in solution, depending on the solubility relationships within the $\text{CH}_3\text{COOH}\cdot\text{CO}(\text{NH}_2)_2 - \text{NH}_2\text{C}_2\text{H}_4\text{OH} - \text{H}_2\text{O}$ system.

The binary $\text{CH}_3\text{COOH}\cdot\text{CO}(\text{NH}_2)_2 - \text{H}_2\text{O}$ system was first examined. Its solubility diagram revealed the presence of two crystallization branches in the solid phase, corresponding to the formation of ice and acetate carbamide. The cryohydrate point of the system was found to correspond to a composition containing 58.0% acetate carbamide and 42.0% water, as shown in Figure 1.

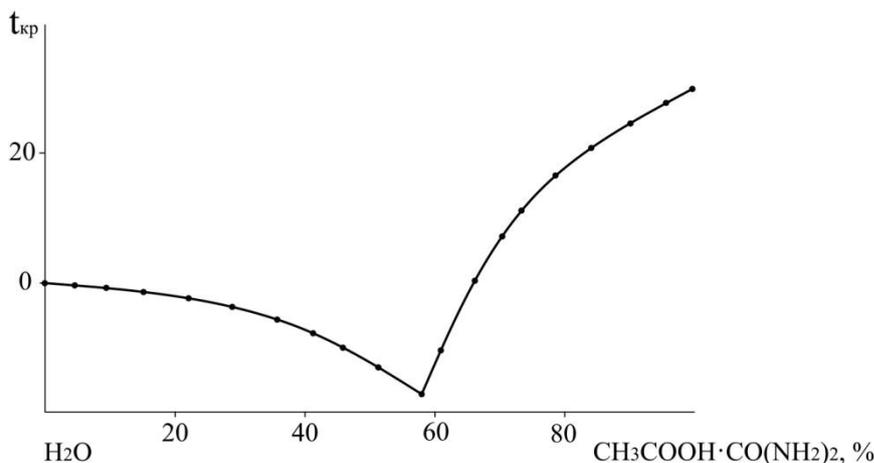


Figure 1. Binary phase diagram of the $\text{CH}_3\text{COOH}\cdot\text{CO}(\text{NH}_2)_2\text{--H}_2\text{O}$ system.

The solubility of the components in the $\text{CH}_3\text{COOH}\cdot\text{CO}(\text{NH}_2)_2 - \text{NH}_2\text{C}_2\text{H}_4\text{OH} - \text{H}_2\text{O}$ system was studied over a wide concentration range and within the temperature interval from -53.0°C to $+20.0^\circ\text{C}$ using the polythermal solubility method. Based on the experimental data, the solubility diagram of the system was constructed. The diagram delineates the crystallization regions of ice, acetate carbamide, acetate carbamide–monoethanolammonium, dihydrate, monohydrate, and anhydrous monoethanolamine (Figure 2). In the polythermal solubility diagram, the isothermal curves were drawn at every 10°C temperature interval.

The constructed phase diagram reveals the presence of four ternary invariant points, which correspond to the following temperatures and compositions: at -41.0°C — 39.2% acetate carbamide, 9.8% monoethanolamine, and 51.0% water; at -53.0°C — 22.0% acetate carbamide,

22,8	42,8	34,4	-38,5	-/-
22,0	44,0	34,0	-53,0	Ice + C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH + NH ₂ C ₂ H ₄ OH·2H ₂ O
20,0	48,0	32,0	-51,0	C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH + NH ₂ C ₂ H ₄ OH·2H ₂ O
16,0	58,6	25,4	-47,0	C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH + NH ₂ C ₂ H ₄ OH·2H ₂ O+ NH ₂ C ₂ H ₄ OH·H ₂ O
15,2	61,6	23,2	-32,0	C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH + NH ₂ C ₂ H ₄ OH·H ₂ O
14,4	68,0	17,6	-18,0	-/-
14,4	74,4	11,2	-14,0	C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH + NH ₂ C ₂ H ₄ OH·H ₂ O + NH ₂ C ₂ H ₄ OH
14,4	76,0	9,6	-11,0	-/-
14,8	78,4	6,8	-6,0	-/-
16,4	83,6	-	-1,5	-/-
10,0	74,8	15,2	-18,0	NH ₂ C ₂ H ₄ OH·H ₂ O + NH ₂ C ₂ H ₄ OH
5,6	75,6	18,8	-20,0	-/-
4,8	76,0	19,2	-21,5	-/-
-	79,2	20,8	-25,2	-/-
7,6	60,8	31,6	-44,5	NH ₂ C ₂ H ₄ OH·2H ₂ O+ NH ₂ C ₂ H ₄ OH·H ₂ O
-	66,6	33,4	-46,1	-/-
10,4	46,4	43,2	-47,5	Ice + NH ₂ C ₂ H ₄ OH·2H ₂ O
-	52,0	48,0	-48,5	-/-
50,8	14,8	34,4	-20,5	CH ₃ COOH·CO(NH ₂) ₂ + C ₃ H ₈ O ₃ N ₂ · NH ₂ C ₂ H ₄ OH
58,2	16,0	25,8	-10,0	-/-
58,8	16,2	25,0	-7,0	-/-
64,8	21,0	14,2	4,0	-/-
68,6	24,8	6,6	12,0	-/-
71,6	28,4	-	16,0	-/-

Ice co-crystallizes with acetate carbamide in the temperature range -22.0 to -17.0 °C, and with monoethanolamine dihydrate in the range -48.5 to -47.5 °C; monoethanolamine monohydrate co-crystallizes with the dihydrate in the range -46.1 to -44.5 °C, and with anhydrous monoethanolamine in the range -25.2 to -18.0 °C.

CONCLUSION

This study established the polythermal solubility and phase equilibria of the acetate carbamide–monoethanolamine–water system over -53.0 to $+20.0$ °C and mapped the corresponding crystallization fields with 10 °C isotherm resolution. The phase diagram reveals well-defined regions for ice, acetate carbamide, monoethanolamine hydrates (mono- and dihydrate), anhydrous monoethanolamine, and a newly formed mixed phase—acetate carbamide–monoethanolammonium. Four ternary invariant points were identified with precisely determined temperature–composition coordinates, providing a consistent thermodynamic framework for the system.

The coexistence intervals show that acetate carbamide–monoethanolammonium crystallizes jointly with acetate carbamide (-20.5 to $+16.0$ °C), with ice (-31.0 to -38.5 °C), with

monoethanolamine dihydrate (at $-51.0\text{ }^{\circ}\text{C}$), with the monohydrate (-32.0 to $-18.0\text{ }^{\circ}\text{C}$), and with anhydrous monoethanolamine (-11.0 to $-1.5\text{ }^{\circ}\text{C}$). These equilibria reflect strong associative interactions among amide, hydroxyl, and amino functional groups and explain the observed temperature-dependent solubility trends.

Practically, the obtained diagram and invariant data create a reliable basis for rational selection of component ratios and processing temperatures when formulating agrochemical defoliant components and physiologically active fertilizer additives derived from aminoalcohol–amide–acid systems. The results enable targeted control of solid-phase formation, product purity, and phase stability—key factors for scalable, environmentally responsible technologies.

Future work should quantify thermodynamic functions (activity coefficients, partial molar properties), apply calorimetry and in-situ diffraction to refine phase assignments, and evaluate field performance and phytotoxicity profiles of compositions guided by the established phase map.

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