

STUDY OF THE SOLUBILITY OF THE CALCIUM CHLORATE - TRIETHANOLAMMONIUM MONOCHLOROACETATE - WATER SYSTEM

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ABSTRACT

The objective of this study was to investigate the physicochemical interactions between calcium chlorate and triethanolammonium monochloroacetate in aqueous systems and to determine their phase behaviour. The ternary system $\text{Ca}(\text{ClO}_3)_2 - (\text{C}_2\text{H}_4\text{OH})_3\text{N}\cdot\text{ClCH}_2\text{COOH} - \text{H}_2\text{O}$ was studied using the visual-polythermal method combined with physicochemical analytical techniques. A polythermal solubility diagram of the system was constructed over the temperature range from -52°C to 47°C . The analysis revealed the crystallization fields of ice, $\text{Ca}(\text{ClO}_3)_3$ hydrates ($\text{Ca}(\text{ClO}_3)_2\cdot 6\text{H}_2\text{O}$, $\text{Ca}(\text{ClO}_3)_2\cdot 4\text{H}_2\text{O}$ and $\text{Ca}(\text{ClO}_3)_2\cdot 2\text{H}_2\text{O}$), triethanolammonium monochloroacetate, and a newly formed crystalline compound with the composition $\text{ClCH}_2\text{COOH}\cdot\text{Ca}(\text{ClO}_3)_2\cdot(\text{C}_2\text{H}_4\text{OH})_3\text{N}$. The formation and individuality of the new compound were confirmed by chemical analysis, IR spectroscopy and scanning electron microscopy. The obtained results provide a physicochemical basis for improving chlorate-based defoliant formulations and optimizing their production technologies.

Keywords: calcium chlorate, triethanolammonium monochloroacetate, phase equilibrium, polythermal solubility diagram, crystallization, defoliant chemistry.

INTRODUCTION

Low-toxicity chlorate-based defoliants are widely used in agriculture to stimulate leaf drop. Commercial formulations based on sodium, calcium, and magnesium chlorates, including Sihat, Sadaf, and the UDM series, have been manufactured industrially and applied to

various crops [1 - 4]. However, the currently available chlorate defoliants do not fully meet modern agricultural requirements, and their performance remains limited.

To develop highly efficient defoliants with a complex mode of action, the $\text{Ca}(\text{ClO}_3)_2\cdot 2\text{CO}(\text{NH}_2)_2$ $\text{C}_4\text{H}_6\text{O}_5\cdot\text{NH}_2\text{C}_2\text{H}_4\text{OH}\cdot\text{H}_2\text{O}$ system was investigated using binary combinations and ten internal sections. On

this basis, a visual polythermal solubility diagram was constructed over the temperature range from -24.2°C to 32.0°C . The diagram identified the crystallization field of ice as well as the precipitation regions of $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{CO}(\text{NH}_2)_2 \cdot 2\text{H}_2\text{O}$ and $\text{C}_4\text{H}_6\text{O}_5 \cdot \text{NH}_2\text{C}_2\text{H}_4\text{OH}$ [5].

Practical application of chlorate-based formulations on various crops has revealed not only their advantages but also several limitations [6]. A key feature of physiologically active substances is their ability to produce the desired effect even at low dosages [7]. Excessive treatment with chlorate-based defoliant can lead to adverse effects, such as contamination of the cotton yield with dried leaves and damage to young bolls. Therefore, incorporating physiologically active substances obtained from triethanolamine salts of carboxylic acids into chlorate formulations increases defoliation efficiency and promotes the proper maturation and opening of young bolls [8 - 10].

From this perspective, the aim of this study is to provide a physicochemical rationale for the development of low-toxicity, physiologically active defoliant formulations based on calcium chlorate and triethanolammonium monochloroacetate.

EXPERIMENTAL

Calcium chlorate and triethanolammonium monochloroacetate were selected as the objects of this study. Calcium chlorate dihydrate was synthesized by converting calcium chloride and sodium chlorate in an acetone medium [11]. In addition, the calcium chlorate-water binary system was examined, and the obtained results were found to be consistent with the literature data [12, 13]. In these studies, physicochemical properties such as solubility, phase composition, and interactions between the components were investigated.

The solubility of the systems was evaluated using the visual polythermal method [14]. Using this method, the formation of solid and liquid phases was monitored as a function of temperature, and the phase boundaries and freezing points were determined. The compositions of the liquid and solid phases were determined by quantitative analytical methods: calcium was measured by volumetric complexometric titration [15], the chlorate ion was determined by volumetric permanganometric titration [16], and carbon, nitrogen, and hydrogen were quantified by elemental analysis [17, 18]. These

methods enabled the quantitative determination of each component and the analysis of phase equilibria in the binary systems. To clarify the interactions among the components, infrared (IR) spectroscopy was employed. IR absorption spectra of the initial components and the synthesized compounds were recorded over the range $4000 - 400 \text{ cm}^{-1}$ using a Shimadzu FT-IR spectrometer. This analysis enabled identification of the presence of hydrogen bonding as well as carbonyl and hydroxyl functional groups and their mutual interactions. The IR spectra were used to examine synergistic effects and to characterize the nature of chemical bonding between the components.

RESULTS AND DISCUSSION

For the first time, the solubility of the ternary system composed of calcium chlorate, triethanolammonium monochloroacetate, and water was comprehensively investigated. Based on the binary systems and internal sections of the polythermal diagrams, a polythermal solubility diagram of the $\text{Ca}(\text{ClO}_3)_2 - (\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH} - \text{H}_2\text{O}$ system was constructed over the temperature range from -52.0°C to 47.0°C . In this study, the visual polythermal method was employed to determine the appearance of phases and the corresponding phase boundaries (precipitation points). Analysis of the diagram indicates the presence of crystallization regions corresponding to ice, $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$, $\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$, $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$, $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH}$, and a newly formed phase of composition $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$. The occurrence of these phases varies with temperature and component proportions. $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH}$ was obtained from monochloroacetic acid and triethanolamine at a 1:1 molar ratio by slow addition in a water bath with constant stirring [23]. The results obtained for the $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH} - \text{H}_2\text{O}$ binary system were found to be consistent with previous studies [24, 25]. These results made it possible to elucidate the interactions between the hydroxyl and carbonyl functional groups of the components. In the polythermal diagram, lines I - V extend from the $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH} - \text{H}_2\text{O}$ side toward $\text{Ca}(\text{ClO}_3)_2$, whereas lines VI - VIII extend from the $\text{Ca}(\text{ClO}_3)_2 - \text{H}_2\text{O}$ side toward $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH}$. Four ternary invariant points were identified in the system (Table 1).

Analysis of the ternary invariant points showed

Table 1. Representation of secondary and tertiary points in the $\text{Ca}(\text{ClO}_3)_2 - \text{CH}_2\text{ClCOOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N} - \text{H}_2\text{O}$ system.

Ternary invariant point	$\text{Ca}(\text{ClO}_3)_2$, %	$(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH}$, %	H_2O , %	Temperature, °C
I	19.0	21.8	59.2	-21
II	38.5	11.0	50.5	-52
III	43.0	14.5	42.5	-42
IV	49.0	21.5	29.5	-20

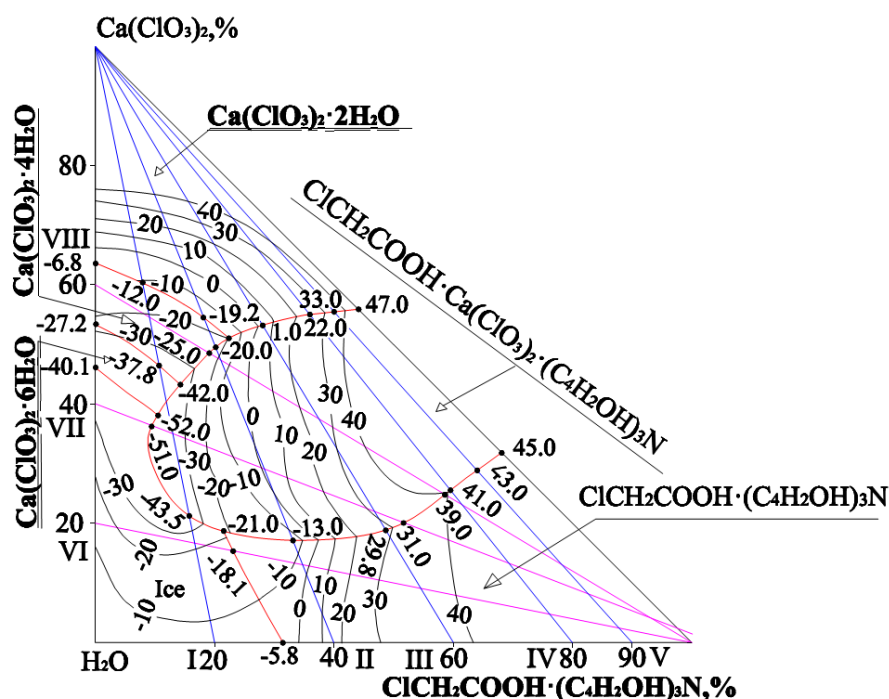


Fig. 1. Solubility diagram of the $\text{Ca}(\text{ClO}_3)_2 - (\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH} - \text{H}_2\text{O}$ system.

that the interaction of $\text{Ca}(\text{ClO}_3)_2$, triethanolammonium monochloroacetate, and water leads to the formation of a new complex, $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$. This complex constitutes a new crystallizing phase and may significantly alter the solubility behaviour of the system. The results indicate that polythermal diagrams constructed using binary systems and internal sections allow physicochemically and pharmacologically significant conclusions to be drawn. They serve as a basis for determining the optimal component ratios and phase relationships required for the development of physiologically active, low-toxicity defoliant for agricultural applications. By analysing the diagrams and the ternary invariant points, clear scientific conclusions were drawn regarding phase stability

and the crystallization behaviour of the investigated system. This, in turn, establishes an important research foundation for improving defoliant performance and further optimizing their physicochemical characteristics in future studies.

In the polythermal solubility diagram of the system, crystallization fields corresponding to ice; calcium chlorate hydrates $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$, and $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$; as well as $(\text{C}_2\text{H}_4\text{OH})_3\text{N} \cdot \text{ClCH}_2\text{COOH}$ and the newly formed double compound $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ were delineated (Fig. 1). These fields are interconnected through four invariant ternary points of the system. To characterize the state of the solution as a function of temperature, solubility isotherms were determined at

10°C intervals (-30, -20, -10, 0, 10, 20, 30°C, and 40°C) on the phase diagram of the polythermal system. These isotherms made it possible to evaluate the solubility behaviour of the system components at different temperatures and to analyse phase equilibria.

Using the isotherms, the boundaries of the crystallization fields at each temperature were determined, and their temperature - dependent shifts were observed. The obtained results are important for assessing changes in phase equilibria in the polythermal system and for characterizing its thermodynamic properties.

Thus, the investigated calcium chlorate - triethanolammonium monochloroacetate - water system was found to belong to a complex eutonic type, and the formation of a new compound with the composition $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ was observed (Table 2).

To confirm the presence of the new compound, its crystals were isolated from the presumed crystallization region. The collected crystals were filtered using a Büchner funnel and washed several times with cold distilled water. The washed product was then dried in a drying oven at 70°C for 6 h.

Subsequently, the obtained compound was examined using chemical and physicochemical analytical methods. The chemical analysis gave the following results: Found (wt. %): Ca^{2+} - 9,11; ClO_3^- - 35,3; N - 3,81. Calculated (wt.%) for $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$: Ca^{2+} - 8,87; ClO_3^- - 37,06; N - 3,10.

To establish the individuality of the newly obtained compound, it was characterized by physicochemical methods, including IR spectroscopy and scanning electron microscopy (SEM) (Fig. 2).

The morphology and elemental composition of the synthesized compound were characterized using scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDS). The morphology of the compound was characterized using the SEM micrograph, which is presented in Fig. 2. The micrograph indicates that the morphology of the compound is crystalline with a plate-like layered structure. The morphology of the compound is indicative of a crystalline nature rather than an amorphous nature. The presence of a layered structure is indicative of the growth of the crystals in an anisotropic manner. The growth of crystals in an anisotropic manner is a common phenomenon in the growth of crystals through a solution

phase crystallization mechanism. The morphology is indicative of the growth of crystals through a nucleation-aggregation mechanism. The relatively small and dense packing of particles indicates that there are strong intermolecular interactions within the crystal lattice, probably mediated through hydrogen bonding and ionic interactions between the chlorate ions and the protonated triethanolamine moiety. The elemental composition of the synthesized compound was also validated through EDS analysis. The detected elements were oxygen (40.7 %), chlorine (24.6 %), carbon (22.2 %), calcium (9.3 %), and nitrogen (3.2 %). The high concentration of oxygen and chlorine indicates that there are chlorate ions (ClO_3^-) within the structure. Calcium was also detected, indicating that there are indeed $\text{Ca}(\text{II})$ ions within the structure. The presence of carbon and nitrogen is a further argument for the presence of the organic part of the triethanolammonium structure. The lack of unexpected impurity elements in the EDS spectrum is a sign of the high purity of the synthesized compound. In addition, the quantitative composition of the elements present is in good agreement with the suggested stoichiometric composition of the synthesized compound, which is $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$. Thus, the results obtained by the combination of the two methods, SEM and EDS, confirm the assumption that the synthesized compound is a new crystalline substance with unique morphology and elemental composition. The results are in good agreement with the data obtained using IR spectroscopy and chemical analysis, which confirm the individuality and structural organization of the synthesized substance.

The structure of the synthesized compound $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ was confirmed by IR spectroscopy (Fig. 3). The spectrum exhibits several characteristic absorption bands corresponding to the functional groups present in the proposed structure. A broad absorption band observed in the region 3380 - 3160 cm^{-1} is attributed to O-H stretching vibrations of hydroxyl groups involved in hydrogen bonding. The broad nature of this band indicates strong intermolecular interactions, confirming the participation of hydroxyl groups from the triethanolammonium fragment in hydrogen bonding within the crystal lattice. The bands at 2919 cm^{-1} correspond to aliphatic C-H stretching vibrations of CH_2 groups, indicating the presence of organic moieties derived from triethanolamine and

Table 2. Representation of binary and ternary points in the $\text{Ca}(\text{ClO}_3)_2 - \text{CH}_2\text{ClCOOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N} - \text{H}_2\text{O}$ system.

Liquid phase composition, %			Crystallization temperature, °C	Solid phase
$\text{Ca}(\text{ClO}_3)_2$	$\text{CH}_2\text{ClCOOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$	H_2O		
1	2	3	4	5
46.0	0	54.0	-40.1	ice + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$
38.5	11.0	50.5	-52.0	ice + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
40.5	12.3	47.2	-49.0	ice + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
43.0	14.5	42.5	-42.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$ + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$ + $\text{CClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
46.8	11.0	42.2	-37.8	$\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$ + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$
55.0	-	45.0	-27.2	ice + $\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$
63.0	-	37.0	-6.8	ice + $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$
49.0	21.5	29.5	-20.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$ + $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$ + $\text{CClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
58.7	8.5	32.8	-12.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$ + $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$
52.5	28.5	19.0	1.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
53.9	32.0	14.1	11.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
55.2	35.5	9.3	22.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
55.9	39.3	4.8	33.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
56.0	44.0	0.0	47.0	$\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$ + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
36.9	9.5	53.6	-51.0	Ice + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
21.0	16.0	63.0	-43.5	Ice + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
19.0	21.8	59.2	-21.0	Ice + $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
17.0	23.8	59.2	-18.1	ice + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
	31.0	69.0	-5.9	ice + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
17.5	33.0	49.5	-13.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
20.5	47.5	32.0	29.8	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
20.7	48.5	30.8	31.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
22.9	53.8	23.3	36.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
25.0	58.0	17.0	39.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
28.7	64.0	13.3	43.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$
31.5	68.2	0.3	45.0	$\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$ + $\text{CClCH}_2\text{COOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$

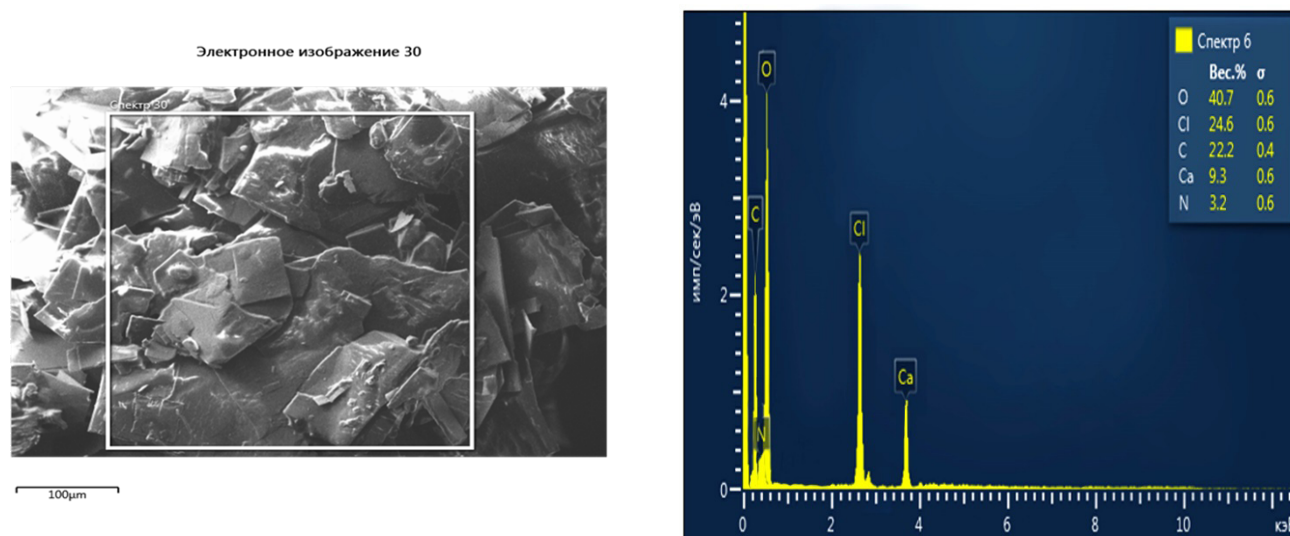


Fig. 2. SEM analysis results of the new compound $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$.

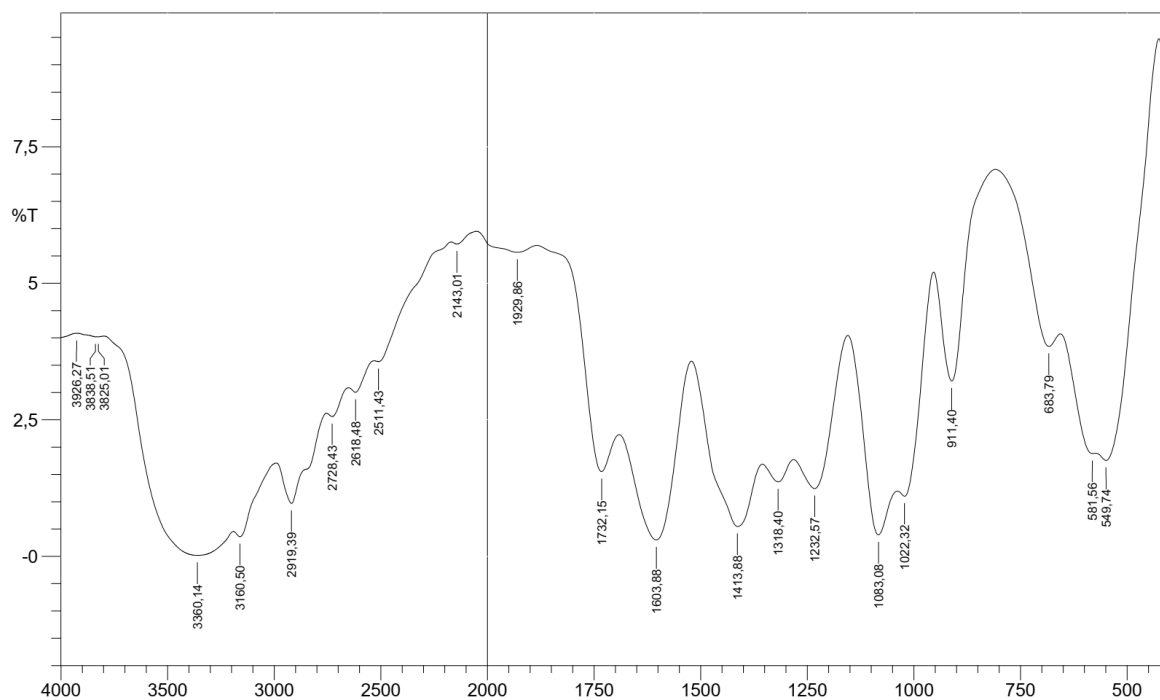


Fig. 3. IR spectra of new compound $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$.

monochloroacetic acid.

A strong absorption band at 1723 cm^{-1} is assigned to the $\text{C}=\text{O}$ stretching vibration of the carboxylic group. The presence of this band confirms the retention of the carboxyl functional group in the structure. The band at 1603 cm^{-1} is associated with N-H bending vibrations

and possible contributions from coordinated carboxylate groups, suggesting protonation of triethanolamine and formation of a triethanolammonium cation. In the region $1413 - 1318\text{ cm}^{-1}$, absorption bands correspond to symmetric and asymmetric stretching vibrations of the carboxylate group (COO^-), indicating partial ionization

of monochloroacetic acid and interaction with Ca^{2+} ions. Strong bands observed at 1083 cm^{-1} and 1022 cm^{-1} are attributed to C-O and C-N stretching vibrations, confirming the presence of the triethanolamine fragment in the compound.

Characteristic absorption bands of the chlorate ion (ClO_3^-) are observed at 914 cm^{-1} and in the region $630 - 580\text{ cm}^{-1}$. These bands correspond to asymmetric and symmetric stretching vibrations of the ClO_3^- group, confirming its incorporation into the structure. The bands at 638 cm^{-1} and $581 - 549\text{ cm}^{-1}$ are additionally associated with C-Cl and Cl-O vibrations, supporting the presence of the chloroacetate fragment. The simultaneous presence of hydroxyl, carboxyl, ammonium, chlorate, and chloroalkyl vibrational bands confirms that the synthesized compound is not a physical mixture, but a new chemically bonded system consisting of calcium chlorate coordinated with triethanolammonium monochloroacetate. Thus, the IR spectral data provide strong evidence for the formation of a new complex compound with the proposed composition $\text{ClCH}_2\text{COO H} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$.

Thus, the disappearance of absorption bands attributed to O-H stretching vibrations, together with the emergence of characteristic vibrational bands of the ClO_3^- ion in the spectrum of the new compound, provides strong evidence for compound formation and confirms a change in its structural organization.

CONCLUSIONS

In this work, the ternary $\text{Ca}(\text{ClO}_3)_2 - \text{CH}_2\text{ClCOOH} \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N} - \text{H}_2\text{O}$ system was investigated, and its polythermal solubility diagram was successfully constructed. Based on the obtained diagram, scientifically reliable information was acquired regarding the interactions among the system components, crystallization behaviour, and phase-equilibrium states. The experimental results indicate that this system belongs to a complex eutonic type and that the components crystallize while largely retaining their individuality.

The obtained findings provide a solid physicochemical basis for improving technologies for producing new physiologically active defoliants. These data are of practical importance for developing new formulations, enhancing their efficiency, and optimizing production processes.

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Authors' contributions

K.T. conceived the research idea and supervised the project. D.Q. and S.X. performed the experimental work. R.J. analysed the data and prepared the manuscript. All authors discussed the results and approved the final manuscript.

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