Investigation of the physicochemical properties of novel urea-organic amine complexes for agricultural applications

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Abstract: *The development of environmentally friendly and highly efficient agrochemical materials is an important objective of modern agricultural chemistry. Among various approaches, the synthesis of urea-based organic complexes has attracted considerable attention due to their potential to improve nutrient availability, enhance physicochemical stability, and increase fertilizer efficiency. In the present study, novel urea-organic amine complexes were synthesized and their physicochemical properties were systematically investigated with the aim of evaluating their potential agricultural applications. The synthesized complexes were prepared through interactions between urea and selected organic amines under controlled experimental conditions. Their physicochemical characteristics were examined using a combination of analytical and instrumental techniques. Particular attention was devoted to structural features, thermal behavior, solubility characteristics, and important physicochemical parameters, including pH, density, viscosity, and refractive index. The influence of organic amine incorporation on the properties of the resulting complexes was also assessed. The obtained results demonstrated the successful formation of stable urea-organic amine complexes exhibiting distinct physicochemical properties compared with the individual starting components. Structural investigations confirmed the presence of intermolecular interactions between urea molecules and organic amines, leading to the formation of new supramolecular systems. Thermal analysis revealed satisfactory thermal stability of the synthesized complexes, while solubility studies indicated favorable dissolution behavior in aqueous media. Significant variations in density, viscosity, and pH values were observed depending on the nature of the organic amine component, reflecting changes in molecular organization and intermolecular interactions. The synthesized complexes exhibited physicochemical characteristics that may contribute to improved nutrient utilization and controlled release behavior in agricultural systems. Their enhanced stability and favorable solubility properties suggest potential applicability as components of advanced agrochemical formulations. Furthermore, the ability to modify the physicochemical parameters of the complexes through selection of appropriate organic amines provides opportunities for tailoring their properties to specific agricultural requirements. The findings demonstrate that novel urea-organic amine complexes represent promising materials for agricultural applications. The comprehensive physicochemical characterization performed in this study provides valuable information regarding their structure-property relationships and establishes a scientific basis for future investigations involving agronomic performance, nutrient availability, and fertilizer efficiency.*

Keywords: *urea, organic amine complexes, supramolecular compounds, physicochemical properties, hydrogen bonding, thermal stability, solubility behavior, density, viscosity, agrochemical applications*

INTRODUCTION

The continuous growth of the global population and the increasing demand for agricultural productivity have intensified the need for efficient and environmentally sustainable fertilizer systems. Modern agriculture requires the development of advanced agrochemical materials capable of improving nutrient utilization efficiency, minimizing nutrient losses, and reducing the environmental impact associated with conventional fertilizers. Among various nitrogen-containing compounds, urea remains one of the most widely used fertilizers due to its high nitrogen content, low production cost, and ease of application. Despite its numerous advantages, the agricultural effectiveness of urea is often limited by several factors, including rapid dissolution, ammonia volatilization, leaching losses, and relatively low nitrogen use efficiency under certain environmental conditions. These limitations have stimulated extensive research aimed at modifying the physicochemical properties of urea through the formation of molecular complexes and supramolecular systems with various organic and inorganic compounds.

Organic amines represent an important class of compounds that possess unique physicochemical characteristics and the ability to form stable intermolecular interactions with urea molecules. The presence of amino and hydroxyl functional groups in many organic amines facilitates the formation of hydrogen-bonded networks and supramolecular assemblies, which can significantly influence the physicochemical behavior of the resulting complexes. Such interactions may alter solubility, thermal stability, viscosity, density, and other properties that are important for agricultural applications. Recent studies have demonstrated that the incorporation of organic amines into urea-based systems can enhance nutrient retention, improve solution properties, and potentially contribute to controlled nutrient release. Monoethanolamine, diethanolamine, and triethanolamine are particularly attractive organic amines because of their high water solubility, low toxicity, and ability to participate in extensive hydrogen-bonding interactions. The formation of urea-organic amine complexes may provide new opportunities for the development of multifunctional agrochemical materials with improved physicochemical performance. The physicochemical properties of fertilizer materials play a crucial role in determining their storage stability, transportation characteristics, application efficiency, and behavior in soil environments. Parameters such as solubility, pH, density, viscosity, refractive index, and thermal stability directly influence the practical performance of agrochemical products. Therefore, comprehensive characterization of newly synthesized urea-organic amine complexes is essential for understanding their structure-property relationships and evaluating their suitability for agricultural use.

Various analytical techniques have been employed to investigate the structural and physicochemical characteristics of urea-based complexes. Spectroscopic methods provide information about intermolecular interactions and structural organization, while thermal analysis enables evaluation of stability and decomposition behavior. In addition, measurements of density, viscosity, refractive index, and solubility contribute to understanding the molecular organization and practical applicability of the synthesized materials. Although numerous studies have investigated urea-containing systems, information regarding the physicochemical properties of newly synthesized urea-organic amine complexes remains limited. In particular, the influence of different organic amines on the structural organization and physicochemical behavior of such complexes has not been sufficiently explored. Further investigation is therefore required to establish the relationship between molecular composition and functional properties relevant to agricultural applications. The present study focuses on the synthesis and physicochemical characterization of novel urea-organic amine complexes intended for agricultural use. Particular attention is devoted to the evaluation of their structural features, thermal behavior, solubility characteristics, and key physicochemical parameters. The obtained results are expected to provide valuable insights into the design of advanced agrochemical materials and contribute to the development of more efficient and environmentally sustainable fertilizer technologies.

MATERIAL AND METHODS

Urea ($CO(NH_2)_2$), monoethanolamine (MEA, C_2H_7NO), diethanolamine (DEA, $C_4H_{11}NO_2$), and triethanolamine (TEA, $C_6H_{15}NO_3$) of analytical grade were used as starting materials for the synthesis of urea-organic amine complexes. Distilled water was employed for the preparation of all solutions. All reagents were used without further purification. The urea-organic amine complexes were synthesized by direct interaction of urea with the corresponding organic amine under controlled laboratory conditions. Predetermined molar amounts of urea and organic amine were mixed and stirred continuously until a homogeneous solution was obtained. The reaction mixture was maintained at 60-80°C for 2-4 h under constant stirring to promote intermolecular interaction and complex formation. After completion of the reaction, the resulting solution was cooled gradually to room temperature and allowed to crystallize. The obtained products were separated, dried under reduced pressure, and stored in airtight containers for further analysis.

The synthesis procedure was performed separately for the urea-monoethanolamine, urea-diethanolamine, and urea-triethanolamine systems. The pH values of aqueous solutions of the synthesized complexes were measured using a calibrated digital pH meter at 25 ± 0.1°C. Measurements were performed in triplicate, and the average values were recorded. Density measurements were carried out using a pycnometric method at 20 ± 0.1°C. The density of each sample was calculated according to the ratio of sample mass to its corresponding volume. Dynamic viscosity was determined using a capillary viscometer at 25 ± 0.1°C. The flow time of each sample was measured several times, and the average viscosity values were calculated. The refractive index of the synthesized complexes was determined using a digital refractometer operating at 20°C. Measurements were conducted using the sodium D-line wavelength (589.3 nm). The solubility behavior of the synthesized complexes was investigated over a temperature range of 0-60°C. Saturated solutions were prepared by adding an excess amount of solid complex to distilled water and maintaining equilibrium under continuous stirring.

After equilibrium was established, undissolved solids were removed by filtration, and the concentration of dissolved material was determined gravimetrically. Solubility values were expressed as mass percentage of dissolved complex. FTIR spectroscopy was employed to investigate the structural features and intermolecular interactions within the synthesized complexes. Spectra were recorded in the range of 4000-400 cm^{-1} using the KBr pellet technique. Particular attention was given to absorption bands associated with N-H, O-H, C=O, C-N, and C-O functional groups. Changes in band positions and intensities were analyzed to identify hydrogen-bonding interactions and complex formation. The crystalline structure of the synthesized complexes was investigated using X-ray diffraction analysis. Diffraction patterns were recorded within a 2θ range of 5-60°. The obtained diffraction data were used to evaluate crystallinity, phase composition, and structural modifications resulting from complex formation. Thermal stability and decomposition behavior were studied using thermogravimetric analysis. Samples weighing approximately 5-10 mg were heated from 25°C to 700°C at a heating rate of 10°C min^{-1} under a nitrogen atmosphere. The mass loss profiles obtained from the thermograms were used to determine decomposition stages, thermal stability limits, and residual mass formation. Differential scanning calorimetry was employed to investigate thermal transitions occurring within the synthesized complexes. Samples were heated from 25°C to 350°C at a constant rate of 10°C min^{-1} under nitrogen atmosphere. Endothermic and exothermic events were analyzed to determine melting behavior, phase transitions, and thermal stability of the complexes. All experimental measurements were performed in triplicate. Results were expressed as mean ± standard deviation. Statistical analysis was conducted using standard descriptive methods to evaluate the reproducibility and reliability of the obtained data.

RESULTS AND DISCUSSION

The interaction between urea and organic amines resulted in the formation of stable supramolecular complexes through intermolecular hydrogen-bonding interactions. During synthesis, homogeneous solutions were obtained for all investigated systems, indicating favorable compatibility between urea and the selected organic amines. Subsequent cooling and crystallization produced solid products with physicochemical characteristics different from those of the initial components. The formation of the complexes can be attributed to hydrogen-bond interactions between the amino groups of urea and the hydroxyl and amino groups of monoethanolamine, diethanolamine, and triethanolamine. These interactions contribute to the stabilization of the supramolecular structure and significantly influence the physicochemical properties of the resulting products.

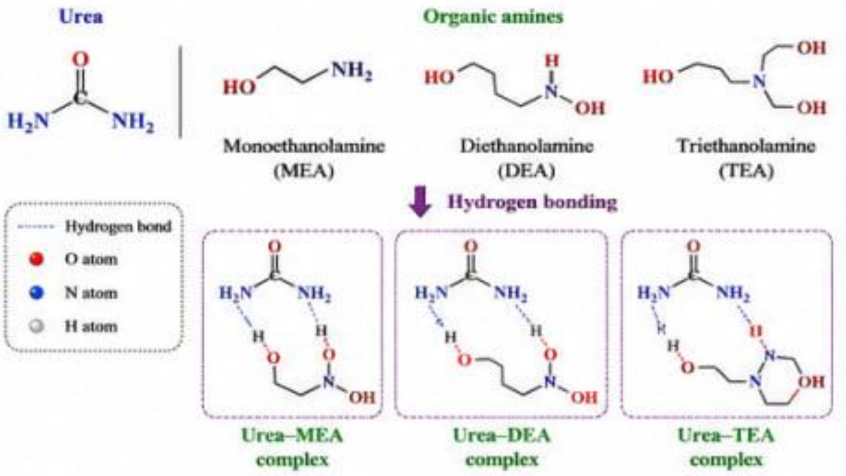

Figure 1. Proposed formation mechanism of urea–organic amine complexes through hydrogen-bond interactions.

FTIR spectroscopy confirmed the successful formation of urea-organic amine complexes. Significant changes were observed in the characteristic absorption bands associated with N-H, O-H, and C=O functional groups. The broadening and shifting of absorption bands in the region of 3200-3500 cm^{-1} indicated the formation of extensive hydrogen-bond networks within the complexes. The carbonyl stretching vibration of urea, typically observed near 1670 cm^{-1}, shifted toward lower frequencies after complex formation, suggesting strong intermolecular interactions involving the carbonyl oxygen atom. Additional changes in the C-N and C-O stretching regions further supported the formation of new supramolecular structures. The observed spectral modifications demonstrate that hydrogen bonding represents the principal driving force responsible for complex formation.

XRD analysis revealed substantial changes in the crystalline structure following interaction between urea and organic amines. Pure urea exhibited sharp diffraction peaks characteristic of a highly crystalline material. In contrast, the synthesized complexes displayed altered diffraction patterns with modified peak positions and intensities. The appearance of new diffraction peaks and the disappearance of several characteristic urea reflections indicate the formation of new crystalline phases. The reduction in crystallinity observed for some complexes may be attributed to increased structural disorder caused by incorporation of organic amine molecules into the crystal lattice. Among the investigated systems, the urea-triethanolamine complex exhibited the greatest reduction in crystallinity, reflecting the influence of the larger molecular structure and higher number of hydroxyl groups participating in hydrogen-bond formation.

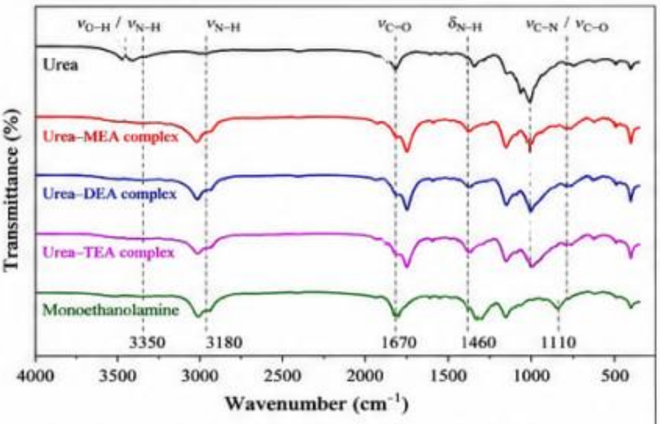

Figure 2. FTIR spectra of synthesized urea–organic amine complexes and initial components.

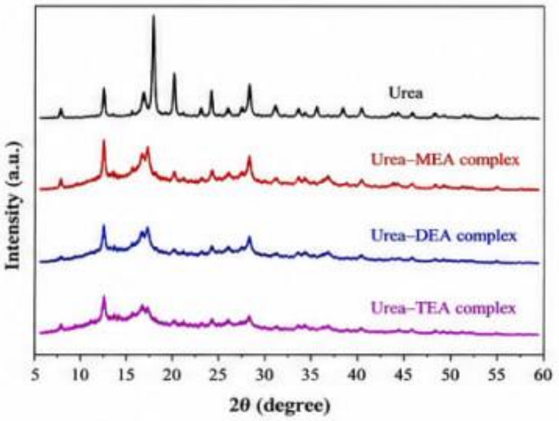

Figure 3. XRD diffractograms of urea and synthesized urea–organic amine complexes.

Thermogravimetric analysis demonstrated that the synthesized complexes possess satisfactory thermal stability. The thermograms revealed several stages of thermal decomposition. The initial mass loss observed below 150°C was attributed to the removal of physically adsorbed moisture and volatile impurities. The major decomposition stage occurred within the temperature range of 180-350°C and was associated with degradation of the hydrogen-bonded supramolecular structure and decomposition of organic components. Compared with pure urea, the synthesized complexes exhibited higher onset decomposition temperatures, indicating improved thermal stability. This enhancement can be explained by the formation of strong intermolecular interactions that increase resistance to thermal degradation.

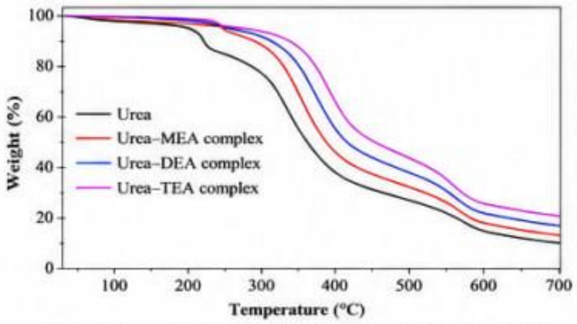

Figure 4. Thermogravimetric (TGA) curves of synthesized urea–organic amine complexes.

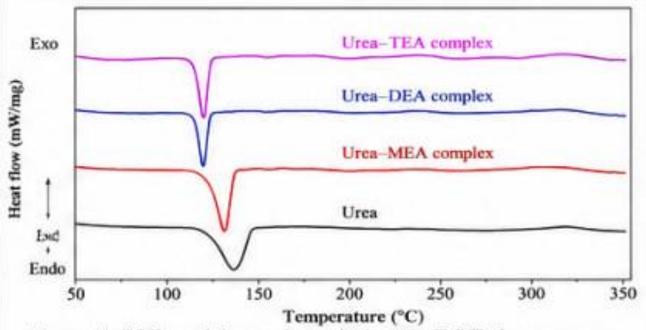

Figure 5. Differential scanning calorimetry (DSC) thermograms of urea–organic amine complexes.

DSC thermograms revealed distinct thermal transitions corresponding to melting and structural rearrangements of the complexes. The melting temperatures of the synthesized products differed from those of the individual components, providing further evidence for complex formation. The endothermic transitions observed in the DSC curves indicate disruption of hydrogen-bond networks and melting of the crystalline phases. The broadening of thermal transitions suggests the formation of structurally heterogeneous supramolecular systems. The urea-triethanolamine complex exhibited the broadest thermal transition region, reflecting its more extensive hydrogen-bonding network and complex molecular organization.

The synthesized complexes exhibited significantly improved aqueous solubility compared with pure urea. Solubility increased progressively with temperature for all investigated systems, indicating an endothermic dissolution process. Among the studied complexes, the urea-monoethanolamine system demonstrated the highest solubility values, while the urea-triethanolamine complex showed relatively lower solubility due to stronger intermolecular interactions within the solid phase. The enhanced solubility characteristics are advantageous for agricultural applications because they facilitate nutrient dissolution and improve the availability of nitrogen-containing species in aqueous environments.

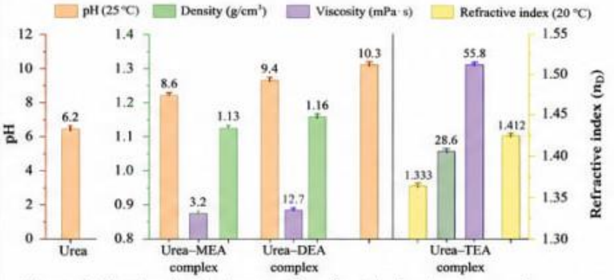

Figure 6. Physicochemical properties of synthesized urea–organic amine complexes.

The physicochemical parameters of the synthesized complexes varied depending on the nature of the organic amine component. The pH values of aqueous solutions increased in the order: Monoethanolamine complex < Diethanolamine complex < Triethanolamine complex. This trend reflects the increasing basicity of the organic amine component and its influence on the acid-base properties of the resulting complexes. Density measurements indicated moderate increases compared with pure urea solutions. The observed density variations suggest changes in molecular packing and intermolecular interactions within the liquid phase. Viscosity values increased significantly with increasing molecular size of the organic amine. The highest viscosity was observed for the urea-triethanolamine complex, which can be attributed to the formation of an extensive hydrogen-bonding network and increased intermolecular association. Refractive index measurements also increased progressively from monoethanolamine to triethanolamine complexes, reflecting changes in molecular structure and electronic polarizability.

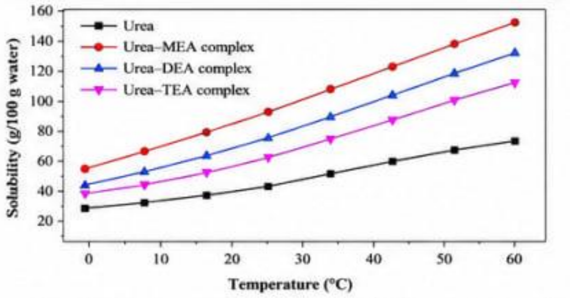

Figure 7. Temperature dependence of solubility of urea–organic amine complexes in water.

The combination of favorable thermal stability, enhanced solubility, adjustable pH, and improved physicochemical characteristics suggests that the synthesized urea-organic amine complexes possess significant potential for agricultural applications. The ability to modify physicochemical parameters through the selection of appropriate organic amines provides opportunities for designing agrochemical materials with tailored properties. Improved solubility and stability may contribute to enhanced nutrient availability and fertilizer efficiency, while controlled physicochemical behavior could reduce nutrient losses during storage and application. The obtained results demonstrate that the synthesized urea-organic amine complexes represent promising agrochemical materials with physicochemical properties suitable for further investigation in fertilizer formulations and agricultural technologies.

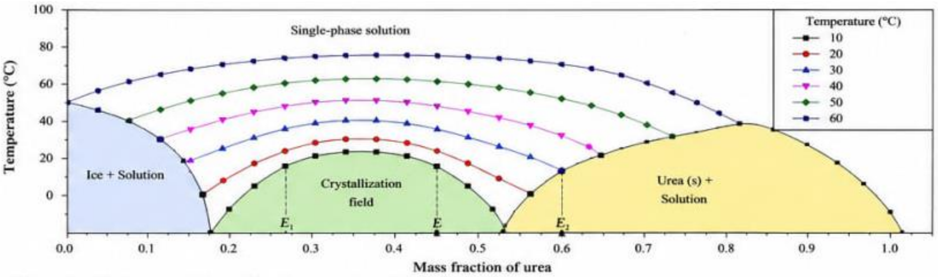

Figure 8. Polythermal solubility diagram of the urea–organic amine–water system.

CONCLUSION

The present study successfully synthesized and comprehensively characterized a series of novel urea-organic amine complexes intended for potential agricultural applications. The obtained results demonstrated that the interaction of urea with monoethanolamine, diethanolamine, and triethanolamine led to the formation of stable supramolecular complexes through extensive intermolecular hydrogen-bonding interactions. These interactions significantly influenced the structural organization and physicochemical behavior of the synthesized products. FTIR spectroscopic analysis confirmed the formation of new intermolecular associations through shifts in the characteristic absorption bands corresponding to N-H, O-H, and C=O functional groups. The observed spectral changes provided clear evidence for hydrogen-bond formation between urea molecules and organic amines. X-ray diffraction studies further revealed substantial modifications in crystalline structure, indicating the formation of new solid phases with physicochemical properties distinct from those of the individual starting components.

Thermal analysis demonstrated that the synthesized complexes possess satisfactory thermal stability. TGA results showed that the complexes exhibited higher decomposition temperatures compared with pure urea, indicating enhanced resistance to thermal degradation. DSC investigations revealed characteristic thermal transitions associated with melting and structural rearrangements, providing additional confirmation of complex formation and differences in molecular organization among the investigated systems. The synthesized complexes exhibited favorable solubility behavior in aqueous media, with solubility increasing as temperature increased. Such characteristics are particularly important for agricultural applications, where rapid dissolution and efficient nutrient availability are essential. The solubility data indicated that incorporation of organic amines can significantly modify the dissolution properties of urea-based materials and may contribute to improved fertilizer performance.

Measurements of pH, density, viscosity, and refractive index demonstrated that the physicochemical properties of the complexes depend strongly on the nature of the organic amine component. Progressive increases in viscosity, refractive index, and solution basicity were observed from monoethanolamine to triethanolamine-containing complexes, reflecting changes in molecular structure and intermolecular interactions. These findings confirm that the physicochemical characteristics of urea-based materials can be effectively tailored through the selection of appropriate organic amines. The obtained results establish clear relationships between molecular composition, structural organization, and physicochemical behavior of the synthesized complexes. The combination of enhanced thermal stability, favorable solubility, adjustable physicochemical parameters, and stable supramolecular structure suggests that these materials possess significant potential for use in advanced agrochemical formulations. The study demonstrates that novel urea-organic amine complexes represent promising agricultural materials with improved physicochemical characteristics compared with conventional urea. The comprehensive characterization presented in this work provides a scientific foundation for future investigations focused on nutrient release behavior, fertilizer efficiency, soil interactions, and practical agricultural performance under field conditions.

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