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Urea and Iron (II) Impurities: Impact on Sulphamic Acid Single Crystal Properties

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Abstract
Characterization and Optical Properties of Doped Sulphamic Acid Single Crystals. Sulphamic acid (SA) single crystals doped with iron (Fe2+) and urea were grown using conventional methods. X-ray diffraction (XRD) analysis confirmed the orthorhombic structure of the doped crystals. UV-Visible spectroscopy revealed the optical transmittance of electromagnetic radiation in the doped crystals. The results showed that the efficiency of the doped crystals followed the order: SA (undoped) > Fe:SA (iron-doped) > Urea:SA (urea-doped). This study highlights the potential of doping sulphamic acid single crystals with iron and urea to modify their optical properties.

1. Introduction
The growth of organic single crystals has experienced significant growth in recent years, driven primarily by their vast applications in optoelectronics and nonlinear optics. Organic materials, with their unique properties and characteristics, have shown tremendous potential in revolutionizing various technological fields. However, cultivating high-quality organic single crystals poses substantial challenges due to their inherent properties. [1]. Some of the key challenges associated with growing organic single crystals include their low thermal conductivity, susceptibility to supercooling, low melting points, and weak mechanical properties. These characteristics can lead to difficulties in controlling crystal growth, achieving uniform crystal quality, and maintaining crystal stability [2]. In contrast, inorganic crystals have been widely employed in various technological applications, including optical modulation, fiber optic communication, and optoelectronics. The popularity of inorganic crystals in these fields can be attributed to their exceptional properties, such as high mechanical stability, chemical inertness, and elevated melting points. These characteristics enable inorganic crystals to withstand harsh operating conditions, maintain their structural integrity, and provide reliable performance [3, 4]. Despite the challenges associated with growing organic single crystals, researchers continue to explore new methods and techniques to overcome these obstacles. By improving our understanding of organic crystal growth and developing innovative strategies to control and manipulate crystal properties, we can unlock the full potential of organic materials and harness their unique characteristics to create innovative technologies and applications [5].

2. Experimental Procedure
2.1. Synthesis and Conventional Growth of Sulphamic Acid Single Crystals
In this research, ferrous chloride (FeCl2) doped sulphamic acid (NH2.SO3H) and urea (CH4N2O) doped sulphamic acid (H2NSO3H) salts were synthesized using high-purity Analar reagent (AR) grade chemicals. Millipore water was employed as the solvent to ensure minimal impurities.

2.2. Solution Preparation and Crystal Growth
Homogeneous saturated solutions of urea: sulphamic acid and Fe2+: sulphamic acid were prepared by adding 1 mol% of MgCl2.6H2O and FeCl2 at room temperature. The solutions were stirred thoroughly and filtered using Whatman filter paper into petri dishes. The dishes were then placed in a dust-free environment at room temperature to facilitate crystal growth.

2.3. Crystal Harvesting
The grown crystals were harvested and photographed. The resulting crystals are shown in Fig. 1 (a), Fig. 1 (b), and Fig. 1 (c).

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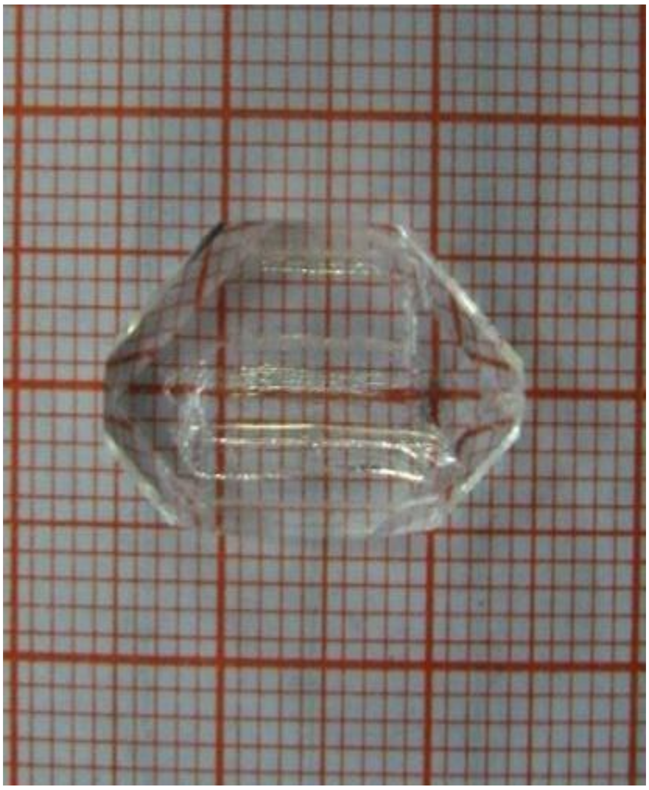

Fig.1.3. (a): Pure Sulphamic acid single crystal

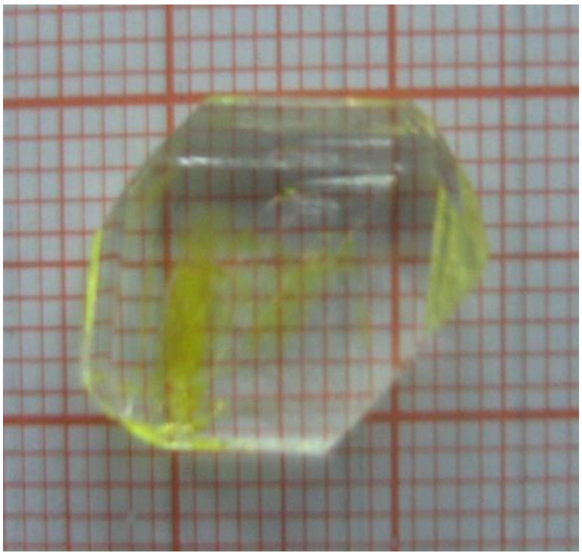

Fig. 1.3. (b). Fe doped Sulphamic acid

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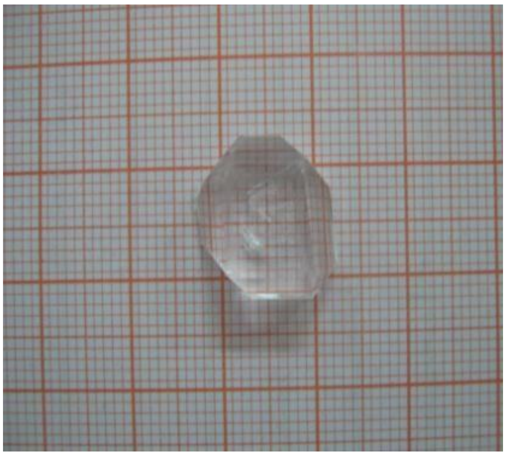

Fig.1.3. (c): Urea: SA single crystal

3. Characterization

3.1. Single crystal X-ray diffraction analysis

The grown pure and doped sulphamic acid (SA) single crystals, including urea-doped SA and Fe2+: SA, were subjected to single crystal X-ray diffraction (XRD) studies. The analysis was performed using an Enraf Nonius CAD4 single crystal X-ray diffractometer with MoKα radiation.

3.2. Crystal Structure and Lattice Parameters

The XRD study revealed that the crystals belong to the orthorhombic system. However, a discrepancy in the 2θ values and lattice parameters was observed, which may be attributed to the incorporation of urea and Fe2+ ions into the sulphamic acid crystal lattice.

The cell parameters obtained from the XRD analysis are summarized in Table 1.
Single crystal data of Urea and Fe^{2+} doped SA single crystals

Crystal	**Fe:SA**	**Urea: SA**
Crystal System	Orthorhombic	Orthorhombic
a (A^0)	8.06	8.19
b (A^0)	8.11	8.33
c (A^0)	9.25	9.40
V ($Å^3$)	605	642
α=β [illegible] (deg)	[illegible]	[illegible]
2 θ	19.27	68.90

3.3. UV-vis transmission spectrum

3.3.1. Optical Transmittance Studies

The optical transmittance spectra of the grown pure, urea-doped, and Fe2+-doped sulphamic acid (SA) crystals were recorded using a Labindia analytical UV3092 spectrophotometer. This study aimed to assess the stability of these crystals for optical applications.

3.3.2. Transmittance Results

The transmittance spectra revealed that the Fe2+-doped SA crystal exhibited a high transmittance of 96%, while the urea-doped SA crystal showed a transmittance of 93%. These results indicate that the doped SA crystals possess excellent optical transparency, making them suitable for various optical applications.

4. Conclusion

High-quality single crystals of Urea-doped Sulphamic Acid (SA) and Fe2+-doped SA have been successfully grown using the conventional slow evaporation solution growth technique from aqueous solutions. The lattice parameters of these crystals were accurately determined through single crystal X-ray diffraction (XRD) analysis. Furthermore, UV-Vis spectroscopy was employed to assess the optical transparency of the Fe2+ and Urea-doped SA single crystals.
Notably, the efficiency of the doped single crystals followed the order: SA > Fe:SA > Urea:SA. These results suggest that metal ions doped Sulphamic acid single crystals exhibit great promise for device applications, owing to their enhanced properties.

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