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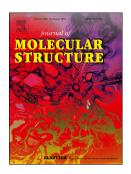
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# Novel 1,3-diethyl-2-thiobarbiturates of 2,2'-bipyridine and 1,10-phenanthroline: synthesis, crystal structure and thermal stability

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#### **Abstract**

Co-crystallization of 1,3-diethyl-2-thiobarbituric acid (HDetba) with 2,2'-bipyridine (Bipy) and 1,10-phenanthroline (Phen) results in preparing a salt co-crystal, BipyH(Detba)(HDetba) (1), and the salt, PhenH(Detba)·H<sub>2</sub>O (2). The compounds are characterized by single-crystal and powder X-ray diffraction and TG-DSC. The nitrogen atoms of BipyH<sup>+</sup> adopt an *cis* conformation and the N—C—C—N torsion angle is  $-17.3(1)^{\circ}$ . There are six intermolecular hydrogen bonds O—H···O, N—H···O, C—H···O and C—H···S in (1) which form a 2D plane network. One Detba<sup>-</sup> ion and one HDetba molecule form a pair by means of O—H···O hydrogen bonds. Detba<sup>-</sup> anions in (2) do not form dimers, they are connected by N—H···O, C—H···S and C—H···O hydrogen bonds only with PhenH<sup>+</sup> cations and water molecules which form a 3D net. Different  $\pi$ - $\pi$  interactions between the rings are found in (1)–(2).

**Keywords**: 1,3-diethyl-2-thiobarbituric acid; 1,10-phenanthroline; 2,2'-bipyridine; salt; salt cocrystal; X-ray diffraction; infrared spectroscopy; thermal stability

#### 1. Introduction

Derivatives of barbituric acid have anesthetic, sedative, anticonvulsive, antimicrobial, antifungal, antiviral and anti-cancer properties [1, 2]. Moreover, the organic salts of barbituric acids and their metal complexes possess potentially useful properties, for instance, biological activities [3, 4], solvatochromism, molecular recognition, photoluminescence, catalytic activity

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