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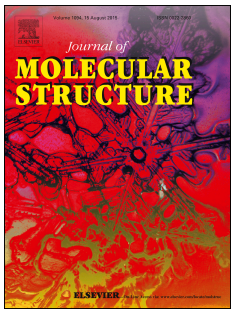

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Novel 1,3-diethyl-2-thiobarbiturates of 2,2'-bipyridine and 1,10-phenanthroline: synthesis, crystal structure and thermal stability

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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_2O (**2**). The compounds are characterized by single–crystal and powder X–ray diffraction and TG-DSC. The nitrogen atoms of $BipyH^+$ adopt an *cis* conformation and the N—C—C—N torsion angle is −17.3(1)º. 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 $Detba^-$ ion and one HDetba molecule form a pair by means of O—H···O hydrogen bonds. $Detba^-$ 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 $PhenH^+$ cations and water molecules which form a 3D net. Different π–π interactions between the rings are found in (**1**)–(**2**).

Keywords: 1,3-diethyl-2-thiobarbituric acid; 1,10-phenanthroline; 2,2'-bipyridine; salt; salt co-crystal; 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