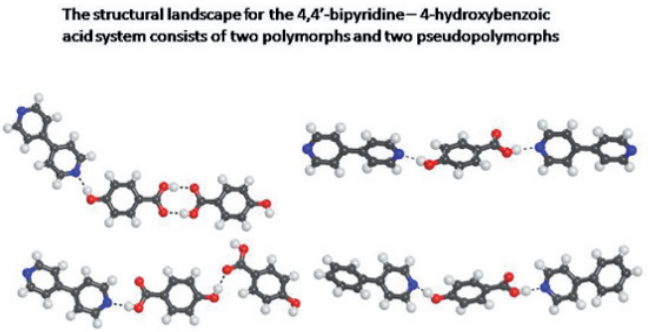

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Keywords: polymorphism, hydrogen bond, crystal engineering.

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Compounds of organic molecules and metal halides: structures and properties

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Organic molecules containing amine, carboxylic acid and/or amide functional groups may be combined with inorganic metal halides to form two different types of hybrid materials, both of which are of technological interest and self-assemble at the nano-scale.

When the components are combined as organic cations and perhalometalate anions, the resulting ionic organic-inorganic hybrid material often retains the properties of the individual parts, with the inorganic component potentially contributing mechanical hardness, thermal stability, electronic properties (conductor, semiconductor, insulator) and magnetic properties, while the organic component may add structural diversity and optical properties (fluorescence and luminescence) [1]. Proven applications of these ionic hybrids include light emitting diodes (LED's) [1].

Coordination compounds or coordination polymers are formed when the organic molecules coordinate to the metal atom of the metal halide component. The coordination polymers may be related to metal organic framework materials (MOF's), and contain both organic linkers and inorganic halide linkers, whereas MOF's typically only have organic linkers. Related coordination polymers have been reported to have interesting properties including non-linear optic behaviour and magnetic properties [2].

In the current study the effect of a change in one of the three parameters (organic component, metal atom and halide atom) on the crystal structures, packing and crystal engineering motifs are reported. In addition, the preliminary results of experimental properties, including band gap and electronic conduction, are presented, and compared to the properties calculated employing the software Materials Studio [3].

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Keywords: crystal engineering, properties

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Tautomeric polymorphism in triclabendazole

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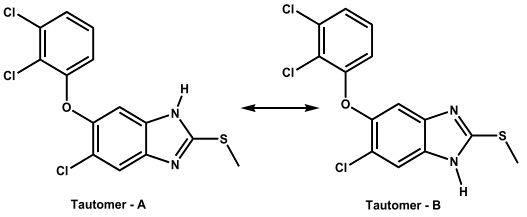
Triclabendazole [1] (TCB), 5-chloro-6-(2,3-dichlorophenoxy)-2-(methylthio)benzimidazole, is a classical veterinary anthelmintic drug active against liver flukes and belongs to the benzimidazole family of anthelmintics. It is known to exhibit polymorphism [2]. Two anhydrates (Form I and II), three solvates and an amorphous form are known. This study reports for the first time the crystal structures of Form I and Form II. The structural features of these crystal forms are interesting in the context of a little known variety of polymorphism, namely tautomeric polymorphism [3] (Scheme 1).

The crystal structure analysis reveals that Form I (Z' = 2) is composed of two molecules of tautomer A and Form II (Z' = 1) contains a 1:1 tautomeric mixture of A and B (Scheme 1) with the N=C–N–H fragment of the imidazole showing positional disorder (H–N=C–N–H). The polymorphs were also characterized using different solid state techniques (DSC, TGA, PXRD, IR and SSNMR). Based on enthalpy of fusion rule[4] and infrared rule[4] Form I and Form II are monotropically related to each other, and Form I is thermodynamically the most stable form. In addition, the tautomeric forms present in Form I and Form II were characterized by variable temperature NMR experiments in DMSO-d_6.

Further, to check the existence of the 100% tautomer B of TCB we carried out various co-crystallization experiments with 3,5-dinitirobenzoic acid and 3,5-dinitrosalicylic acid in different solvents and elucidated their crystal structures. In solvated cocrystals of dinitrobenzoic acid (methanol, acetone, acetonitrile and DMF) and dinitrosalicylic acid (methanol and DMF), the TCB molecule exists as a 100% tautomer B. However, in the latter case there is a proton transfer observed from the carboxylic acid to N(1) of the benzimidazole ring. In the absence of a carboxylic acid co-former TCB forms a 1:1 dimethylacetamide/water solvate with tautomer A. The presence of 100% tautomer B in cocrystals/salts of TCB strongly supports tautomeric polymorphism in TCB and confirms the coexistence of both tautomers A and B in Form II. The intriguing structural and thermodynamic features of these tautomorphs will be discussed in detail.



Scheme 1. Two possible tautomeric forms of TCB

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Keywords: crystal engineering, polymorph, drug.