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Crystal and molecular structure of eight organic acid–base adducts from 2-methylquinoline and different acids

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HIGHLIGHTS

- Eight organic acid–base adducts have been prepared and structurally characterized.
- The different hydrogen bond interaction modes of the 2-methylquinoline and acidic compounds have been ascertained.
- All structures adopted hetero supramolecular synthons.
- The classical hydrogen bonds are the primary intermolecular force in a family of structures containing the OH···2-methylquinoline synthons.
- The secondary propagating interactions also play an important role in the solid-state packing of the compounds.

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ABSTRACT

Eight supramolecular complexes with 2-methylquinoline and acidic components as 4-aminobenzoic acid, 2-aminobenzoic acid, salicylic acid, 5-chlorosalicylic acid, 3,5-dinitrosalicylic acid, malic acid, sebacic acid, and 1,5-naphthalenedisulfonic acid were synthesized and characterized by X-ray crystallography, IR, mp, and elemental analysis. All of the complexes are organic salts except compound **2**.

All supramolecular architectures of **1**–**8** involve extensive classical hydrogen bonds as well as other noncovalent interactions. The results presented herein indicate that the strength and directionality of the classical hydrogen bonds (ionic or neutral) between acidic components and 2-methylquinoline are sufficient to bring about the formation of binary organic acid–base adducts. The role of weak and strong noncovalent interactions in the crystal packing is ascertained. These weak interactions combined, the complexes **1**–**8** displayed 2D–3D framework structure.

Introduction

Cocrystal/salt formation is rapidly gaining popularity as a method for the synthesis of new materials [1]. Important in this regard is the fact that cocrystals/salts provide an opportunity to synthesize organic solids by design, through the use of supramolecular synthons [2]. Thus, cocrystals/salts can be engineered with the intention to design, or improve upon, a particular solid-state property of a molecule (e.g. reactivity, dissolution, mechanical, electrical or optical properties) without affecting its intrinsic structure [3]. The major driving force in cocrystal/salt formation is hydrogen bonding and other nonbonding interactions [4–8].

Because of the predictable supramolecular properties and the ability to form strong hydrogen bonds, carboxylic acids were frequently chosen as building blocks for crystal engineering [9–11]. Numerous heterodimers composed of carboxylic acids and a variety of N-containing basic building blocks have been documented recently [12–16]. The hydrogen bonding between hydroxyl groups of carboxylic acids and heterocyclic nitrogen atoms has been proved to be a useful and powerful organizing force for the formation of supramolecules. It should be noted that these structures are normally held together by hydrogen-bonding, and in this regard, the most frequently used moieties with hydrogen bonding capability are pyridyl and carboxyl. As a pyridyl derivative, besides the methyl group, 2-methylquinoline bears more aromatic π electrons, which can be a better group in creating aromatic stacking interactions. To the best of our knowledge there are very few reports involving the organic acid–base adduct concerning the Lewis base of 2-methylquinoline.

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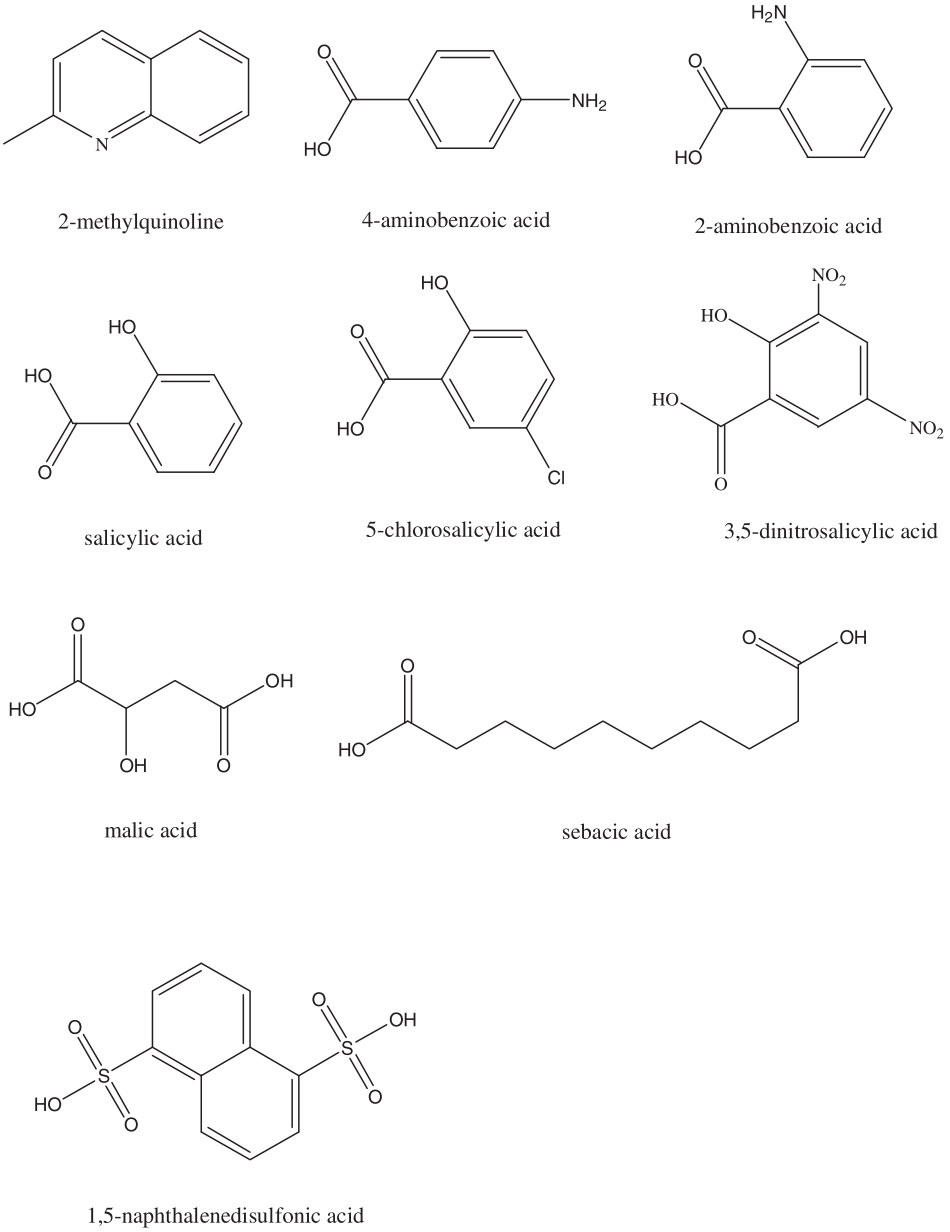
Following our previous works of acid–base adducts based on N-aromatic derivatives and carboxylic acids [17–19], herein we report the synthesis and crystal structure of eight supramolecular complexes assembled through hydrogen bonding interactions between acidic synthons and 2-methylquinoline. In this study, we got eight organic acid–base adducts composed of acidic units and 2-methylquinoline (L) (Scheme 1), namely 2-methylquinoline: (4-aminobenzoic acid) $[(HL)^+ \cdot (4\text{-aba}^-)$, 4-aba$^-$ = 4-aminobenzoate] **(1)**, 2-methylquinoline: (2-aminobenzoic acid) [(L) · (2-Haba), 2-Haba = 2-aminobenzoic acid] **(2)**, 2-methylquinoline: (salicylic acid) $[(HL)^+ \cdot (sal^-)$, sal$^-$ = salicylate] **(3)**, 2-methylquinoline: (5-chlorosalicylic acid) $[(HL)^+ \cdot (csal^-)$, csal$^-$ = 5-chlorosalicylate] (**4**), 2-methylquinoline: (3,5-dinitrosalicylic acid) $[(HL)^+ \cdot (3,5\text{-dns}^-)$, 3,5-dns$^-$ = 3,5-dinitrosalicylate] **(5)**, $(2\text{-methylquinoline})_2$: (L-malic acid) $[(HL)^+ \cdot (L) \cdot (Hmal^-)$, Hmal = L-hydrogenmalate] (**6**), $(2\text{-methylquinoline})_2$: (sebacic acid) $[(HL)_2^{2+} \cdot (seba)^{2-}$, seba = sebacate] (**7**), and $(2\text{-methylquinoline})_2$: (1,5-naphthalenedisulfonic acid): $2H_2O$ $[(HL)_2^{2+} \cdot (nsa)^{2-} \cdot 2H_2O$, nsa = 1,5-naphthalenedisulfonte] (**8**) (Scheme 2).

Experimental section

Materials and methods

All reagents were commercially available and used as received. The C, H, N and S microanalysis were carried out with a Carlo Erba 1106 elemental analyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000–400 cm^{-1} on a Mattson Alpha-Centauri spectrometer. Melting points of new compounds were recorded on an XT-4 thermal apparatus without correction.

(1,5-naphthalenedisulfonic acid) : $2H_2O$ $[(HL)_2^{2+} \cdot (nsa)^{2-} \cdot 2H_2O$, nsa = 1,5-naphthalenedisulfonte] (**8**) (Scheme 2).



Scheme 1. Hydrogen bond synthons discussed in this paper.