

Proton-transfer and non-transfer in
compounds of quinoline and quinaldic
acid with L-tartaric acidGraham Smith,^{a*} Urs D. Wermuth^b and Jonathan M.
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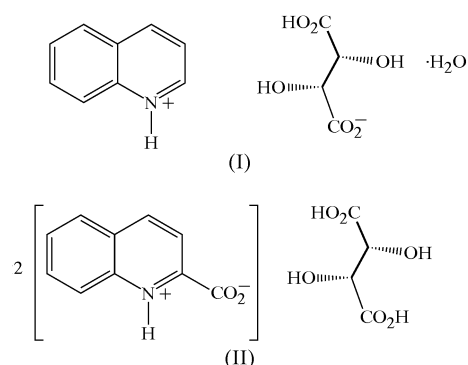
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The structures of two compounds of L-tartaric acid with quinoline, *viz.* the proton-transfer compound quinolinium hydrogen (2*R*,3*R*)-tartrate monohydrate, C₉H₈N⁺·C₄H₅O₆[−]·H₂O, (I), and the anhydrous non-proton-transfer adduct with quinaldic acid, bis(quinolinium-2-carboxylate) (2*R*,3*R*)-tartaric acid, 2C₁₀H₇NO₂·C₄H₆O₆, (II), have been determined at 130 K. Compound (I) has a three-dimensional honeycomb substructure formed from head-to-tail hydrogen-bonded hydrogen tartrate anions and water molecules. The stacks of π -bonded quinolinium cations are accommodated within the channels and are hydrogen bonded to it peripherally. Compound (II) has a two-dimensional network structure based on pseudo-centrosymmetric head-to-tail hydrogen-bonded cyclic dimers comprising zwitterionic quinaldic acid species which are interlinked by tartaric acid molecules.

Comment

Tartaric acid is a relatively strong diprotic chiral α -hydroxy acid ($pK_{a1} = 2.93$ and $pK_{a2} = 4.23$) and, therefore, is potentially capable of forming both 1:1 and 1:2 proton-transfer salts with most Lewis bases. However, with stoichiometric control it is possible to selectively form 1:1 hydrogen tartrates, and the crystal structures of a large number of these 1:1 salts have been reported, particularly since these compounds usually have good crystal morphology, allowing structure determination by single-crystal X-ray analysis, which is often not possible with the parent Lewis base. Applications have been with drugs such as epinephrine (Carlström, 1973), dextromoramide (Bye, 1975), amosulalol (Furuya *et al.*, 1989), alprenolol (Główska & Coddington, 1989), phendimetrazine (Glaser *et al.*, 1994) and tolterodine (Košutić-Hulita & Žegarac, 2005), as well as natural products such as alkaloids, *e.g.* strychnine (Gould *et al.*, 1987), brucine (Smith, Wermuth & White, 2006), quinine (Ryttersgaard & Larsen, 2004),

cinchonine (Puliti *et al.*, 2001), cinchonidine (Ryttersgaard & Larsen, 2003; Zhang *et al.*, 2003) and quincoridine (Kania *et al.*, 2004), and amino acids, *e.g.* L-alanine (Rajagopal *et al.*, 2002), L-proline (Subha Nandhini *et al.*, 2001), D-, L- and DL-histidine (Marchewska *et al.*, 2003; Rajagopal *et al.*, 2003; Johnson & Feeder, 2004*a,b,c*), and L-lysine (Debrus *et al.*, 2005).



Because of the ready availability of L-(+)-tartaric acid, which has the confirmed 2*R*,3*R* absolute configuration, it has been very useful for both resolution and the crystallographic determination of absolute configuration in chiral molecular species, *e.g.* with the anticholinergic agent *R*-(−)-1,1-diphenyl-3-piperidinobutan-1-ol (Schjelderup *et al.*, 1990). More recently, its utility as an agent for the introduction of chirality in achiral organic compounds for the generation of crystalline materials with potentially useful non-linear optical properties has been explored (Aakeröy *et al.*, 1992; Fuller *et al.*, 1995; Marchewska *et al.*, 2003; Debrus *et al.*, 2005; Manivannan *et al.*, 2006).

We have found that 1:1 stoichiometric interactions of the relatively strong carboxylic acids 5-sulfosalicylic acid (5-SSA) (Smith *et al.*, 2004) and 3,5-dinitrosalicylic acid (DNSA) (Smith, Wermuth, Healy & White, 2006) with a series of bicyclic heteroaromatic amines, including quinoline, tetrahydroquinoline, 8-hydroxyquinoline, 8-aminoquinoline and

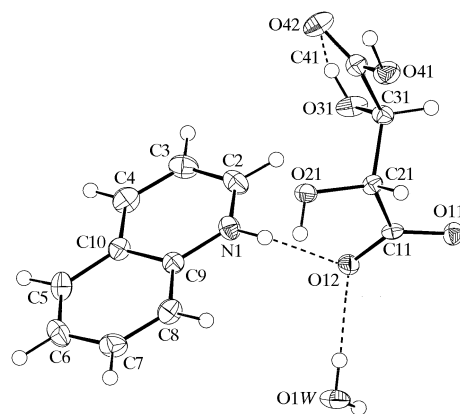


Figure 1

The molecular configuration and atom-numbering scheme for the quinolinium cation, the hydrogen L-tartrate anion and the solvent water molecule in (I). Non-H atoms are shown as 50% probability displacement ellipsoids.