

(H₂O) is essentially part of the crystal structure. Fe(II) ion having electronic configuration [Ar]3d⁶ is in a high-spin state since both H₂O and oxalate anion are weak field ligands (Moore 2004). Hence the electron configuration of Fe(II) ion is somewhat asymmetric that Fe(II)-polyhedron is vertically contracted by Jahn-Teller effect (Burns 1993). Bond-valence analysis (Brown 2002) of the crystal structure of Fe(II)-oxalate suggested that the polyhedral distortion gives rise to the strong hydrogen bond.

Keywords: hydrogen bonding of coordination compounds, Jahn-Teller effect, Raman spectroscopy

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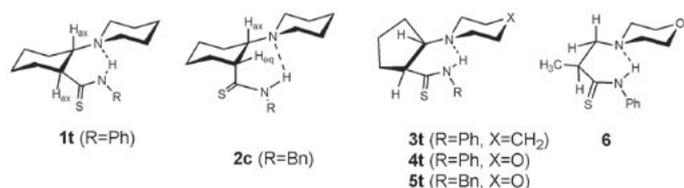
Secondary thioamide group deformations caused by intramolecular hydrogen bond

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Structures of several *b*-aminofunctionalized secondary thioamides capable to form intramolecular hydrogen bond N-H...N have been determined by X-ray diffraction (Scheme 1). Particular attention has been directed to the deformations of the thioamide group caused by steric strain. Out-of-plane deformations of the thioamide group are described in terms of bending (χ_C and χ_N) and twisting (τ) parameters [1]. The X-ray results show that the thioamide group displays high resistance to steric stress which is in this case caused by the intramolecular hydrogen bond and deviations of the thioamide group from planarity are small if any. On the other hand, some sp² bond angles in the thioamide group of the molecules under exploration as well some tetrahedral bond angles in the saturated parts are substantially changed from the ideal values in order to retain the thioamide group planarity.

[1] J.D. Dunitz, F.K. Winkler, *Acta Cryst.* B31 (1975) 251-263.



Keywords: secondary thioamides, intramolecular hydrogen bond, deformations of the thioamide group

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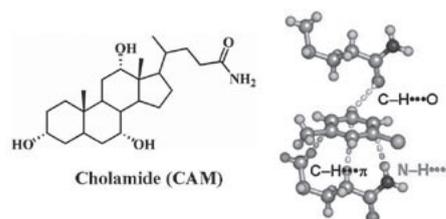
Weak hydrogen bonds in cholamide inclusion crystals with aromatic guests

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Steroidal cholamide (CAM) forms inclusion crystals with more than twenty aromatic compounds in 1:1 or 2:1 host-to-guest molar ratios. The 1:1 crystals have guest-dependent host frameworks, where

weak hydrogen bonds such as N-H/ π , C-H/ π , and C-H/O play a key role in linking the host and guest molecules. The steroidal side-chains involving methyl, methylene, and amide groups serve as the hydrogen bond donors, and aromatic guest molecules serve as the acceptors. Three kinds of such weak hydrogen bonds are visualized by the Hirshfeld surfaces of the guest molecules. Comparisons of the inclusion crystals of CAM and cholic acid (CA) with the same guests clarify a profound effect of the weak hydrogen bonds. In the case of the 1:1 crystals, the N-H/ π hydrogen bonds explain the fact that CAM always employs a β -*trans*-type framework, while CA employs either an α -*gauche*- or β -*trans*-type framework. On the other hand, the 2:1 crystals, termed DCA-type, have only C-H/ π hydrogen bonds. The guest-dependent isomerization of these frameworks is examined in terms of the weak hydrogen bonds as well as compatibilities in size and shape.



Keywords: hydrogen bonding, inclusion compounds, supramolecular chemistry

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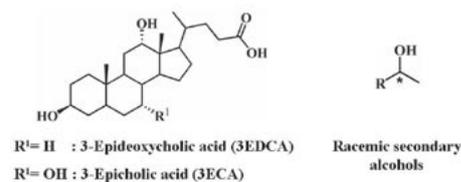
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Chiral recognition for inclusion compounds of 3-epicholic and 3-epideoxycholic acids with alcohols

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Chiral recognition mechanism is still an interesting subject for efficient enantioresolution of racemates by using inclusion crystals. We perform a systematic study on cholic acid derivatives as the host compounds for enantioresolution of various alcohols. So far, we reported that cholamide includes a wide variety of the alcohols and exhibits a specific ability for recognizing (*S*)-2,2-dimethyl-3-hexanol. Moreover, it was found that 3-epicholic and 3-epideoxycholic acids showed efficient enantioresolution towards aliphatic secondary alcohols, such as 2-pentanol, 2-hexanol, 2-heptanol, and so on. The enantioresolution for two stereogenic carbons was ascertained toward (2*R*,3*S*)-3-methyl-2-pentanol (over 95 ee%). Here we describe crystal structures of these inclusion compounds as well as a plausible mechanism for such chiral recognition. The mechanism is based on a four-point location model which demands a disordered structure of the guest molecules in a concaved surface of host channels.



Keywords: chiral recognition, inclusion compounds, supramolecular chemistry