# Molecular Structure of the Hydrated Complex of 1,4-dimethylpiperazine di-betaine with L-tartaric Acid Studied by X-ray Diffraction and FTIR

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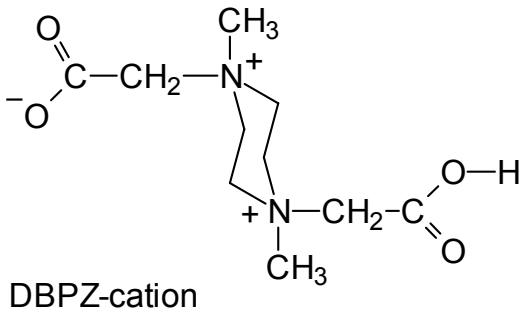
1,4-Dimethylpiperazine di-betaine (1,4-dicarboxymethyl-1,4-dimethylpiperazinium inner salt, DBPZ) forms two kinds of 1:1 complexes with L-tartaric acid (TA), anhydrous DBPZ·TA and hydrated DBPZ·TA·2.5$H_2O$.

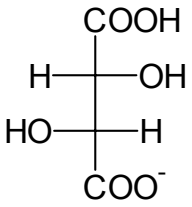
In the first one, DBPZ·TA, DBPZ and TA molecules are linked into infinite chains by two asymmetric hydrogen bonds of 2.485(3) and 2.566(3) Å, the carboxylic group of TA and the carboxylate group of DBPZ, without the proton transfer. The piperidine ring has a chair conformation with the methyl groups in the axial positions and the $CH_2COO$ substituents equatorial [1].

In this contribution we report the molecular structure and spectroscopic properties of the DBPZ·TA·2.5$H_2O$ complex studied by the X-ray diffraction, FTIR and Raman spectroscopies and optimized by at the B3LYP/6-31G(d,p) level of theory.

In the complex investigated the piperazine ring has a chair conformation, however the substituents assume the opposite orientations than in the DBPZ·TA complex, e.g. the methyl groups are equatorial and the $CH_2COO$ substituents are axial. One proton from the carboxylic group of TA is transferred to the carboxylate group of DBPZ. The DBPZ cations are linked by the asymmetric, short COOH···OOC hydrogen bonds of 2.476(3) Å into chains, while the semi-tartrate anions are linked by the short and symmetric COO·H·OOC hydrogen bonds of 2.464(3) Å into separate chains. The chains of the positively charged, $DBPZ^+$, and negatively charged, $TA^-$, molecules are joined together only by a weak O-H···O=C hydrogen bond of 3.230(4) Å, into layers. Water molecules are involved in the hydrogen bonds with the TA chains.




DBPZ-cation




Semi-tartrate

The solid-state FTIR spectrum is consistent with the crystal structure. The broad band, attributed to the $\nu_{OH}$ vibration, appears in the 3600-3100 $cm^{-1}$ region. A broad absorption in the 1500-400 $cm^{-1}$ region is characteristic of the short OHO hydrogen bonds.

[1] Z. Dega-Szafran, A. Katrusiak, M. Szafran, J. Mol. Struct. (2008) in press.