Experimental and Theoretical Evaluation of N-H…O Hydrogen Bonds in Alkylamine Oxalate Crystals

Krzysztof Ejsmont, Jacek Zaleski, *Institute of Chemistry, University of Opole, Poland.* E-mail: zaleski@uni.opole.pl

Design of new materials possessing interesting structure and properties has become an important area in organic crystal engineering. This strategy is based on existence the hydrogen bond interactions between molecules in crystals [1]. Dicaboxylic acids generally interact through intermolecular hydrogen-bonding to form the linear chains. This is the reason why these molecules has been recently used as new building block in crystal engineering [2].

Due to this development we are interested in studying the hydrogen-bonded supramolecular systems of oxalic acid and alkylamines. Oxalates of *t*-butylamine, *n*-ethylamine, *n*-diethylamine and *n*-ethyldimethylamine has been obtained and characterized by X-ray diffraction method, IR and quantum-mechanical calculations. An examination of the crystal structure of these compounds indicated two distinct types of hydrogen bond patterns, involving linear chains of hydrogen bonded monohydrogen oxalate anions and isolated oxalate anions surrounded by the monoprotonated *t*-butylamine cations. The quantum-mechanical calculations were performed to optimize geometries of complexes linked by N-H…O using the Gaussian 98 suite of programs [3].

[1] Desiraju G.R., *Acc. Chem. Res*., 2002, **35**, 565. [2] Vaidhyanathan R., Natarajan S., Rao C.R.N., *J. Mol. Struct.,* 2002, **608**, 123. [3] Gaussian 98, Revision A.7, Frisch M.J., et. al., *Gaussian, Inc., Pittsburgh PA*, 1998.

Keywords: alkylamine oxalate, hydrogen bonds, ab-initio calculation