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Imidazolium Salts of Dicarboxylic Acids -Crystal Structure in the Low Temperature Range 12K -120K

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Crystal engineering is currently a topical area of research, with many examples of target architectures in the literature. The salts of dicarboxylic acids are especially interesting due to their molecular packing in the structure and possible hydrogen bond formation. The room temperature crystal structure of new imidazolium salts of dicarboxylic acids (imidazolium malonate, imidazolium glutarate, diimidazolimu suberate, imidazolium sebacate) has been determined earlier by one of us [1] and all crystals were found to triclinic. Here we describe the crystal structure of two new single crystalline salts of imidazolium: imidazolium pimeline and imidazolium azelaine. The main goal of the paper is however, a characterization of the hydrogen bonds in the crystal structure of the all six compounds in low temperature range from 120K to 12K. The XRD of single crystalline samples was measured using Xcalibur diffractometer with HeliJet attachment at 120K, 60K and 12K. The molecules in the crystal structure of the imidazolium dicarboxylic salts form hydrogenbonded chains, in which the imidazolium cations are bonded together by strong N-H..O hydrogen bonds and the carboxylate anions are coupled by strong O-H..O type bonds. The both types of the chains are self-assembled into a supramolecular network or layers [2]. At room temperature the imidazolium cations "are hot" - exhibit intensive thermal motions and the refinement of crystal structure at low temperatures allows more precise determination of the character of the hydrogen bonds. We determined also the inter- and intra-molecular thermal expansion for the all crystals of imidazolium dicarbolic acid salts.

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Fulgide Photochromism in Crystal: Loss of Crystalline Order in the Photochromic Transformation of 3-Furylfulgide

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The 3-furylfulgide E-form is a photochromic dye which undergoes a reversible electrocyclic ring-closure when irradiated with UV light at λ >300 nm to give a red dye, C-form. The C-form is bleached with white light to revert back to the E-form. The modification of the conformation of the photochromic 3-furylfulgide molecule has been studied in relation with its crystal structure. Intense two photon irradiation of an initial pale yellow single crystal led to a red-colored material which is no longer crystalline, but still photochromic. Conversely, starting from a colored crystal, grown from an irradiated solution, X-ray diffraction gave the first determination of the molecular conformation and crystal structure of the colored form and showed that after visible irradiation the bleached material lost its crystalline structure. The photoinduced molecular displacements responsible for this behavior are pointed out.

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^[2] J.C. MacDonald, Crystal Growth & Design (2001), V1, 29-38