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Structure and Molecular Dynamics of Bis-1,2,4-Triazole Succinic Acid Molecular Crystals. A. Pietraszko[a], J. Baran[a], K. Pogorzelec-Glaser[b], B. Hilczer[b], J. Małecki[b] and M. Połomska[b], [a]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland,* [b]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*
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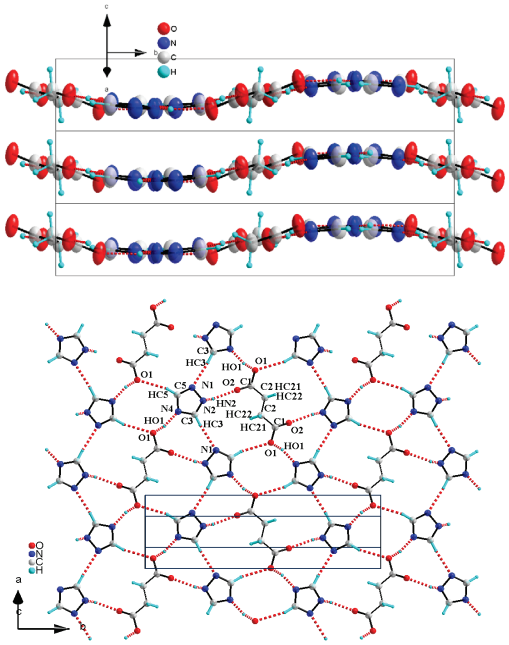
Bis-1,2,4-triazole succinic acid belongs to the family of dicarboxylic acid compounds of nitrogen containing heterocyclic molecules which are expected to exhibit proton conductivity [1,2]. We studied the molecular structure of bis-1,2,4-triazole succinic acid by X-ray diffraction and semi-empirical molecular orbital calculations with the MP3 approximation. Zig-zag-type layer structure with layers parallel to the $(10\bar{2})$ plane of the $P2_1/c$ monoclinic space group was ascribed to the compound. We consider the structure to be formed as a result of a competition between strong specific interaction within a single layer and weak interlayer hydrogen interactions of the N-H…π type. The calculated distributions of the charge density as well as the electrostatic potential in the plane parallel to the triazole pentagon are in good agreement with those obtained from XRD data. Bis-1,2,4-triazole succinic acid formation leads to an increase in the frequencies of the O-H bending modes and decreases the O-H and C=O stretching frequencies of the succinic acid molecule. Moreover, new bands in the 2900-3300 cm^{-1} range are apparent in the bis-1,2,4-triazole succinic acid.



Crystal packing and a single layer of bis-1,2,4-triazole succinic acid.

[1] J.C. Mac Donald et al., Crystal Gowth and Design 1, 29 (2001). [2] K. Pogorzelec-Glaser et al., J. Power Sources 173, 800 (2007).

Keywords: Triazole; Dicarboxylic acids; Molecular structure; Raman spectra