Poster Presentation

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Ultra short H-bond in potassium monobasic 1,4-butodioxybis(4'-benzoic) acid

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Hydrogen bonds have been exhaustively investigated in order to understand their role in intermolecular interactions [1]. The importance of the hydrogen bonds follows from their particular role in the molecular association thanks to their variable strength and geometry. Indeed depending on the chemical nature of the donor/acceptor as well as on the physical parameters such as temperature and pressure, hydrogen bonds can give rise to directional and/or to hydrophilic like interactions which play a crucial role both in stabilizing static structures and in mediating dynamic biological processes. Among the hydrogen bonds the less common ones are the strongest (and shortest) ones, characterized by donor–acceptor interatomic distances shorter than 2.6 Å with D–H...A angle close to 180º [2]. Most of the short hydrogen bonds observed and reported so far are intramolecular interactions, nevertheless, both the bridging as well as the coordination of the metal ions by carboxylate groups and oxalate anions can provide the possibility of short interactions [3]. During the refinement of the structure of the potassium-monodeprotonated salt of 1,4-butodioxybis(4'-benzoic) acid it was observed a high electron density maxima over the mirror symmetry element. This electron density indicates a hydrogen atom doing an ultra short intermolecular hydrogen bond (2.4846(1) Å) between the deprotonated and non-deprotonated carboxylic acid groups. The seven fold coordinate potassium atom ties the organic moieties pushing the hydrogen atom closer to the deprotonated and negatively charged, carboxylate oxygen atom. The hydrogen atomic displacement parameter suggests, however, a possible positional disorder, which could be interpreted both as symmetrical O–H–O or asymmetrical O–H...O interaction.

[1] *M. Nishio, et. al. CrystEngComm, 2009, 11, 1757-1788.,* ***[2]*** *G. Gilli, P. Gilli. J. Mol. Struct. 2000, 552, 1-15.,* ***[3]*** *M. Hamdouni, et. al. J. Chem. Crystallogr. 2011, 41, 11, 1742-1750.*

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