

in the Br- and NO₂- derivatives of 1-phenylethanones (1,2). However, when the N atom in these structures is pyramidal, no distant dimers are formed and the N-H...C(aryl) contacts become evident.

References:

1. Saraogi, I., Mruthyunjayaswamy, B. H. M., Ijare, O. B., Jadegoud, Y. & Guru Row, T. N. (2003). *Acta Cryst.* E59, o443-o444
2. Abdulla, R. F., Boyd, D. B., Jones, N. D. & Swartzendruber, J. K. (1985). *J. Org. Chem.* 50, 3502-3505.

Keywords: hydrogen bonds in organic crystals, small molecules organic, long-range contacts

P08.13.81

Acta Cryst. (2008). A64, C443

The interaction between H-bond and polyhedral network in the polymorphs of aluminium hydroxide

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We have investigated several polymorphs of aluminium hydroxide in the last few years. The most important of these is the structural investigation under pressure of the hydrogen bond (H-bond) in δ -AlOOH, a phase which is a potential water reservoir in cold subducted slabs, transporting water into the lower mantle. Structures of aluminium hydroxides could be characterized as a combination of 0D (D: dimensional) or 1D H-bonding network and 2D or 3D dimensional Al(O, OH)₆ polyhedral network. For example, δ -AlOOH is considered to be a combination of 0D H-bond and 3D polyhedral networks. The H-bond and polyhedral networks are not isolated, but interacted each other via valence sum of the oxygen atoms. For example if we consider a fictitious 1D network consists of 0D H-bond and 0D AlO molecule like: -O-Al-O-H_a...O-Al-O-H_b...O-Al-O-H_c..., where H_a is not able to move independently to acceptor site due to the electrostatic valence principle. This can be considered as a kind of 'ice rule.' In this study, we will present the results of x-ray and neutron diffraction studies for δ -AlOOH, β -AlOOH (boehmite), η -Al(OH)₃ and δ -Al(OH)₃. The last two polymorphs are high pressure modifications of γ -Al(OH)₃ (gibbsite), and their structures had remained unknown for quarter of a century after their discovery. η -Al(OH)₃ has the layered structure like gibbsite, and δ -Al(OH)₃ has the A-site deficient perovskite (ReO₃-type) structure. Although the polymorphs of aluminium hydroxide have a large variety of structures, some features of their phase transitions can be understood by the concept that the H-bonding network interacts with the polyhedral network.

Keywords: hydrogen bonding network, high pressure, aluminium hydroxide

P08.13.82

Acta Cryst. (2008). A64, C443

Rationalizing polymorph stability using hydrogen bonding propensities

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Hydrogen bonding is crucial to structural stability in organic crystals, with impact widely reported in the pharmaceutical industry, and elsewhere [1,2]. Here, in an informatics-based approach, the relative stability of polymorphic structures is assessed based on the hydrogen bonding they exhibit. The implicit connection is made between most probable and energetically favourable interactions. The Logit Hydrogen Bonding Propensity method [3] is used to predict preferences for hydrogen bond formation. The method applies data derived from other known compounds to fit a probability model that creates propensity scores for hydrogen bonding atoms to interact in a crystal structure. This flexible method is parameterized to molecular, chemical and crystal structure descriptors. Once a model is derived, target 2D connectivity information at most is required to calculate propensity predictions specific to that target. In this presentation three contrasting drug-like systems will form an application of the method. The examples are modelled using crystal structure datasets from the Cambridge Structural Database (CSD) [4]. The method is also naturally extendable to use of additional e.g. internal company databases. Focus will be paid to statistical relevance and the influence of the model descriptors, which have physically meaningful interpretations. Relevant feedback into the hydrogen bond prediction from those parameters will also be discussed.

[1] Bernstein, J. (1993). *J. Phys. D: Appl. Phys.* 26, B66-76.

[2] Singhal, D & Curatolo, W (2003). *Adv. Drug. Del. Revs.* 56, 335-347.

[3] Galek, P.T.A., Fabian, L., Allen, F.H., Motherwell, W.D.S. & Feeder, N. (2007). *Acta Cryst.* B63, 768-782.

[4] Allen, F. H. (2002). *Acta Cryst.* B58, 380-388

Keywords: polymorphism, cambridge structural database, hydrogen bonding

P08.13.83

Acta Cryst. (2008). A64, C443-444

The hydrogen bonds in transition-metal oxalate complexes: Influence of Jahn-Teller distortion

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Single crystals of transition-metal oxalate complexes [M(C₂O₄)₂·2H₂O: M = Mn(II), Fe(II), Co(II), Ni(II)] were synthesized and analyzed by micro-Raman scattering spectroscopy; the O-H stretching bands of the complexes were located at 3324.7 cm⁻¹ for Mn(II), 3305.5 cm⁻¹ for Fe(II), 3324.6 cm⁻¹ for Co(II) and 3340.2 cm⁻¹ for Ni(II), respectively. The stretching wavenumber of O-H decreases considerably with increasing strength (decreasing length) of the hydrogen bond (Libowitzky 1999), and thus the Raman spectra indicated that Fe(II)-oxalate has the strongest hydrogen bonds among the present complexes. The crystal structure of Fe(II)-oxalate was analyzed using single-crystal X-ray diffraction method and refined to the agreement index R1 = 3.22 % calculated for 595 unique observed reflections. This oxalate crystallizes in the monoclinic system, space group C2/c, with unit cell dimensions of a = 12.011(11), b = 5.557(5), c = 9.920(9), β = 128.53(3), V = 518.0(8), and Z = 4. In the crystal structure, the alternation of oxalate anions [(C₂O₄)²⁻] and Fe(II) ions constitute one-dimensional chain structures parallel to [010]; water molecules (H₂O) form hydrogen bonds to link the chains, where