Compound 2 crystallizes in monoclinic space group C2/c with $a=11.697(3), b=18.756(4), c=8.549(4)Å, \beta=94.50(1)^{\circ}$ and Z=4. In the binuclear molecule 1 (Figure) each Cd(II) cation is hexacoordinated in the N₃O₃-environment in the shape of square bipyramid. Its basal plane is defined by a bidentate NioxH₂ molecule and two monodentate acetate anions; water molecule and bidentate bpetha ligand occupy the apical sites, bpetha being coordinated to a symmetry-related metal atom in a bridge function and provides Cd Cd separation of 13.86 Å. The water molecule in the apical position of the metal polyhedron demonstrates its cross-linking function being involved in hydrogen bonding with oxygen atoms of acetate anions via two $R_2^2(16)$ H-bonded cycles giving rise to the ordered layer where each binuclear unit is involved in 8 OH ... O hydrogen bonds and is linked with four symmetryrelated neighbors. The assembling of four molecules generates voids with the linear dimensions of *ca*. 11.16 x 22.24 Å, thus demonstrating the gradual increase in comparison with $[Cd_2(NioxH)_2(bpy)(CH_3COO)_4(H_2O)_2]$ (where bpy=4,4'bipyridine) [1], where the voids have dimensions of ca. 11.12 x 20.47 Å.

[1] Croitor L., Coropceanu E.B., Jeanneau E., Dementiev I.V., Goglidze T.I., Chumakov Yu.M., Fonari M.S., *Crystal Growth & Design*, Vol. 9, No. 12, 2009, p.5233-5243.

Keywords: cadmium compounds, coordination compounds, single-crystal X-ray crystallography

FA4-MS26-P13

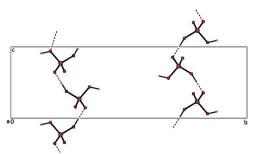
Hydrogen-Bonding Graph-Set Motifs in p-Aminobenzoic Acid Derivatives. <u>Amani Direm</u>, Nourredine

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The present work is devoted to the analysis and the comparison of hydrogen-bonding graphs in crystal structures of six previously studied p-aminobenzoic acid salts : p-Carboxyanilinium dihydrogenphosphate (I) [1], p-Carboxy-anilinium hydrogensulfate (II) [2], p-carboxyphenyl-ammonium dihydrogenmonophosphate monohydrate (III) [3], bis (p-carboxyphenylammonium) sulfate (IV), p-carboxy-phenylammonium perchlorate monohydrate (V) and p-carboxyphenylammonium nitrate (V) [4].

These structures are dominated by N-H...O and O-H...O hydrogen bonding networks between the p-carboxyphenylammonium cations and the ionic molecules. O-H...O interactions between anions are present in the dihydrogenphosphate derivatives (I) and (III) giving rise to a $C_2^{-2}(8)$ infinite chains. While intermolecular cation-cation H-bonds are only observed in the three compounds (IV), (V) and (VI).

The first-level graph set [5] of these compounds contains only D descriptors. Furthermore, the dihydrogenphosphate anions in (I) self-assemble to form supramolecular C(4) chains along the c direction (see Figure below). While, the high-level graph sets of all six structures comprise essentially ring and chain motifs.



The C(4) chain motifs running parallel to the [001] direction.

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FA4-MS26-P14

Polymorphic salts of the antibiotic 4-aminosalicylic acid. <u>M. Teresa Duarte</u>,^{a*} Vânia André,^a Dario Braga,^b Fabrizia Grepioni^b, ^aCentro de Química Estrutural, DEQB, Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisbon, Portugal, ^bDipartimento di Chimica "G. Ciamician'', Universita di Bologna, Via Selmi 2, 40126 Bologna, Italy E-mail:teresa.duarte@ist.utl.pt

4-aminosalicylic acid (ASA) is an antibiotic used in the treatment of tuberculosis. ASA has also shown to be safe and effective in the treatment of inflammatory bowel diseases [1]. Solvates, molecular salts and cocrystals of ASA have recently been disclosed and fully characterized by our group, using 6membered non-aromatic rings, such as dioxane, morpholine and piperazin [2] or bigger cyclic compounds, such as 4,4'bipyridine and DABCO [3] as crystal coformers. Furthermore, studies on salt formation were conducted and three polymorphic ammonia salts of ASA have been synthesized and characterized. Different synthetic routes and methods lead to different final forms: liquid-assisted grinding and gas-solid diffusion yield pure polymorphic form II while the forms obtained by solution techniques are highly dependent on solvent and solution preparation conditions. These crystal forms are also obtained using slurry technique. The crystal structures of the three forms were determined and further characterization has been performed by XRPD, DSC, TGA and HSM.

