Castro,[c] João D. B. Ribeiro,[b] Teresa M. R. Maria,[b] João Canotilho,[c] M. Ermelinda S. Eusébio,[b] *[a]CEMDRX, Physics Department, University of Coimbra, P-3004-516 Coimbra, (Portugal). [b]Department of Chemistry, University of Coimbra, P-3004-535 Coimbra, (Portugal). [c]Faculty of Pharmacy, University of Coimbra, P-3000-548, (Portugal)* E-mail: xelo@teor.fis.uc.pt

In the last decade, the synthesis of pharmaceutical co-crystals has emerged as an innovative strategy to successfully improve biopharmaceutical quality. Co-crystals are made up of two or more molecular neutral species linked by non-covalent bonds [1]. In this work the structure of a new equimolar co-crystal of (*S*)-naproxen, a nonsteroidal anti-inflammatory drug, and isonicotinamide is reported.

Single crystals were prepared by crystallization from 1:2.8 naproxen:isonicotinamide ethanolic solution at 2 ºC. The pure crystals melt at T_{fus} = 125 ºC.

In the new co-crystal structure the homosynthon amide···amide between two isonicotinamide molecules is retained, as in isonicotinamide polymorph I [2], and acid···$N_{aromatic}$ and amide···acid heterosynthons link naproxen to isonicotinamide.

[1] N. Blagden, M. de Matas, P.T. Gavan, P. York, *Advanced Drug Delivery Reviews* **2007**, *59*, 617-630. [2] C.B. Aakeröy, A.M. Beatty, B.A. Helfrich, M. Nieuwenhuyzen, *Crystal Growth & Design* **2003**, *3*, 159-165.

Keywords: co-crystal, NSAID, isonicotinamide

MS53.P30

Acta Cryst. (2011) A**67,** C570

Growth and Characterization of p-CADHP and p-CAHS Single Crystals

Amani Direm, Wahiba Falek, Zina Boutobba, et Nourredine Benali-Cherif, *Laboratoire des Structures, Propriétés et Interactions Inter Atomiques (LASPI2A). Institut des Sciences Exactes, Technologie et Informatique. Centre Universitaire ''Abbes Laghrour'', Khenchela 40000, (Algérie).* E-mail: Amani_Direm@yahoo.fr

Hybrid materials including dihydrogenmonophosphate and bisulfate anions have received increasing attention [1, 2] owing to their interesting ferroelastic [3], NLO [4], phase transitions properties [5] and their potential application in pharmaceutical industry [6].

In order to contribute to the systematic investigation of the hydrogen bonding in those compounds, we have synthesized two new hybrid materials : p-Carboxyanilinium dihydrogenphosphate [7], p-CADHP and p-Carboxyanilinium hydrogensulfate [8], p-CAHS.

The packing of both compounds show alternating anionic ($H_2PO^-_4$ or HSO^-_4) and cationic ($COOH\text{-}C_6H_4\text{-}NH^+_3$) moieties which are linked together by a three-dimensional hydrogen bonding network. In order to study different interactions between hydrogen bonds present in our compounds, we have applied the graph theory [9]. The graph set analysis of hydrogen-bond patterns present in our compounds gives rise to binary graph sets involving rings R and infinite chains C.

[1] M.T. Averbuch-Pouchot, A. Durif, J.C. Guitel. *Acta Cryst*, **1988,** *C44*, 99-102. [2] N. Benali-Cherif, F. Allouche, A. Direm, L. Boukli-H-Benmenni, K. Soudani,. *Acta Cryst*, **2007,** *E63*, 2643-2645. [3] J. Fábry, V. Petrícek, I. Cisarova, J. Kroupa, *Acta Cryst*, **1997,** *B53*, 272-279. [4] J. Pécaut, Y. Le Fur, R. Masse, *Acta Cryst*, **1993,** *B49*, 535-541. [5] N.L. Speziali, G. Chapuis. *Acta Cryst*, **1991,** *B47*, 757-766. [6] J.R. Rubin, P. Swaminathan, M. Sundaralingam .*Acta Cryst*, **1992,** *C48*, 379-382. [7] N. Benali-Cherif, A. Direm, F. Allouche, S. Soudani *Acta Cryst*, **2007,** *E63*, 2272–2274. [8] N. Benali-Cherif, A. Direm, F. Allouche, L. Boukli-H-Benmenni, S. Soudani *Acta Cryst*, **2007,** *E63*, 2054–2056. [9] J. Bernstein, R.E. Davis, L. Shimoni, N.–L. Chang, *Angew. Chem. Int. Ed. Engl*, **1995,** *34*, 1555-1573. [10] L.J. Farrugia. *J. Appl. Cryst*, **1999,** *32*, 837-838.

Keywords: hybrid compounds, single cristals, hydrogen bonds.

MS53.P31

Acta Cryst. (2011) A**67,** C570

Crystal structure of Cytosinium–hydrogen maleate–cytosine

Wahiba Falek, Amani Direm, Zina Boutobba, et Nourredine Benali-Cherif, *Laboratoire des Structures, Propriétés et Interactions Inter Atomiques (LASPI2A). Institut des Sciences Exactes, Technologie et Informatique. Centre Universitaire ''Abbes Laghrour'', Khenchela 40000, (Algérie).* E-mail: falek_wahiba@yahoo.fr

The pyrimidine base, Cytosine, leads to the nucleoside cytidine and its corresponding nucleotide: cytidine 5'-monophos-phate. It may be found in very small quantities as a post-modified form, 5-methylcytosine, in certain nucleic acids such as in tuberculinic acid. More recently, 5-fluoro-cytosine (5-FC) has been used as a prodrug in suicide gene therapy of cancer with the crystal structure of bacterial cytosine deaminase (bCD).

The crystal structures of cytosine [1] and cytosine monohydrate were determined many years ago. Many inorganic cytosinium salts have been previously synthesized: chloride [2], nitrate [3] and dihydrogenphosphate [4,5].

Cytosinium salts of organic acids are also common, the structures of a number of these including trichloroacetate, Cytosinium 3,5-dinitrosalicylate [6] and hydrogen maleate [7] have been recently reported.

[1] D.L. Barker, R.E. Marsh *Acta Cryst*. **1964,** *17*, 1581–1587. [2] N.S. Mandel *Acta Cryst*. **1977,** *B33*, 1079–1082. [3] A. Cherouana, K. Bouchouit, L. Bendjeddou, N. Benali-Cherif, *Acta Cryst*. **2003,** *E59*, o983–o985. [4] M. Jasko ´ lski, *Acta Cryst*. **1989,** *C45*, 85–89. [5] M. Bagieu-Beucher, *Acta Cryst*. **1990,** *C46*, 238–240. [6] G. Smith, U.D. Wermuth, P.C. Healy,. *Acta Cryst*. **2005,** *E61*, o746–o748. [7] T. Balasubramanian, P.T. Muthiah, W. T. Robinson, *Bull. Chem. Soc. Jpn*, **1996,** *69*, 2919–2922.

Keywords: transfer of protons, single-crystal X-ray study, hydrogen bonds.

MS53.P32

Acta Cryst. (2011) A**67,** C570-C571

Crystal structure and hydrogen graph motifs in Anilinium hydrogensulfate

Zina Boutobba, Amani Direm, Wahiba Falek et Nourredine Benali-Cherif, *Laboratoire des Structures, Propriétés et Interactions Inter Atomiques (LASPI2A). Institut des Sciences et Techniques. Centre Universitaire ''Abbes Laghrour'', Khenchela 40000, (Algérie).* E-mail: zinab.zina@hotmail.fr

Hydrogen bonding is one of the most versatile noncovalent forces in supramolecular chemistry and crystal engineering [1]. Therefore, in the past decades assessment of discrete hydrogen bonding patterns had received great attention [2] because of its widespread occurrence in biological systems.

The aim of this paper is to discuss hydrogen patterns assuring the connection between anilinium and hydrogensulfate entities and to establish their different graph-set motifs [3]. Bis (anilinium hydrogensulfate) is one of the hybrid compounds, rich in H-bonds [4-5], which could have potential importance in constructing sophisticated assemblies from discrete ionic or molecular building blocks due to the strength and the directionality of hydrogen bonds [6].

Recently, similar structures containing anilinium cations have