

MS21-P03

Intermolecular interactions in the cyanuric acid dihydrate on the basis of experimental charge density

Barbara Gruza¹, Paulina Dominiak¹, Damian Trzybiński¹

1. Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Warsaw, Poland

email: barbara.gruza@student.uw.edu.pl

The structure of anhydrous cyanuric acid, its intermolecular interactions and thermal parameters have been described in 1971 by G.C. Verschoor [1]. In the following years, i.a., strong donor-acceptor interactions connected with occurrence of N–H and C=O functional groups were investigated by T.C. Lewis [2] for the anhydrous form as well for readily formed solvates and co-crystals. Possibility of satisfying all the hydrogen bonding functionalities and its influence on the crystal structure were verified.

I am presenting experimental charge density analysis for the cyanuric acid dihydrate. Electron density distribution was described with Hansen and Coppens pseudoatom model. Crystal structure, occurring interactions and vibrational parameters were compared with periodic theoretical calculations both for dihydrate and anhydrous form. Molecular interactions with water molecules were also justified basing on the TGA/DSC measurements.

References:

[1] Verschoor, G.C. and Keulen, E. (1971). *Acta Cryst.* B27, 134.

[2] Lewis, T.C. et al. (2005). *Cryst. Growth Des.* 5(3), 983–993

Keywords: cyanuric acid dihydrate, intermolecular interactions, charge density

MS21-P04

Hierarchy and the nature of intermolecular interactions in systems containing aromatic N-heterocyclic rings

Tomasz Sierański¹

1. Lodz University of Technology, Institute of General and Ecological Chemistry, Łódź, Poland

email: tomasz.sieranski@p.lodz.pl

Non-covalent interactions involving N-heterocyclic aromatic rings have recently received greater attention. They play an important role in many chemistry-related fields such as structures of biomolecules, the reactivity of molecules, crystal engineering, molecular recognition, and nanoengineering. Such rings, because of their distinctive electronic properties, are involved in different interaction patterns including π -stacking and hydrogen bonds. Hence, they are considered as useful recognition elements in many biological systems and became key components in most known drug molecules [1, 2].

Though some significant progress has been definitely made in the study of interactions involving N-heterocycles, most studies only focus on analyzing of stationary geometries and say nothing of a whole range of many other configurations. Accurate potential energy surfaces (PES) of such systems are not available and it is impossible to see how the stability of a particular system changes along with various geometrical parameters. Such maps, if they were present, would literally give a new way to look into the interactions patterns that may be formed.

For this reason, the extremely extensive analysis of potential energy surfaces of model N-heterocyclic dimers has been performed. The interaction energies of hundreds of thousands of dimers have been calculated. As the studied N-heterocycles the following ones have been selected: pyrrole, purine, pyridine, imidazole, pyrazole, 1,2,3-triazole, and 1,2,4-triazole. Since the interaction energies of a large number of systems were to be calculated, all the calculations have been carried out using a dispersion-corrected density functional. Other calculations, such as natural bond orbital and energy decomposition, have also been applied. The obtained results were then related to the statistical analysis made on the data gathered from Cambridge Structural Database [3].

The appliance of multidimensional analysis provides much deeper insight into the “landscape” of the interaction energies of the particular systems and enables one to see “a bigger picture” of what really occurs. The performed study, involving the combination of many different methods, has revealed the complexity of the formed intermolecular interactions. Apart from providing a “literal new look” into the present interaction patterns, another picture has emerged. Intermolecular interactions, especially stacking, present in the studied N-heterocycles, are seen” as a combination of many different sources of the interaction energy. The presented results may be a key importance in a prediction of crystal structures and may find a use in modeling of a crystal possessing desired properties.

Participation in this conference is financed by National Science Centre, Poland, 2017/01/X/ST4/00952

References:

-
- [1] Sierański, T. (2017) *J. Mol. Model.* 23, 338-353
 [2] Kruszynski, R. & Sierański, T. (2016) *Cryst. Growth Des.* 16, 587–595
 [3] Groom, C. R. et al. (2016) *Acta Cryst.* B72, 171-179
-

Keywords: intermolecular interactions, density-functional theory, cambridge structural database

MS21-P05

Understanding disorder in a $Z'=4$ structure with computationally cheap tools

Christophe Vande Velde¹, Wim Van Beek², Kourosh Abbaspour Tehrani²

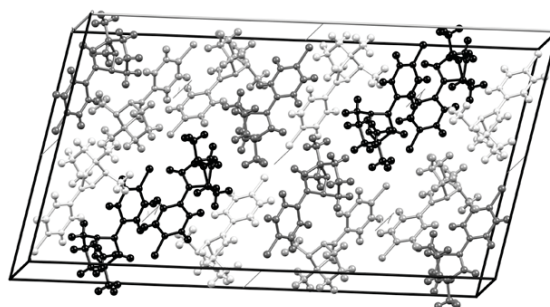
1. University of Antwerp, Faculty of Applied Engineering, Advanced Reactor Technology, Antwerpen, Belgium
2. University of Antwerp, Department of Chemistry, Orsy, Antwerpen, Belgium

email: christophe.vandavelde@uantwerpen.be

As computationally cheap tools have recently become available to better understand crystal packing, we have applied the CE-B3LYP method as implemented in Crystal Explorer 17 [1] to an interesting structure with $Z'=4$, and whole molecule disorder in each of the four molecules in the asymmetric unit.

The structure itself contains many subtle features which are interesting to discuss all by themselves, but we are interested to see whether the energy calculations will aid in providing a reasonable explanation why the structure crystallizes as it does.

The average nature of the coordinates obtained from the crystallographic experiment will obviously be the largest challenge, as it conflicts with the basic premise of a calculation that does not optimize the atomic coordinates before calculating energies.



References:

-
- Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A., (2017) *CrystalExplorer17*, University of Western Australia. <http://hirshfeldsurface.net>
-

Keywords: whole molecule disorder, crystal explorer, high Z'