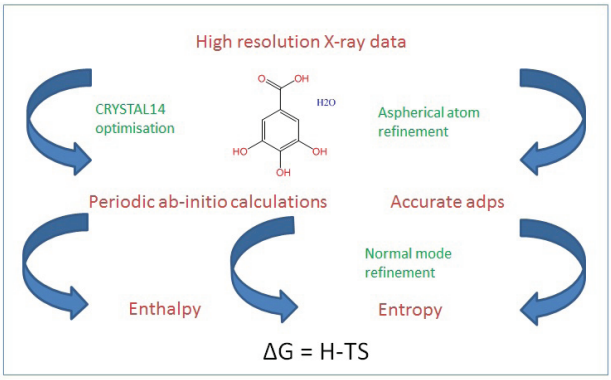

Figure 1.

Keywords: high resolution X-ray diffraction, periodic ab-initio calculations, gallic acid

MS28-P6 Experimental electron density of cytosinium chloride in crystalline state

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Comprehensive goal of my work is to analyze charge density distribution and intermolecular interactions between nucleobases in crystalline state. It is crucial to know precisely potential of this molecules to form particular type of interactions, especially in the context of RNA structure predictions. Presented work is focused on cytosinium chloride.

Single crystals of cytosinium chloride were obtained by slow evaporation of solvent from mixture of cytosine and 4-thiouracil dissolved in water with small amount of hydrochloric acid. High resolution (0.5 Å) X-ray diffraction data were collected on monocrystal diffractometer at 90 K. The data were next subject to data reduction, structure solution, independent atom model refinement and finally multipolar refinement procedures. Several strategies of data reduction and multipolar refinement were tested to obtain the best model of crystal electron density.

Cytosine chloride crystallizes in $P2_1/n$ group in monoclinic system. Unit cell consists of one protonated cytosine molecule and one chloride ion located almost in the same plane. Cytosine forms dimers through double hydrogen bond between O2 and N3 atoms (see Figure 1). Hydrogen bonds, besides cation – anion interactions, play important role in building the crystal structure and determination of crystal lattice energy.

I will present comparison of chosen data reduction and refinement strategy with others and discuss which parameters decided on its superiority. The second part will be dedicated to more profound description of cytosine chloride structure and evaluation of intermolecular interactions based on charge density.

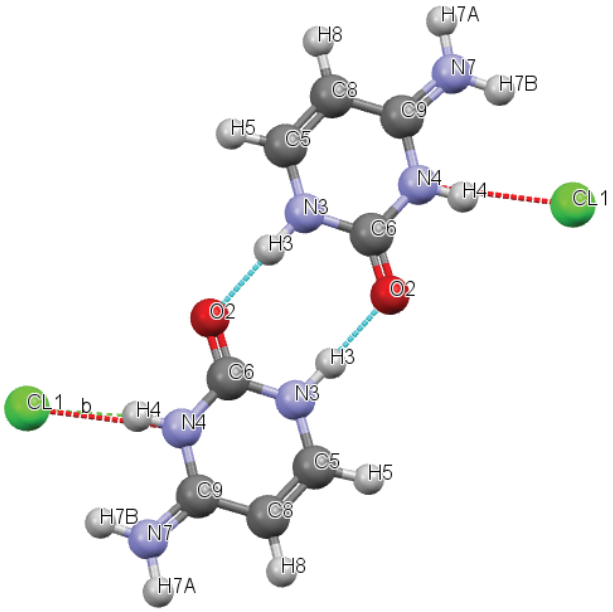

Figure 1. Cytosine dimer

Keywords: charge density, cytosine, hydrogen bonds

MS28-P7 Experimental deformation electron density studies of (-)-cytisine and its simply salts

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The interest in cytisine, a naturally occurring alkaloid, and related compounds has been growing recently, stimulated by the realization of their biological activity. (-)-Cytisine (Scheme 1) is an alkaloid, naturally occurring in plants of the *Leguminosae* family, which interacts with nicotine-acetylcholine receptors and has been applied in investigation of the central nervous system and in anti-nicotine therapy. This alkaloid has been found to moderately increase the concentration of dopamine alleviating the symptoms of nicotine deprivation (the so-called nicotine hunger). Therefore, cytisine has been employed in nicotine withdrawal therapy in the form of Tabex® (Eastern and Central Europe), Chantix® (USA) or Champix® (Canada and Europe) formulations. According to literature data, cytisine derivatives have been tested also for their use in the treatment of Alzheimer's and Parkinson's diseases. In this communication we will present the details of electron density distribution in the cytisine and some of its salts (chloride, nitrate etc.), determined by means of high-resolution X-ray diffraction and described within Hansen-Coppens multipolar model. The deformation electron density of the alkaloid and its salts will be compared and the changes occurring upon protonation will be discussed. Additionally, the topological analysis of the electron density distribution will be applied to describe and analyze the details of the bonds and intermolecular interactions in the crystal structures. This is a part of the wider project which is supposed to compare the biological activity (defined by the ability of making complexes with the DNA fragments) of the known and newly synthesized cytisine derivatives, with the details of the electron density distribution, determined by means of high resolution X-ray diffraction. The result should be the library of the multipolar expansion coefficients for cytisine neutral molecule and cytisinium cations, applicable in similar studies of more complicated derivatives, dimers etc., for which the complexation studies will be also performed. This work is supported by a grant from the Polish National Science Center, 2013/11/B/ST5/01681 (to MK).