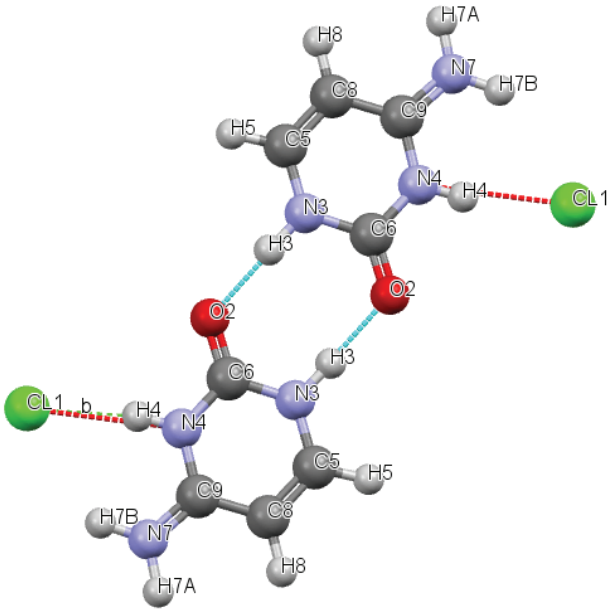

Figure 1. Cytosine dimer

Keywords: charge density, cytosine, hydrogen bonds

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

Maciej Kubicki[1], Agata Owczarzak[1]

1. Faculty of Chemistry, Adam Mickiewicz University in Poznan, Poland

email: mkubicki@amu.edu.pl

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).

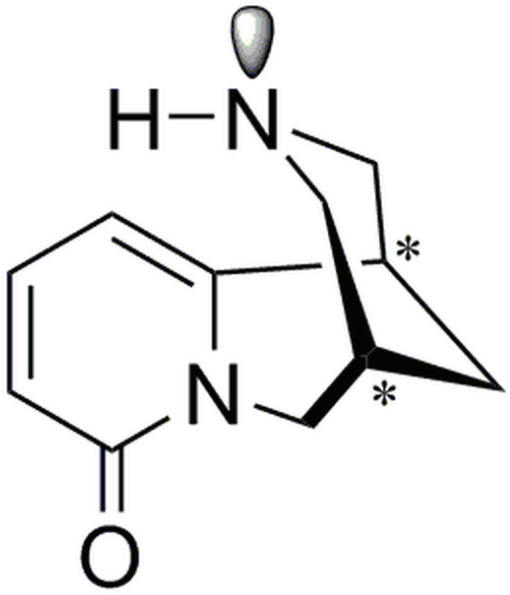

Figure 1. Scheme of (-)Cytisine

Keywords: cytisine, salts, electron density, topological analysis

MS28-P8 The influence of data collection quality on the multipolar parameters of sulfur and chlorine atoms in 5-chloro-2-mercaptobenzimidazole (CMBZT)

Anita M. Owczarzak[1], Maciej Kubicki[1]

1. Adam Mickiewicz University

email: aniow@amu.edu.pl

During our studies of charge density distribution in thioamide compounds, we very often were faced with the evidence of electron density depletion around the nuclei of sulfur atoms , which can be observed as a certain ring in the deformation charge density maps (fig 1.). As such a “ring effect” is observed regularly in charge density studies not only for sulfur but also for other heavier atoms (chlorine, bromine ect.) we decided to look more closely at this subject.

The high resolution data has been collected using Xcalibur diffractometer with Eos detector at 100K for two 5-chloro-2-mercaptobenzimidazole (CMBZT) crystals of deliberately different quality,. The structures have been refined using Hansen-Coppens multipolar model [1] implemented in MoPro software [2], using (almost) exactly the same procedure for both cases. In a communication we will focus on a comparison of the multipole parameters and topological analyses of CMBZT compound. In addition, the influence of cutting off the data on the results of refinement has been also studied.

[1]Hansen, Coppens, P.*Acta Crystallographica Section A* **34,** 909–921 (1978).

[2]Jelsch,Guillot, Lagoutte, Lecomte, *J. Appl. Cryst.* 38,38-54