

**MS18-P7** **Charge Density Study on the Quinazoline Derivative Crystals** Akmal Tojiboev<sup>1</sup>, Ulli Englert<sup>2</sup>, Kambarali Turgunov<sup>3</sup> <sup>1</sup>Department of Physic, Namangan State University, Uychi str., 316, Namangan-160100, Uzbekistan. <sup>2</sup>Institute of Inorganic Chemistry, RWTH Aachen University, Landoltweg 1, Aachen D-52056, Germany. <sup>3</sup>S.Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences Uzbekistan, Mirzo Ulugbek str. 77, Tashkent - 100170, Uzbekistan.  
E-mail: a\_tojiboev@yahoo.com

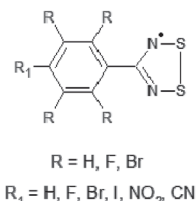
Quinazoline represents the heterocyclic core of natural alkaloids and pharmaceutically active ingredients [1-3]. We have made a charge density study of derivatives quinazoline. 2,3-Trimethylene-3,4-dihydroquinazoline shares the heterocyclic core with natural compounds and synthetic drugs. The hydrochloride of the compound forms excellent crystals of a dihydrate which have allowed to collect high-resolution X-ray diffraction data and obtain the experimental charge density. The solid may be understood as built up from pairs of heterocyclic cations and chloride anions; a direct hydrogen bond links the halide to the formally cationic pyrimidine NH group. The hydrate water molecules interact with the anions, forming an infinite chain along the crystallographic a axis between stacks of the heterocyclic cations. Based on the experimental charge density, a dipole moment of 16.1 Debye is calculated for a pair of hydrogen-bonded quinazolinium cation and chloride anion in the extended crystal structure.

- [1] S.Johne; Pharmazie, **36**, 583 (1981).  
[2] M.V.Telezhenetskaya, S.Yu.Yunusov; , **6**, 731 (1977).  
[3] S.Yu.Yunusov, N.Tulyaganov, M.V.Telezhenetskaya, F.Sadritdinov, Kh.Khashimov; USSR Patent No. 605614, Anticholinesterase agent, Byull. Izobret.(Russ.), 17 (1978).

**Keywords: Quinazoline, electronic structure, high-resolution X-ray diffraction, charge density, topological analysis.**

**MS19-P1** **Dithiazyl Radicals - Structures and Charge Densities of their Crystals and Co-Crystals.** Krzysztof Wozniak<sup>1</sup>, Krzysztof Kości<sup>1</sup>, Sean W. Robinson<sup>2</sup>, Sławomir Domagala<sup>1</sup>, Delia A. Haynes<sup>2</sup> <sup>1</sup>Department of Chemistry, University of Warsaw, Warszawa, Poland. <sup>2</sup>Department of Chemistry and Polymer Science, Stellenbosch University, Republic of South Africa.  
E-mail: kwozniak@chem.uw.edu.pl

Purely organic systems can exhibit conductivity, superconductivity or magnetically ordered phases - properties usually thought as restricted only for crystals containing metallic centres (Cu, Mn, etc.). One of the most intriguing groups of such systems is a family of thiazyl radicals.



These radicals are chemically stable, so they can be arranged in closely packed structures. Relatively high electrostatic polarization allows for inter- and intramolecular S...N interactions. In the crystal phase, the thiazyl group often co-exists with a phenyl molecular fragment, which further stabilizes the crystal lattice by introducing an intermolecular  $\pi$ ... $\pi$  aromatic interactions (e.g. phenyl...perfluorophenyl stack interaction). The spin structure of these compounds is strongly coupled to the crystal structure. One can then try to adjust the magnetic properties (e.g. FM-AFM ordering) of such systems by small changes of structural parameters (e.g. distances between molecules in stack). This and other intriguing properties suggest that the dithiazyl radicals are promising candidates for the construction of molecular devices. No experimental electron density distribution of such system in the crystal phase has been accomplished so far. The scope of the work was to determine the quantitative electron density distribution and its parameters ( $\rho$  and  $\Delta\rho$  at the critical points, integrated charges, etc.) for the three very interesting model crystals of thiazyl radicals belonging to dithiadiazolyl family (chosen examples are depicted below). The Hansen-Coppens multipole expansion of electron density model was refined against the high resolution ( $\sin\theta / \lambda > 0.7\text{\AA}^{-1}$ ) X-ray diffraction data to obtain the best models of the electron density distribution in given crystals. These models were then used to calculate quantitative electron density properties using the Bader's QTAIM theory such as critical points parameters ( $\rho_{CP}$ ,  $\Delta\rho_{CP}$ , bond paths), atomic basins or integrated electron density parameters (integrated charges, atomic multipoles and volumes, etc). The obtained results and detailed analysis of dithiadiazolyl radicals should hopefully help in a better understanding of the magnetic phenomena in organic systems. In spite of that obtaining a reliable model of charge density distribution in a highly reactive radical crystal is a difficult task, such a model was successfully refined. Our results concerning critical points and intra- and intermolecular bonds and bond paths are shown on the pictures below. Preliminary analysis of the properties of  $\rho$  at the critical points and electrostatic potential distribution in the H-DR leads to a hypothesis that the T - shape packing of radical dimers induces a charge transfer between the two independent dimers. Details of this charge transfer are at present subject of our studies.

**Keywords: charge density; dithiazyl radicals; co-crystals**