Poster Presentation

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Charge density studies of nucleobase analogues - the case of DAP and isocytosine

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Nucleobases belong to purine and pyrimidine family and constitute a biologically crucial group of compounds thank to their relation to nucleic acids. Specific interactions between these moieties are responsible for maintaining a proper structure of DNA, namely: hydrogen bonding and π-π stacking interactions (between aromatic ring fragments). Furthermore, many modifications of natural nucleobases serve as drugs, but some could be extremely harmful. In view of the above, investigating the properties of analogues of nucleobases may contribute to our knowledge about nucleic acid properties in general and give an opportunity to find novel ligands binding to DNA, what is essential for drug design. Within this project two modified nucleobases were examined: 2,6-diaminopurine (DAP) and isocytosine (iC). DAP is a derivative of the adenine and iC is an isomer of cytosine. These compounds do not appear naturally in nucleic acids, however, can be used to compare Watson-Crick pairing in DNA and pairing of alternative bases. High resolution X-ray diffraction experiments were carried out to obtain appropriate data for charge density analysis. A comprehensive study of crystal packing and energetic features of the analysed systems was conducted. The nature of intermolecular interactions, structural motifs and crystal packing was analysed via Hirshfeld surface analysis [1], charge density distribution examination, QTAIM (Quantum Theory of Atoms in Molecules) [2] and theoretical calculations (gas phase dimers and periodic). Implications of the observed interactions for biological systems are discussed. This study was supported by the Polish Ministry of Science and Higher Education within the Diamond Grant No DI 2011012441.

[1] *M. Spackman, D. Jayatilaka, CrystEngComm, 2009, 11, 19–32,* ***[2]*** *R. Bader, Atoms in Molecules: A Quantum Theory, Oxford University Press, USA, 1994*

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