s7.m25.p5 **Characterization of (*E*)- and (*Z*)-ajoene inclusion complexes with α-, β-, γ- and permethylated-β-cyclodextrin using PXRD, single crystal X-ray diffraction and thermal analysis.** Vincent J Smith, Mino R Caira, Roger Hunter and Susan A Bourne, *Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa. E-mail: xrayvin@science.uct.ac.za*

Keywords: Isostructurality; X-ray structures; Cyclodextrins

Cyclodextrin inclusion studies with (*E*)- and (*Z*)-ajoene (4,5,9-trithiadodeca-1,6,11-triene 9-oxide), isolated from garlic (*Allium Sativa, L.*), yielded inclusion complexes with the following cyclodextrins: α-, β-, γ-cyclodextrin and TRIMEB (heptakis(2, 3, 6-tri-O-methyl)-β-cyclodextrin). Complexes with α-, β-, and γ-cyclodextrin were characterized with the aid of powder X-ray diffraction (PXRD) while the complexes with TRIMEB were subjected to characterization by thermal analysis (TGA, DSC and HSM) as well as PXRD and single crystal X-ray diffraction. For the complexes with the native cyclodextrins PXRD was used to establish complex formation. Matching of the PXRD diagrams with a series of published patterns based on isostructural cyclodextrin inclusion complexes allowed unequivocal assignment of complex space groups [1]. In the case of TRIMEB, DSC revealed a melting onset of 143.8°C for TRIMEB·(*E*)-ajoene·0.5H_2O (**1**) and 140.5°C for TRIMEB·(*Z*)-ajoene (**2**). Single crystal X-ray diffraction showed that for 1 the crystals are orthorhombic with space group $P2_12_12_1$ while for 2 the crystals are monoclinic and the space group is $P2_1$. It also revealed the distinctly different modes of inclusion of the guests, (*E*)- and (*Z*)-ajoene as well as details of the binding of their stereoisomers. These results represent the first definitive thermal and structural data for cyclodextrin inclusion complexes of a major, pharmacologically active component from garlic.

[1] Caira M. R. *Rev. Roum. Chim*., 2001, **46**, 371-386.

s7.m26.p1 **The Hydrogen Bonding Network in a New Purine Hybrid Compound.** L. Benguedouar[a] and N. Benalicherif[b], [a]*Department of Biology, Faculty of Sciences, University of Jijel. 18000 Algeria.* [b]*Institut des Sciences Exactes, des Technologies et de l'Informatique Centre Universitaire de Khenchela, 40000 Algeria. E-mail: benguedouar.lamia@caramail.com*

Key words : Hybrid compounds; Hydrogen-bonding; Weak bonds

The study of functional and structural properties of the biologic macromolecules can be investigated by the use of hybrid compounds which mimic the interactions between the macromolecules in vivo.

The present study is part of a research axis on new hybrid compounds based on purine bases and various mineral acids [1,2], the crystal structure determination of these molecule and especially the hydrogen-bonding engineered by the different entities (fig.1), can be used in the comprehension of the active site interactions of enzymes and their cofactors the substrates.

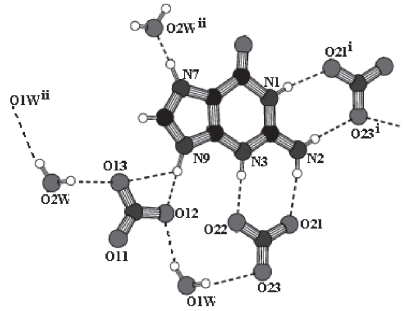

Fig.1 Intramolecular hydrogen bonding

In this way, we have synthesized the new hybrid compound Guaninium Dinitrate Dihydrate, using a mixture of purine base guanine and nitric acid in water. This compound crystallizes in the $P2_1/c$ space group of the monoclinic systemwith the cell parameters a = 6.6340(4)Å, b = 11.9800(5)Å, c = 15.8040(3)Å and β= 91.010°

The crystal structure is solved with SIR 92 program. The refinement of the structure leads to R(F) = 4.5% and S = 1.07. The structure consists of layers of guaninium ions, nitrate anions and water molecules linked by strong hydrogen bonds. These layers are parallel to the diagonal of the ac plane and liked the cohesion of the crystal structure is ensured by weak Van Der Waals bonds between the organic cations and water molecules of the adjacent layer.

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