

m27.p04

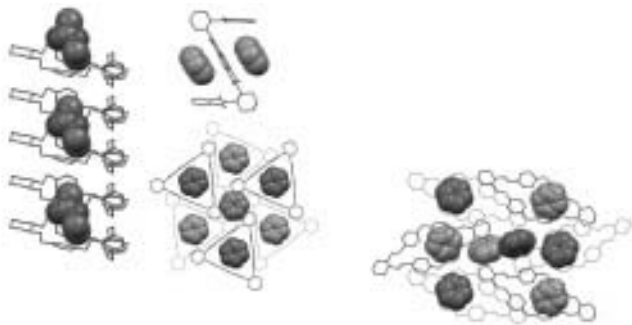
New Class of Chiral, Inclusion Forming Crystals with Host Molecules Derived from trans-1,2- Diaminocyclohexane

Urszula Rychlewska, Agnieszka Plutecka

Faculty of Chemistry, Adam Mickiewicz University Grunwaldzka 6, 60-780 Poznań, Poland

Keywords: inclusion, macrocycles, foldamers

Inclusion properties of several crystals containing as host molecules trans-1,2-diaminocyclohexane units connected by various types of aliphatic and aromatic spacers will be demonstrated [1]. The chiral host molecules are present either in a form of S-shaped chains, involved in face-stacking interactions with aromatic guest molecules, or in a form of rhombs or triangles, only very weakly interacting with the guests. Macrocyclic host molecules display versatile types of inclusion, which involve molecular inclusion, one-dimensional stack with chain molecules as guests in channels passing through the macrocyclic cavity, and various modifications of channel type inclusion with planar aromatic molecules as guests. Provided examples illustrate that the type of inclusion depends not only on the type of included solvent molecule(s) but also on the type of spacer in the host molecule and the host rigidity. The results presented highlight the potential of this new class of molecules as flexible hosts for various solvent molecules.



[1] Samples for X-ray analysis have been obtained from prof. Jacek Gawroński, Dept. of Organic Stereochemistry Adam Mickiewicz University, Poznań, Poland.

m27.p05

A new salt of halofantrine

Agata Semeniuk, Agnieszka Niedospial, Justyna Kalinowska-Fluscik, Barbara J. Oleksyn

Faculty of Chemistry, Jagiellonian University, Krakow, orlow@chemia.uj.edu.pl

Keywords: halofantrine, antimalarials, crystal structures

The crystal structure of methanol solvate of racemic halofantrine (Hf) acetate monohydrate, $C_{26}H_{31}Cl_2F_3NO^+ \cdot CH_3COO^- \cdot CH_3OH \cdot H_2O$, has been investigated in order to establish the effect of the anion and co-crystallizing molecules on the Hf conformation.

Crystal data: $a=9.6452(8)\text{\AA}$, $b=11.7239(11)\text{\AA}$, $c=14.6265(16)\text{\AA}$, $\alpha=103.138(3)^\circ$, $\beta=102.340(3)^\circ$, $\gamma=92.625(3)^\circ$, P1, Z = 2, V = 1.295g/cm³

The conformation of Hf molecule is similar to that observed by Karle&Karle [1] in the racemic Hf hydrochloride, but it differs slightly from that determined in (-)-Hf hydrochloride. The water and methanol molecules, as well as acetate anion, form intermolecular hydrogen bonds with the Hf cations, stabilizing their conformation. H₂O, CH₃OH and CH₃COO⁻ are also linked by hydrogen bonds.

It is interesting that despite the hydrogen bonding system, which remarkably differs from that in halofantrine hydrochlorides [1, 2], the molecular conformation of Hf is relatively well preserved. This contribution has been supported by grant of Polish Ministry of Education and Science: 1 T09A 06930

[1] Karle J.M, Karle I.L *Acta Cryst.* 1989 (C45), 1248.

[2] Karle J.M. *Antimicrobial Agents and Chemotherapy* 1997 (41), 791.