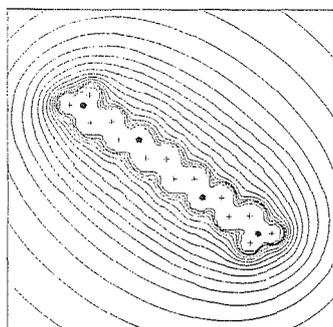


PS05.06.07 THE ELECTROSTATIC POTENTIAL FOR SPERMINE PHOSPHATE HEXAHYDRATE. A. E. Cohen, J. R. Ruble, and B. M. Craven, Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260

Spermine, a water soluble, tetra-basic polyamine, is widely found in nature and may function to stabilize DNA secondary structures. The crystal structure of spermine phosphate hexahydrate ($[(C_{10}H_{30}N_4)^{4+} 2[HP0_4]^{-2} \cdot 6H_2O]$) was first determined by Iitaka and Huse (1965) from X-ray Weissenberg photographic data. Their proposed hydrogen-bonding has been confirmed by low temperature neutron diffraction (Cohen, Klooster & Craven). Now a high resolution X-ray data set has been collected at 125 K using Mo K α radiation and the charge density distribution has been determined. The map of the electrostatic potential of the isolated spermine cation (below) shows that the electrostatic potential is an almost uniformly electropositive cylinder. The spermine cation while attracted to the negatively charged phosphate groups would have freedom to slide along the major groove of native DNA.



The electrostatic potential of the isolated spermine cation is shown. The nitrogen atoms are labeled with black dots. Contours are at intervals of 0.05 e \AA^{-1} .

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PS05.06.08 DIMORPHISM OF THE ALKALOID COLCHICINE HYDRATE. L. Yu. Izotova, K.M. Beketov, B.T. Ibragimov, M.K. Yusupov. Institute of Bioorganic Chemistry, H. Abdullaev str., 83, Tashkent, 700143, Uzbekistan, e-mail root@ibc.tashkent.su

Alkaloid colchicine having different types of the biological activity forms two inclusion compounds with water depending on crystallization conditions.

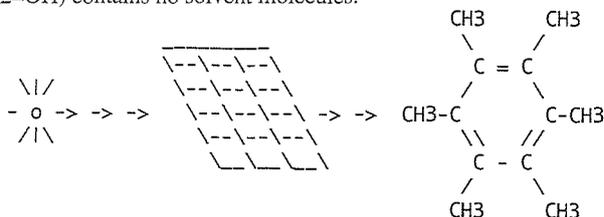
First of them is dihydrate and it was obtained nearly twenty years ago [1]. X-ray structure analysis of colchicine was carried out namely on this host-guest complex. In the colchicine dihydrate hydrogen bonds of the host-host, host-guest and guest-guest type are existed. Colchicine and water molecules are linked to bilayers by these H-bonds.

We have obtained monohydrate of colchicine and solved its crystal structure. Crystal data are: orthorhombic, P212121, a=9.14, b=13.27, c=17.94 Å, Z=4 and R=0.06 for 2100 reflections. The conformation of colchicine molecule is not distinct from one in dihydrate. Water molecules are connected with three alkaloid molecules by means of H-bonds that gives rise to H-bonded three dimensional network. In the result of this a solubility and melting point of monohydrate is substantially different from ones in other hydrate.

I. Lessinger L., Margulis T.N. Acta Crystallogr.

PS05.06.09 CRYSTAL AND MOLECULAR PACKING OF SIX RYANIA ALKALOIDS: THE PREDOMINANCE OF A MULTI-DIMENSIONAL H-BOND NETWORK. Marc Drouin, Marco Dodier and Luc Ruest. Département de Chimie, Université de Sherbrooke, Sherbrooke, Québec, Canada, J1K 2R1.

Originally extracted from *Ryania speciosa* Vahl plant, the natural insecticide ryanodine is also a calcium release channel modulator in mammalian muscle. In order to identify structural features which are necessary to keep biological activity, several polyhydroxylated diterpene compounds were isolated from the plant or synthesized upon testing their biological activity. Their respective crystal structures were elucidated to confirm their stereochemistry and exact molecular structure. The general aspect of the molecules show a highly polar face with many OH groups opposite to a relatively hydrophobic face. The molecular packing are dominated by a two- or a three-dimensional hydrogen bonding network with many intra- and intermolecular hydrogen bonds. Elaborate crystal packing are presented, highlighting minor changes in molecular structures inducing major differences in H-bond network systems. As example, the cinnzeylanol compound (R1=OH, R2=H) display a highly disordered water channel whereas 2-deoxy 3-epiryranodol (R1=H, R2=OH) contains no solvent molecules.



Other Synthetics

PS05.07.01 STRUCTURE AND CONFORMATION OF SOME SULFONE DERIVATIVES. Y.S. Chen, S. Narasinga Rao, Elizabeth J. Holt*, K.V. Narayana Raju and M. Krishnaiah*, Department of Physics, University of Central Oklahoma, Edmond, Oklahoma, Dept. of Chemistry, Oklahoma State University, Stillwater, Oklahoma*, Dept. of Physics, Sri Venkateswara University, Tirupati, India*.

Sulfones are antibacterial and antifungal agents. The antifungal activity of some unsaturated sulfones has been found to be dependent upon substituent and stereochemical effects. (E)-3-[2(phenylsulfonyl) ethenyl]-4H-1-benzopyran-4-one has been observed to display antifungal activity against *Curularia lunata* and *Fusarium oxysporum* (Mukundam, 1990). In the interest of exploiting and increasing this activity, we have synthesized a series of compounds which are derived from these active antifungal agents but with substituents at the 6 position of the 4H-1-benzopyran-4-one ring and with variation of the parasubstituent on the phenyl ring: (I) none (II) para-chloro (III) para-chloro, 6-chloro (IV) para-bromo, 6 bromo and (V) para-chloro, 6-methoxy. Our aim is to observe the influences of these changes upon the conformation of the ethenylsulfone moiety.

The solid state structures of molecules confirm the transconformation at C7-C8 for I & II, and C9-C10 at III, IV and V. Bond distances reflect electron delocalization in the 04-C10-C9- C8C7 (I), 03-C6-C5-C8-C7 (II) and 01-C2-C3-C9-C10. (III, IV and V), chains. There are no significant differences in details of angles and distances for all five structures. All molecules show coplanarity of the sulfur, ethene and chromanone ring moieties. However, in the methoxy substituted chromanone derivative (V), O3 lies on that plane (d=0.05) whereas in III & IV, O3 is respectively 0.569 and 0.548 Å from that plane. Thus the S11, O1, O3, C2-C10 plane bisects the C12-S11-O4 angle in (III) as seen in a projection down the S11-C10 bond, but is perpendicular to the S11-C12 bond in the same projection for IV & V.

Mukundam, (1990), Ph.D. Thesis, Sri Venkateswara University, Tirupati, India.