03.2-12 THE CHARACTERIZATION OF VARIOUS CRYSTALLINE FORMS OF ASPARTAME (A DIPEPTIDE SWEETENER). By N. Nagashima, C. Sano, S. Kishimoto, and Y. Iitaka*, Central Research Labs., Ajinomoto Co., Inc., Kawasaki, Japan and *Faculty of Pharmaceutical Sciences, University of Tokyo, Tokyo, Japan.

Aspartame, a dipeptide L-α-aspartyl-L-phenylalanine methyl ester: a sweetener, tends to crystallize from an aqueous solution as extremely fine needles (or fibres) with diameters of 10μm or less, unsuitable for industrial process operations.
Crystals obtained by a new industrial crystallization method (S. Kishimoto et al., Chem. & Ind., in press) are relatively large, however, most of them appear to be bundle-like.
For the purpose of elucidation of a correlation between crystallization and structure, we have tried to solve the crystal structure. One of the crystal forms, applicable for X-ray diffraction examination, was found and crystal structure determination is underway.
The space group is $P2_1$, with a=22.959(23), b=4.964(5), c=22.124(22)Å, β=117.17(12)°. This crystal is different from the reported one (M. Hatoda et al., J. Am. Chem. Soc., 1985, 107, 4279-4282), which was crystallized from a quaternary solvent system (water, ethanol, acetone, Me_2SO) in space group $P4_1$, with a=b=17.685(5), c=4.919(2)A.
We have also found that the present crystal changes its form during the loss of water of crystallization upon drying. In this transition, four forms have been confirmed by powder X-ray diffraction.

03.2-13 STRUCTURE AND CONFORMATION OF A NUCLEOSIDE ANALOG 5-NITRO-ARAU. By G. Biswas & A. Banerjee, Department of Biophysics, Bose Institute, Calcutta-54, India.

As chemotherapeutic agents many C-5 substituted pyrimidine nucleosides have been shown to exhibit activity against Herpes Simplex and Vaccinia Viruses, some acting as inhibitors of certain enzymes. The structure determination of 5-NO_2-AraU was undertaken as part of a series of structure determinations of nucleic acid components and their analogs of antitumor, antiviral or anticancer activities to correlate, if possible, their structure function relation. The 5-NO_2-AraU conformation reveals a similar type of structure function correlation in line with other.

Crystals of 5-NO_2-AraU (David Sugar & W. Duax) were obtained from ethanol in the form of transparent needles. Crystals belonged to the space group $P2_12_12_1$ with unit cell parameters: a = 9.241, b = 20.518, c = 6.187 Å, $\alpha = \beta = \gamma = 90°$, D_x = 1.29 gm cm^{-3}, Z=4. 3D intensity data were collected on a CAD-4 diffractometer at room temperature in the ω-2θ mode using Mo K_α radiation. The structure was solved by MULTAN 78 and refined by full matrix least squares to a final R of 0.055 for 1155 reflections with $I > 2\sigma(I)$. The sugar pucker, C(2') endo, is similar to that in the related analog of AraU structures. The glycosidic torsion angle defined for the sequence of atoms O(5)-C(1')-N(1)-C(6) = -27.5°. The conformational features of the nucleoside include a glycosidic bond conformation in the anti range and the C(5')-O(5') bond that is trans to C(4')-O(1') but gauche to C(4')-C(3'). The structure consists of successive layers of hydrophobic and hydrophilic zones, with the layers running parallel to the bc plane.

03.3-1 CRYSTAL STRUCTURE OF A SYNTHETIC ANTI-LEUKAEMIC AGENT-5,5', 10,10'- DIOXO-1,1',3,3'-TETRAPHENYL-10,10' - BI (BENZ (G) ISOQUINOLINE), $C_{50}N_2O_2H_{32}$.

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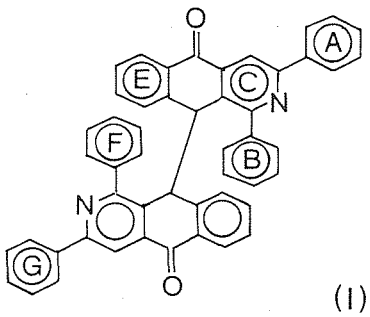
The title compound was synthesised from Indan-1,3-dione as the starting material. Yellowish crystals were obtained from glacial acetic acid and belong to the space group $P\bar{1}$ with a=10.4411(9), b=11.746(1), c=15.929(1) Å, α =86.21(1), β =82.83(1), γ =64.57(1)° and Z=2. The structure was solved by direct methods using the program MULTAN80 after several trails and was refined to R=0.041 for 3636 observed reflections.

The molecule (I) consists of two similar fragments (a dimer) linked through a weak $C(Sp^3)$ - $C(Sp^3)$ bond of length 1.617(6)Å . The angles around the Sp^3 carbon deviate from the normal tetrahedral values due to strain caused by dimer formation. The planes through rings A,B,E,F and G respectively are planar while the two pyridine rings are distorted. The central rings are in distorted sofa conformation. Planes A&B make an angle of 14.5° and 63.3° with C and F&G make 47.6° and 16.1° with H. The tricyclic groups take a butterfly shape with the angle between outer rings being 17.5° and 18.9° in the two fragments. The angle between the mean plane through the tricyclic groups is 27.8° .

There is one C-H...O intermolecular hydrogen bond and the molecules are stabilised by vander Waals forces. Probable intercalation of the monomer (one fragment) with DNA may account for the reported anti-leukaemic activity.



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