03.5-2 THE CRYSTAL AND MOLECULAR STRUCTURE OF ROTENONE. By M. Rossi and P. Fule, Department of Chemistry, Vassar College, Poughkeepsie, NY 12601, USA and M.R. Taylor, School of Physical Sciences, The Flinders University of South Australia, Bedford Park, S.A. 5042. Australia.

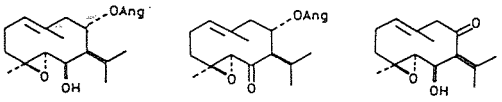
The crystal and molecular structure of the mitochondrial and mitotic spindle inhibitor, rotenone, was solved by direct methods. Rotenone crystallizes in an orthorhombic space group, $P2_12_12_1$ with Z = 8, with two molecules per asymmetric unit; a = 8.413(1)Å, b = 19.840(1), c = 23.581(1), V = 3936Å^3. The structure was refined by least squares methods to a final R = 0.0671, using 5133 observed reflections. Rotenone crystallizes in two distinct conformations: I forms a twisted butterfly shape with a dihedral angle between the aromatic rings of 77.3°; II forms a V-shape with a dihedral angle of 169.0°. Both molecules had the 6αS, 12αS, 5'R configuration. The packing of the two molecules is such that they are able to fit together tightly, maximizing intermolecular interactions and forming a dense structure. This tight packing provides an explanation for the presence of the two conformations. Neither two V-shaped molecules nor two of the other conformation could pack into such a dense, almost spherical unit.

03.5-3 CRYSTAL AND MOLECULAR STRUCTURE OF MALTITOL. By Young Ja Park and Jung Mi Shin, Department of Chemistry, Sook Myung Women's University, Seoul 140, KOREA.

Maltitol, 4-O-α-D-glucopyranosyl-D-glucitol($C_{12}H_{24}O_{11}$) is orthorhombic, space group $P2_12_12_1$, with a = 8.171(1), b = 12.735(2), c = 13.675(2)Å and Z = 4. The structure was solved by the direct method. The α-glucose ring has $^4C_1$ chair conformation. The carbon atom chain of the glucitol residue has the bent ap, Psc, Psc conformation and differs from those observed in the other crystal structures of D-glucitol (Y. J. Park, G. A. Jeffrey and W. C. Hamilton, 1971, Acta Cryst., B27, 2393), glucitol-pyridine complex (H. S. Kim, G. A. Jeffrey and R. D. Rosenstein, 1971, Acta Cryst., B27, 307), 4-O-β-D-glucopyranosyl-D-glucitol (W. P. J. Gaykema and J. A. Kanters, 1979, Acta Cryst., B35,1156) and D-glucitol hexaacetate (Myung Hee Park, 1987, Master Theses, Sook Myung Women's University, Korea). The conformation of the terminal hydroxyl group is ap, Msc in the glucitol residue. The molecules are linked by very complicated hydrogen bonds, and there is one intramolecular hydrogen bond between glycosidic linkage O(1) and O(6') of the glucitol residue. Research supported by Korea Science and Engineering Foundation.

03.5-4 CONFORMATIONAL CHARACTERIZATION OF SHIROMODIOL DERIVATIVES. By G. Appendino, M. Calleri, G. Chiari, P. Ugliengo and D. Viterbo - Dipartimento di Scienza e Tecnologia del Farmaco, Dipartimento di Scienze della Terra and Istituto di Chimica Fisica, University of Torino, Italy.

The X-ray analysis of the related germacrane epoxides Shiromodiol 8-O-angelate (1) and its 6-ketone (2) has been recently reported [Appendino, Calleri & Chiari, J.Chem.Soc, Perkin II,1986, 205], while the analysis of the ketol (3) has just been carried out.



(1) (2) (3)

The three similar molecules show three distinct conformations in the solid state. The dynamic behaviour of these molecules in solution has also been studied by NMR spectroscopy. We have therefore attempted to rationalize the X-ray and NMR findings by means of molecular mechanics calculations. Both the energy minima and the interconversion barriers have been analyzed and a detailed comparison of these calculations with the experimental results will be presented.