09.2-3 CRYSTAL STRUCTURE OF 1-(5-CARBOMETHOXY-2-FURYL)-2,2,2-TRICHLOROETHANOL. By F. Pajardo and R. Pons, University of Oriente and Academy of Sciences of Cuba, Santiago de Cuba, Cuba.

C₈H₁₀O₂Cl₃, orthorhombic, space group Pbcn, a = 21.00(1), b = 13.72(1), c = 7.13(1)Å, β = 90°, 406 P(hkl). A three-dimensional data set was collected at room temperature with MoKα radiation (λ = 0.70928Å), using a pentagonal beam diffractometer with a graphite monochromator. Data were recorded by the θ-2θ scan technique to a maximum 2θ value of 80°. The structure was solved by direct methods. The coordinates and the anisotropic temperature factors of the non-hydrogen atoms were refined by full-matrix least-squares methods to a final R value 0.046.

Molecular structure of C₈H₁₀O₂Cl₃

09.2-4 ON THE MOLECULAR STRUCTURES OF 4- AND 5-ARYLCYCLOPHOSPHAMIDES. By Ling-Kang Liu Institute of Chemistry, Academia Sinica, Nankang, Taipei, Taiwan 115, ROC.

As antitumor agents, the cyclophosphamides have been studied metabolically as well as structurally. Mono substitution of cyclophosphamide with an aryl group at C-4 or C-5 creates a second chiral center at C-4 or C-5 in addition to the original chiral P=O. Racemization of 4- or 5-arylcyclophosphamides may simply be described as cis or trans by considering the P=O and the aryl group. Referring to their separation by silica-gel column, the faster eluting components, for both 4- and 5- aryl substitution, have the cis structure as confirmed by single crystal x-ray diffraction studies, while the slower diastereomers are trans, although IR and NMR data for 4- and 5- aryl substitution have shown reverse trends.


The structure and conformation of the trisaccharides, mannotriose, are reported. The crystal structure space group is P2₁, a = 11.834(2), b = 12.274(1), c = 9.223(2)Å, β = 112.34(2)°, solved by using SHELX and refined using SHELXL, with anisotropic scale factors, from 1769 reflections with D3(001). Final R = 0.048 with unit weights. The conformation of the molecule is stabilized by intra-molecular hydrogen bonds 0(13)-0(5) and 0(23)-0(12). Each molecule is extended, has its long axis at about 45° to the a and b axes, and is approximately perpendicular to the c axis, producing a pattern which resembles a herring-bone brick bond.

Water molecules in the interstices take part in hydrogen bonds reinforcing the inter-layer connections.

The central residue, with torsion angles of φ(1) = -94.3°, χ(1) = -169.0°, φ(2) = -73.8° and χ(2) = -132.1° provides a good model for a poly(1+4)mannoside, c.f. α-cellotrioside undecaacetate (Perez, S. & Brisse, F. Acta Cryst. 1977, 33, 2578-2584) for a poly(1+4) glucoside.