The crystal structures of 1 and 2 were determined by a single crystal X-ray diffraction technique. Crystal data are:

\[
\begin{align*}
& \text{Space group} \\
1 & a = 8.467 \ b = 13.210 \ c = 16.413 \ \text{P}2_12_12_1 (Z=4) \\
2 & a = 7.519 \ b = 11.853 \ c = 22.428 \ \text{P}2_12_12_1 (Z=4)
\end{align*}
\]

The absolute configurations of silicon atoms were obtained by anomalous X-ray scattering. Conformational analysis using molecular mechanics method and crystallographic data will be also presented.

**06.04 - Crystal and Molecular Packing, Hydrogen Bonding**

**PS-06.04.01 MOLECULAR AND CRYSTAL STRUCTURE OF A NEW X-RAY CONTRAST AGENT, C_{38}H_{44}ClN_2O_5**

By L. Ehrenew and B. Fjorros Pedersen, Institute of Pharmacy, University of Oslo, Norway.

The title compound, Iodixanol, is a water soluble non-ionic dimeric contrast agent for use in diagnostic imaging. The structure of a non-ionic monomer has previously been reported (Ganazelli, P. 1981). *Acta Cryst.* C39, 1570-1572.

The intensity data from a single crystal were collected on a Nicolet P3 diffractometer at liquid nitrogen temperature. 12 132 reflections were measured, out of which 4779 were considered observed (I>2.50σ(I)). Iodixanol crystallizes in the triclinic space group P1, a = 16.864(4), b = 18.64(3), c = 19.360(4), α = 95.68(2), β = 102.43(2), γ = 143.56(2), V = 5147(2) Å^3, Z = 4. λ(MoKα) = 0.7107 Å. The structure was solved by direct methods (Gilmore, C.J. 1983), MITHRIL Version 1.0 University of Glasgow, Glasgow, Scotland), and refined by full-matrix least-squares minimization of Σw(ΔF)^2, where w = 1/(Mullinpson, P.R. and Muri, K.W. 1985). *J. Appl. Cryst.* 18, 51-55. The structure was corrected for absorption, and anisotropic vibration was included for the iodine atoms. The high flexibility of the side chains makes the determination difficult. The structure has an R-factor of 7.5%, and an e.s.d. in the bond distance 0.04 Å is about 0.15 Å for the outermost atoms. There are two different conformations of the molecule in the asymmetric unit. One of them has a paramolecular hydrogen bond, which gives it a folded conformation.

**FIG. 1 PERSPECTIVE VIEW OF IODIXANOL MOLECULE**

**FIG. 2 CRYSTAL STRUCTURE OF IODIXANOL VIEKED AGO N X-RAY**