SPECTROSCOPIC METHODS USED FOR STRUCTURE INVESTIGATION OF SOME NEW DIOXANE DERIVATIVES

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New 2-aryl-5-hydroxy-1,3 dioxane derivatives were obtained by the acetalization reaction of glycerol with several aldehydes (MURZA & SAFAROV, 1987; GARDINER et al., 2002). The compounds were investigated by X-ray diffraction techniques and high-field ¹H and ¹³C NMR spectroscopy. The assignment of the signals is based on bidimensional NMR spectra. The complex NMR spectra suggest anancomeric structures.

We succeeded to isolate adequate crystals for some of these compounds which could be analyzed using X-ray diffraction techniques. The DIAMOND diagrams (Fig. 1) revealed the chair conformation of the 1,3-dioxane rings, the equatorial or axial preference of the aromatic substituents and important intramolecular and intermolecular aromatic π stacking interactions (GROSU et al., 2003; BALOG et al., 2004).

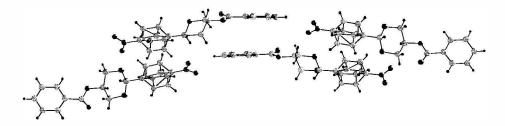


Fig. 1. DIAMOND diagram for trans-5-benzoiloxy-2(p-NOz-phenyl)-1,3-dioxane

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