MITT.ÖSTERR.MINER.GES. 149 (2004)

SYNTHESIS, STEREOCHEMISTRY AND REACTIVITY OF SOME 2-METHYL-2-(3'-NITROPHENYL)-4-HYDROXYMETHYL-1,3-DIOXOLANES

Gâz, S.A., Gropeanu, R., Roiban, D. & Grosu, I.

Babeş-Bolyai University, Organic Chemistry Department (Arany Janos Str., 11, 400028, Cluj-Napoca, Romania)
e-mail: agaz@chem.ubbcluj.ro

The efficient synthesis (SOLOMONS & GRAHAM, 1996) of new dioxolane compounds used in treatment of contaminated water with heavy metals like mercury, cadmium or lead was performed. Two stereoisomers were identified using ^{1}H and ^{13}C NMR (MAGER et al., 1996; SILVERSTEIN, 1997) and X-ray diffraction techniques.

The ^{1}H-NMR spectra showed major differences in aliphatic area (McCLELLAND et al., 1993), differences which lead to the separation of two pure stereoisomers. Only the *anti* stereoisomer was used in the further steps of the synthesis due to the π stacking interactions (STEED & ATWOOD, 2000) observed, which influenced the final conformation of the structure.

The ORTEP plot of the *anti* stereoisomer crystals (Fig. 1) highlighted π stacking interactions that confirm in this way the NMR data (STENBERG & KILIK, 1974).

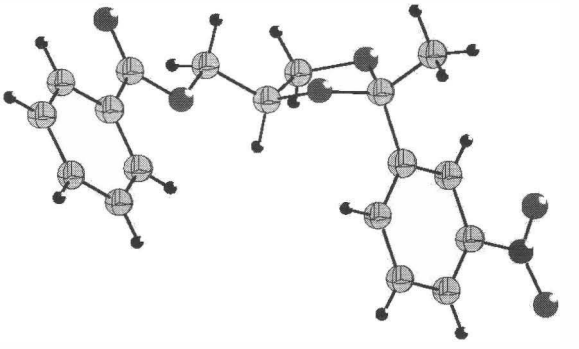

Fig. 1. ORTEP plot for anti 2-methyl-2-(3'-nitrophenyl)-4-hydroxymethyl-1,3-dioxolane

References

GRAHAM SOLOMONS T.W. (1996): Fundamentals of Organic Chemistry. John Wiley & Sons, 724 p.

MAGER, S., GROSU, I., PLE, G. & DARABANTU, M. (1996): Aplicatii ale RMN in analiza structurala organica. University Press, Cluj-Napoca.

McCLELLAND, A.R., WATADA, B. & LEW C.S.Q. (1993): J. Chem. Perkin Trans. 2, **10**: 1723-1728.

SILVERSTEIN R.M. (1997): Spectrometric Identification of Organic Compounds. Wiley Text Books.

STEED, W.J. & ATWOOD, J.L. (2000): Supramolecular Chemistry. John Wiley & Sons, New York, 443 p.

STENBERG, V.I. & KILIK, D.A. (1974): J. Org. Chem., **39**: 215-219.