

Structure of *trans*-Isoshinanolone in the Crystal and in Solution*

Gerhard Bringmann^a, Robert-Michael Pfeifer^a, Matthias Breuning^a,
Matthias Reichert^a, Kim Messer^a, Michaela Schraut^a, and Gabor Tóth^{b,c}

^a Institute of Organic Chemistry, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

^b Institute of General and Analytical Chemistry, Budapest University of Technology and Economics, Szt. Gellért tér 4, H-1111 Budapest, Hungary

^c Present address: IVAX Drug Research Institute, H-1045 Budapest, Berliini u. 47-49, Hungary

Reprint requests to Prof. Dr. G. Bringmann. Fax: +49 931 888 4755.
E-mail: bringman@chemie.uni-wuerzburg.de

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The first X-ray structure analysis of authentic, not derivatized (racemic) *trans*-isoshinanolone, a wide-spread acetogenic tetralone, is described. In the crystal, two slightly different conformers are found, along with the corresponding enantiomers. The ‘homomeric’ conformers differ by their H-bonding interactions with the respective neighboring molecules. Rows of a single enantiomeric species, but with the two conformers linked ‘head-to-head’, ‘tail-to-tail’, are surrounded by four analogous rows of the corresponding enantiomers. Apparently the interactions between these heterochiral rows are the reason for the enhanced crystallization tendency of the racemate as compared to that of enantiomerically pure isoshinanolone. The structures in the crystal are compared with those calculated (gas phase) and with the structure in solution.

Key words: Natural Products, Crystal Structure, Quantum Chemical Calculations, NMR Methods