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Journal of Molecular Structure 344 (1995) 95–106

Journal of
MOLECULAR
STRUCTURE

# Molecular structure and conformations of eight-membered cyclic acetals with 1,4-diplanar fragments

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Received 20 May 1994

**Abstract**

The molecular structures of nine eight-membered cyclic acetals containing two planar fragments in the ring, the derivatives of dibenzo- and dinaphtho[*d,g*][1,3]dioxocines, have been studied by x-ray single crystal diffraction. Steric interactions were found to determine the conformation realized in the crystalline phase. Depending on the type of planar fragments in the cycle and the group bridging them, boat–chair (BC), distorted boat (DB), twist (T) or twist–boat (TB) conformations were observed. The BC conformation was found for derivatives of 6*H*,12*H*-dibenzo[*d,g*][1,3]dioxocine containing methyl groups in the benzo fragments or one methyl substituent in the bridge methylene group. The T and TB conformations are realized for molecules with the carbonyl group bridging the planar fragments. 8*H*,16*H*-Dinaphtho[2,1-*d*,1′2′-*g*][1,3]dioxocine exhibits the first example of BC conformation among all eight-membered cyclic compounds containing two naphtho groups at the expense of large deviations of its geometrical parameters from their unstrained values. Other dinaphtho derivatives exist in the DB conformation. The molecular geometry and the possibility of weak intramolecular C–H···O hydrogen bonding are discussed.

## 1. Introduction

For several years, eight-membered cyclic compounds with 1,4-diplanar fragments in the cycle have been studied extensively by IR, Raman and NMR spectroscopy and X-ray diffraction. The presence of planar fragments significantly decreases the number of possible conformations which may be realized in these molecules compared with saturated cycles. However, the number of conformations, including a rigid one and a family of flexible forms, remains reasonably large.

The experimental data on the conformations of eight-membered cyclic compounds with 1,4-diplanar fragments were first summarized by Renaud et al. [1], and four possible low-energy conformations were reported. Later studies of 1,3,2-diazaphosphocines [2], 1,3,2-dioxaphosphocines [3–10], 2-oxo-1,3,2-dioxathiocines [11–16] and azocines [17] were carried out both in liquid and crystalline phases. Summarizing these structural data and using Cremer–Pople puckering parameters, Arshinova and co-workers [18–20] derived the following low-energy conformations including one rigid boat–chair (BC) form and a family of flexible boat–boat (BB), distorted boat (DB), twist (T) and twist–boat (TB) forms:

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*SSDI* 0022-2860(94)08429-7