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CONFORMATIONAL STUDY OF DIBENZO[d,g][1,3]DIOXOCIN-12-ONE BY VIBRATIONAL SPECTROSCOPY AND MOLECULAR MECHANICS

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ABSTRACT

Two of the four possible dibenzo[d,g][1,3]dioxocin-12-one conformers are identified in solution from IR and Raman spectra. The experimental enthalpy difference between boat–chair (*BC*) and twist (*T*) conformers of 0.7 kcal mol^{-1} is obtained from temperature dependent IR spectra. Structural parameters and the potential energy difference (1.4 kcal mol^{-1}) for these conformers are calculated by molecular mechanics. Band shape simulations and normal coordinate analysis are applied when they are necessary for interpretation of the experimental results. The conformational equilibria seems to be non-typical for cyclic systems with two planar units in 1,4 position.

INTRODUCTION

Distinctive features in the conformational behaviour of 8-membered rings with two planar units in 1,4-position were described in a review article [1], devoted to three-dimensional structures of 8-membered cyclic systems. As a rule, two conformations, boat–chair (*BC*) and distorted boat (*DB*), exist in such systems. However, if the methylene bridge between annulated aromatic rings is replaced by an sp^2-hybridized atom (for instance, a carbonyl group) certain changes may occur in the conformational behaviour.

NMR ^1H spectral tests for conformational identification of such systems are mainly based on considering methylene bridge coupling constants, which obviously cannot be used when the methylene group is absent. Distinctive IR spectral conformational criteria are not found for these molecules either.

Preliminary NMR and IR spectral studies indicated that the same di-

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