

Stereochemistry of seven-membered heterocycles. Communication 14. Synthesis and three-dimensional structure of 4-methyl-1,3-dioxo-5,6-benzocycloheptenes

Klimovitskii E., Sergeeva G., Strel'nik D., Arbuzov B.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

1. On the basis of data obtained by the dipole moment method, cis-2-methyl (or phenyl)--methyl-1,3-dioxo-5,6-benzocycloheptenes have an equilibrium of chair and twist forms that is close in quantitative respects to the related 2-R-phthalylacetals; the spiroketal of cyclohexanone is realized in the e-Tw form; the methylal is conformationally inhomogeneous. 2. The isomeric 2-tert-butyl-4-methyl-1,3-dioxo-5,6-benzocycloheptenes, according to ^{13}C NMR data, are realized in chair conformations. An analysis has been made of the influence of the 4-methyl group on the chemical shifts of the carbon atoms of the seven-membered ring. © 1985 Plenum Publishing Corporation.

<http://dx.doi.org/10.1007/BF00954082>
