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

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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.

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