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Study of the structure of p-tert-butyl-substituted thiacalix[4]arenes containing amide fragment by one- and two-dimensional NMR spectroscopy

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Abstract

Structures of 5,11,17,23-tetra-tert-butyl-25,26,27-trihydroxy-28- and 5,11,17,23-tetra-tert-butyl-25,26-dihydroxy-27,28-[N-(4′-nitrophenyl) aminocarbonylmethoxy]thiacalix[4]arenes (I, II) (solutions in CDCl3) were studied by 1H and 13C 1D and 2D (NOESY) NMR spectroscopy combined with the use of computational simulation (semiempirical quantum-chemical calculations, method PM3). Compound I was found to exists in the cone conformation, and the bulky substituent OCH2C(O)NHPhNO 2, in contrast to the crystalline state, was located in the exo position to the macrocycle cavity; for compound II the cone conformation was observed, where the substituents are turned to the inside of the cavity of the macrocycle (endo position).

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