Russian Journal of General Chemistry 2013 vol.83 N4, pages 698-702

# One- and two-dimensional NMR study of structure of 1,2-disubstituted p-tert-butylthiacalix[4]arene containing amide fragment

Karataeva F., Vagizova R., Stoikov I., Antipin I., Klochkov V.
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

## Abstract

The structure of 5,11,17,23-tetra-tert-butyl-25,27-dihydroxy-26,28-bis[N- (4′-nitrophenyl)aminocarbonylmethoxy] thiacalix[4]arene I was examined by 1D and 2D (NOESY) 1H and 13C NMR methods in a CDCl 3 solution using numerical simulation (semi-empirical quantum-chemical calculations, PM3 method). Compound I was found to exist in the 1,2-alternate conformation, where bulky substituents OCH2C(O) · NHPhNO2 are in the endo-position relative to the macrocycle cavity. © 2013 Pleiades Publishing, Ltd.

http://dx.doi.org/10.1134/S1070363213040154