

The use of a lyotropic liquid-crystalline medium and residual dipolar coupling constants for determination of the spatial structure of thiacalix[4]arenes in solutions

Klochkov V., Khairutdinov B., Klochkov A., Tagirov M., Thiele C., Berger S., Vershinina I., Stoikov I., Antipin I., Konovalov A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The possibility of using an approach for the elucidation of the spatial structure of functionalized thiacalix[4]arenes based on the determination the residual dipolar coupling constants between the ^1H and ^{13}C nuclei separated by one chemical bond ($^1\text{D CH}$) in lyotropic liquid-crystalline media (poly- γ -benzyl-L-glutamate and CDCl_3) is demonstrated for the first time. This approach was used to distinguish between the cone and 1,3-alternate conformations of 5,11,17,23-tetr-tert-butyl-25,26,27,28-tetrakis(2-oxopropoxy)-2,8,14,20-tetrathiacalix[4]arene. The results were confirmed by the data from 2D NMR ($^1\text{H} - ^1\text{H}$) NOESY experiments for these compounds in an isotropic solvent (CDCl_3).

<http://dx.doi.org/10.1023/B:RUCB.0000046242.55417.1c>

Keywords

conformations, lyotropic liquid-crystalline media, NMR, residual dipolar coupling constants, thiacalix[4]arene