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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

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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).

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Keywords

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