

## Conformational diversity and dynamics of distally disubstituted calix and thiacalix[4]arenes in solution

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### Abstract

According to the quantum chemical calculations and Dynamic NMR experiments in the distally disubstituted classical and thiacalix[4]arenes (CCA and TCA) in addition to the C<sub>2v</sub> symmetrical pinched cone (PC) conformation, the distorted cone (DC) form with an approximate C<sub>s</sub> overall symmetry (with two OH groups bonded to one oxygen atom) also corresponds to the energy minimum. Moreover, in DC form, two different mutual orientations of O-R groups at a lower rim lead to two stable conformations: the first - with both these groups directed outward, the second - with both these groups pointing toward the same direction. In CCA, the PC is essentially favoured over the DC, while in TCA, energies of these forms are similar or the latter may be even preferable. Copyright © 2013 John Wiley & Sons, Ltd.

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### Keywords

conformation, DNMR, dynamics, quantum chemistry, solution state