Collection of Czechoslovak Chemical Communications 2001 vol.66 N4, pages 641-662

New calix[4]arene-based amides - Their synthesis, conformation, complexation

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Abstract

New chiral calix[4]arene-based diol-diamides 1a, 1b, tetraamides 2a, 2b and 7 as well as achiral diamide 3 and tetraamides 4-6 were prepared. The conformation of 1 has been studied in solution by NMR and in solid state by X-ray crystallography. The pinched-cone conformation of the calix[4]arene skeleton in 1 was found to be stabilized by a circular array of hydrogen bonds formed by two phenolic O-H and two amidic N-H bonds at lower rim. Whereas no significant complexation of Na+ was observed in solution for diamides 1 and 3, tetraamides 2, 4, 5, and 6 give strong complexes with Na+ as confirmed by NMR titrations of 2 and 4. The influence of anions and the solvents used on complexation ability of 2 towards Na+ is negligible.

http://dx.doi.org/10.1135/cccc20010641

Keywords

Calix[4, arenes, Calixarenes, Complexation, Conformation analysis, NMR spectroscopy, Receptors, Recognition, X-Ray diffraction