An Integrated approach to the study of complexation of alkali-metal cations by calix[4]arene amide derivative

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Complexation of alkali-metal cations by calix[4]arene derivative (L) in benzonitrile was studied by means of microcalorimetric titrations, molecular dynamics simulations and single-crystal X-ray diffraction. The inclusion of acetonitrile molecule in the calixarene hydrophobic cone was also studied using the same methods.

The stability constants of the LiL+, NaL+, LiLMeCN+ and NaLMeCN+ complexes in benzonitrile were determined along with the enthalpies and entropies of complexation reactions. All investigated reactions were found to be enthalpy driven. In the case of LiL+ complex the inclusion of benzonitrile molecule in the calixarene cone was observed, and the corresponding molecular and crystal structures were determined. This finding was in accordance with the results of molecular dynamics simulation of LiL+ complex in benzonitrile.