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

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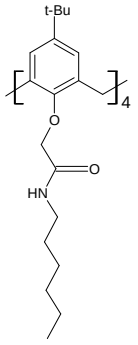
Complexation of alkali-metal cations by calix[4]arene derivative (**L**) in benzonitrile was studied by means of microcalorimetric titrations, molecular dynamics simulations and single-crystal X-ray diffraction. The inclusion of acetonitrile molecule in the calixarene hydrophobic *cone* was also studied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



Structure of **L**.

The stability constants of the Li**L**$^+$, Na**L**$^+$, Li**L**MeCN$^+$ and Na**L**MeCN$^+$ 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 Li**L**$^+$ 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 Li**L**$^+$ complex in benzonitrile.