Molecular Dynamics Simulations of tetramethylketone p-tert-butyl calix[4]arene

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We describe the results of Molecular Dynamics simulations of the calixarene tetramethylketone p-*tert*-butyl calix[4]arene in vacuum, in pure acetonitrile and in the presence of Pb^{+2} ions solvated by acetonitrile. The mean goal of these calculations is to validate the parametrization of the system model using experimental thermodynamics and crystallographic data and to describe the process by which the calixarene traps one Pb^{+2} ion in its hydrophilic cavity and one acetonitrile molecule in its hydrophobic one. This information allows us to determine the relevance of several structural parameters in the process of complexation, thus adding to the rational building of more efficient ligands. The initial state of the simulations is taken from X-ray diffraction results[1] which are also used to verify that the simulations predictions are in agreement with experimental data.

[1] de Namor A.F.D., Chahine S., Kowalska D., Castellano E.E., Piro O.E., *J. Am. Chem. Soc.*, 2002, **124**, 12824-12836.

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