Calculation of crown-ether binding energies: methods comparison

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Crown ethers and their modifications are compounds with unique affinity properties to a vast range of cations. Molecular dynamics can facilitate the search of crown ethers most affinitive to a cation in a solution. To do so one has to choose a proper method of investigation of affinity properties.

We perform a comparative analysis of two calculation methods of cation to crown binding free energies. In the first method, as proposed by Dang [1] and employed by Bakulin [2], a potential of mean force is utilized to calculate the binding free energy. In this method, a simulation cell consists of 1 crown ether molecule, 1 ion pair and a solvent of choice with a trajectory length of ~ 7 ns. The second method, introduced by Jing [3], requires simulation of $\gtrsim 100$ crown ether molecules with as many ion pairs on a time scale of ~ 50 ns. The binding free energy is calculated as the scaled energy difference between the end and the beginning of the simulation.

OPLS-AA/CM1A force field [4] is used to describe interactions in the system. General complexity and time-efficiency of the methods under study is evaluated. Precision of each method is assessed by comparing calculated binding free energies to experimental data [5, 6] on a wide range of crown ether species, cations and solvents.

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