Volumetric properties of binary mixtures of carbon tetrachloride with *tert*-butyl alcohol: a molecular dynamics simulation study

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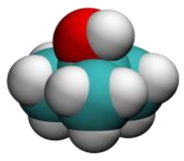
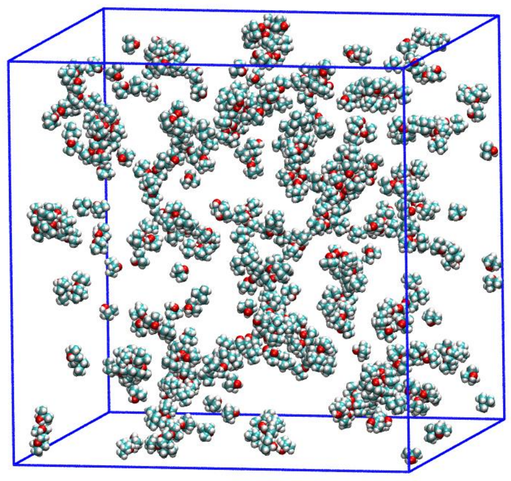
Motivation

tert-Butyl alcohol (TBA) in simple non-polar CCl_4 solvent is a useful comparison system for intriguing aqueous TBA solutions.

CCl_4



t-BuOH (TBA)

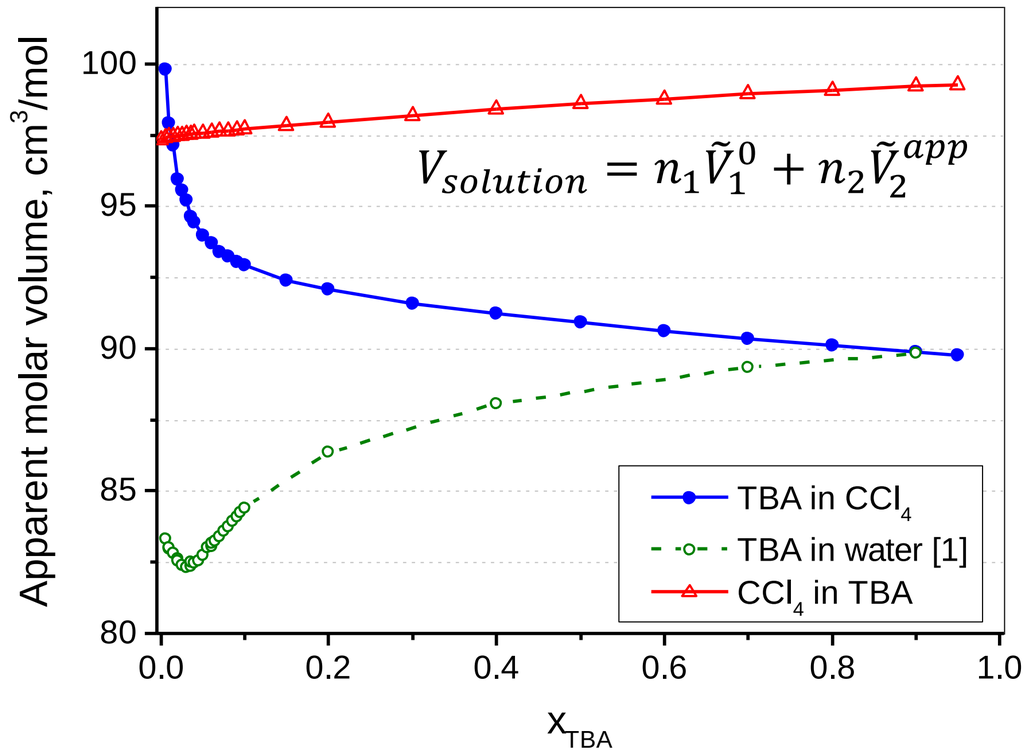


TBA molecules in CCl_4+*TBA* solution, x_{TBA}=*0.05*

MD models

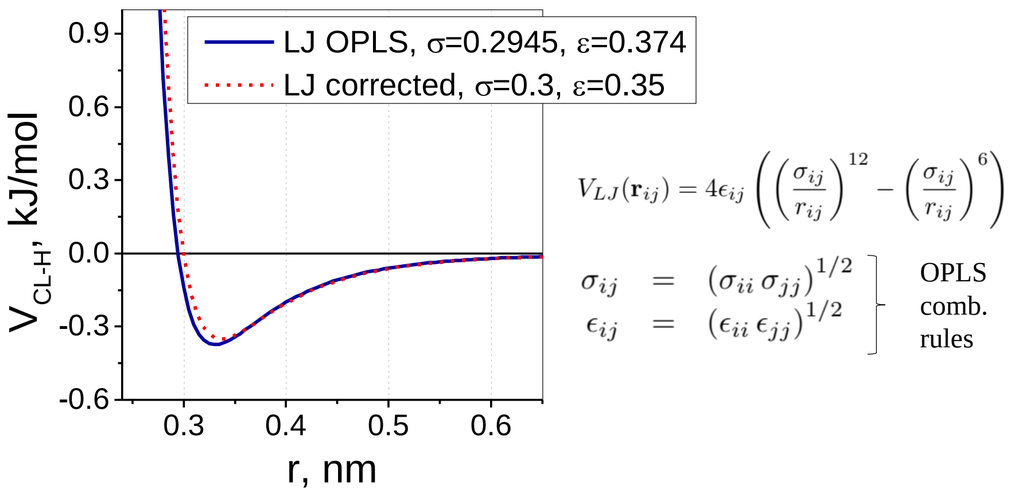
- GROMACS 2021 package
- OPLS-AA interatomic potentials with corrected LJ cross term
- 10 000 molecules in each model
- 100 ns production run trajectories
- full range of concentrations at T=298 K, P=1 bar

Results: apparent and geometric molar volumes



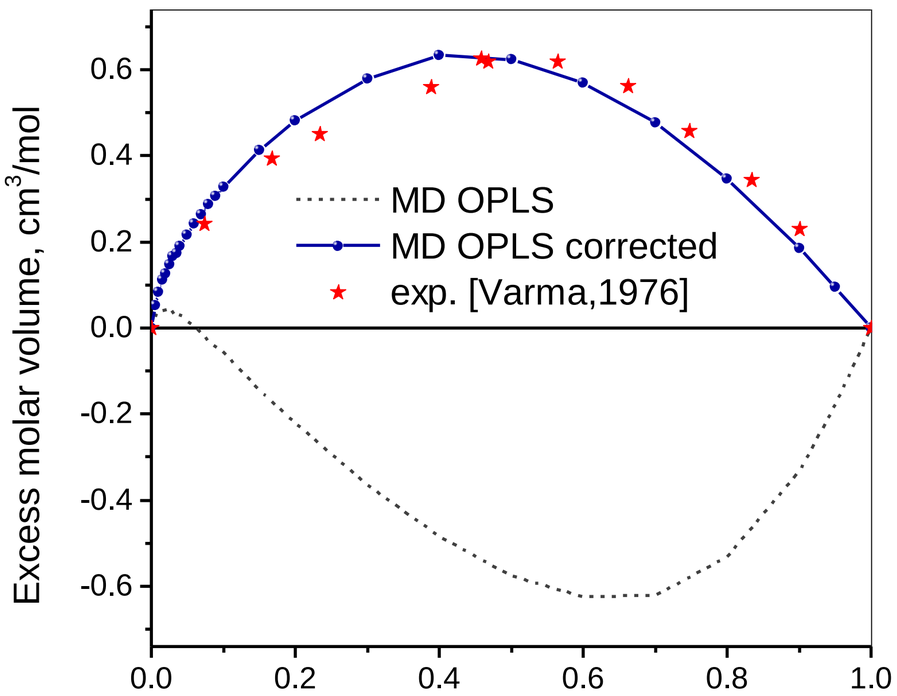
[1] E.D. Kadtsyn et al., *J. Mol. Liq.* **349** (2022) 118173.

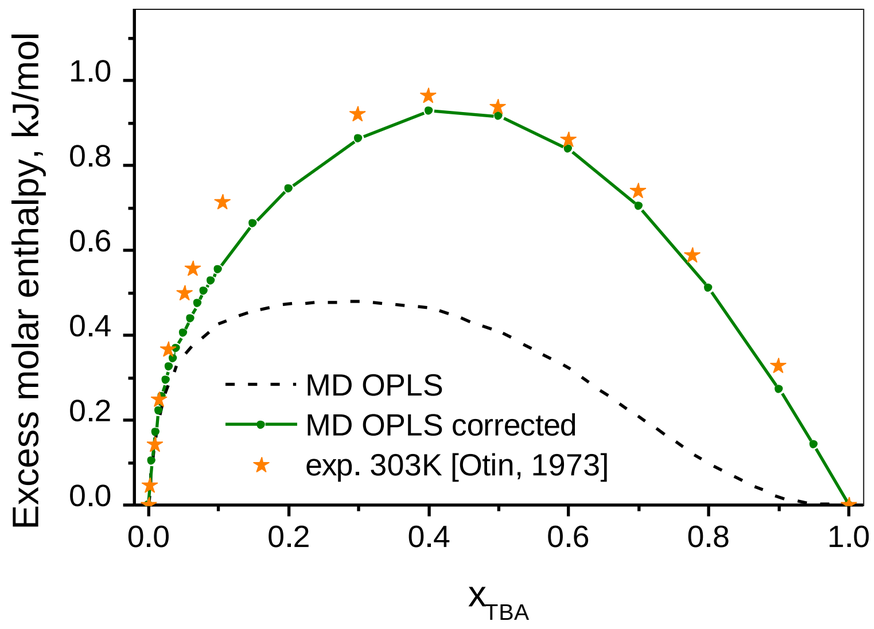
Correcting Lennard-Jones cross term for *Cl–H* interaction



Results: excess mixing properties of CCl_4 + *TBA*

$$V_m^E = V_m - x_1V_1^0 - x_2V_2^0$$





Conclusions

- Models with corrected OPLS interatomic potentials reproduce experimental mixing properties of CCl_4 + *TBA* system quite well;
- Geometric (Voronoi) molecular volumes provide new perspective on volumetric properties of solutions.

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