A New Database of Rigid Molecular Models for Simulations of Thermodynamic Properties of Fluids

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A new database is presented which contains information on molecular models of over 150 pure fluids. Most technically relevant small and medium sized molecules are included. They are described by rigid multi-centre Lennard-Jones 12-6 based models with electrostatic sites. The models were developed in a consistent way and are known to describe vapor-liquid equilibrium data (saturated densities, vapour pressure, enthalpy of vaporization) well, as such data were used in the parameterization. In many cases, also predictions of other properties, like transport and interfacial properties were tested and found to be in good agreement with experimental data. As all molecular models belong to the same class, they can easily be combined for describing mixtures using mixing rules, like that of Lorentz-Berthelot. Furthermore, also ion models are included. They were developed such as to form an ion model family in which any anion can be combined with any cation, yielding reasonable descriptions of thermodynamic properties of the corresponding salt in water and often also in other solvents. The database contains a full specification of the models including references to the literature. It provides a wide range of search functionalities and offers downloading of input files for several molecular simulation codes, like LAMMPS [1], GROMACS [2], *ms*2 [3], and ls1 mardyn [4].

The database development was conducted under the auspices of the Boltzmann-Zuse Society of Computational Molecular Engineering (BZS) and it focusses on validated models developed by its members in the last 20 years.

References:

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[3] C.W. Glass et al.: Computer Physics Communication 185 (2014) 3302–3306.
[4] C. Niethammer et al.: Journal of Chemical Theory and Computation 10 (2014) 4455-4464.