

## Analytical model for 3D Mercedes-Benz water molecules

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We developed a statistical model which describes the thermal and volumetric properties of water-like molecules. A molecule is presented as a three-dimensional sphere with four hydrogen-bonding arms. Each water interacts with its neighboring waters through a van der Waals interaction and an orientation-dependent hydrogen-bonding interaction. This model, which is largely analytical, is a variant of a model developed before for a two-dimensional Mercedes-Benz model of water [1]. We explored properties such as molar volume, density, heat capacity, thermal expansion coefficient and isothermal compressibility as a function of temperature and pressure. We found that the volumetric and thermal properties follow the same trends with temperature as in real water and are in good general agreement with Monte Carlo simulations [2], including the density anomaly, the minimum in the isothermal compressibility, and the decreased number of hydrogen bonds upon increasing the temperature.

## References

- [1] T. Urbic and K. A. Dill, *J. Chem. Phys.* **132**, 224507 (2010).
- [2] C. L. Dias, T. Ala-Nissila, M. Grant and M. Karttunen, *J. Chem. Phys.* **131**, 054505 (2009).