Towards a spectroscopic potential energy surface of Methanol CH3OH –

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Ab initio electronic potential energy surfaces form the basis of spectroscopic calculations. Achieving spectroscopic accuracy in such calculations remains a difficult task. Here we apply the approach previously used to obtain the highly accurate surface computed for methyl chloride (Owens et al. 2015). The main contribution is computed using the explicitly correlated CCSD(T)-f12b method extrapolating to the complete basis set limit using the aug-cc-pVTZ-f12b/aug-cc-pVQZ-f12b basis sets. We then consider core valence effects, higher order correlation, the diagonal Born-Oppenheimer correction and scalar relativistic corrections. The potential energy function is represented by a fully symmeterised series expansion fit using weighted least squares on the ab initio data consisting of 49537 grid points.

References:

Owens, Alec, Sergei N. Yurchenko, Andrey Yachmenev, Jonathan Tennyson, and Walter Thiel. “Accurate *Ab Initio* Vibrational Energies of Methyl Chloride.” *The Journal of Chemical Physics* 142, no. 24 (June 28, 2015): 244306. https://doi.org/10.1063/1.4922890