

Methanol Potential Energy Surface

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Methanol is a prototype for hydrogen bonding in liquids, and has been the subject of many experimental studies. Theoretical models, however, disagree with many of the basic experimental properties of methanol. To develop an improved model of methanol, *ab initio* electronic

structure calculations were performed using the NWChem electronic structure code at the MP2 level of theory with an aug-cc-pVTZ basis set on several orientations of the methanol dimer. These were then used to fit a polarizable molecular dynamics model, which was subsequently adjusted to give better agreement with experiment. The new model is a significant improvement on existing models, but suggests significant 3-body effects may be present.

