SIMULATION STUDIES OF THE VIBRATIONAL DYNAMICS OF $para$-HYDROGEN CLUSTERS

NABIL F. FARUK, JING YANG, ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

This paper discusses the construction and application of reduced-dimensional potential energy surfaces for use in performing simulation of para-hydrogen clusters. Simple spherical averaging and 'adiabatic-hindered-rotor' averaging[a] treatments of the angular degrees of freedom are considered and compared. The resulting one-dimensional surface is used in quantum Monte Carlo simulations of para-hydrogen clusters of varying sizes. Energetic, and structural properties are computed and compared to previously published results, and vibrational frequency shifts are predicted and compared to available experimental measurements.

[a] H. Li, P.N. Roy and R.J. Le Roy, *J. Chem. Phys.* **133**, 104305 (2010).