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Vibrationally Averaged Properties Using Monte Carlo Methods
STEVEN ALEXANDER, Southwestern University, R.L. COLDWELL, University of Florida — Using explicitly correlated wavefunctions and variational Monte Carlo methods we have computed potential energy surfaces for several small molecules. These surfaces include both relativistic corrections and non-Born Oppenheimer corrections. From this surface we then computed several of the lowest rotational and vibrational energies and wavefunctions again using Monte Carlo methods. With our molecular wavefunctions we next evaluated a number of properties for each molecule as a function of the nuclear positions. When we finally integrated these properties over the rotational/vibrational wavefunctions, the result is a set of vibrationally averaged properties.

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