Abstract Submitted
for the TS4CF08 Meeting of
The American Physical Society

Computing Energies and Properties of Small Molecules Using Fully Nonadiabatic Wavefunctions STEVE ALEXANDER, Department of Physics, Southwestern University, R.L. COLDWELL, Department of Physics, University of Florida — Using variational Monte Carlo methods and compact, explicitly-correlated fully nonadiabatic wavefunctions we have computed the energies and properties of several rovibrational states for several small molecules. We have extensively examined the form of the wavefunctions that are needed to accurately describe the excited vibrational and rotational states of these systems. Examples of each form will be discussed. Our results will be compared with previous calculations and we will show that the accuracy of this method is similar to comparable Born-Oppenheimer calculations.

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Date submitted: 11 Sep 2008 Electronic form version 1.4