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Energy and Properties of Fully Nonadiabatic Molecules Using Monte Carlo Methods STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, University of Florida — Recent advances in the area of Quantum Monte Carlo allow fully nonadiabatic wavefunctions to be computed for a number of chemically interesting molecules. These explicitly-correlated wavefunctions are compact, capture a high percentage of the correlation energy and automatically include all nonadiabatic corrections. They also eliminate the need to form potential energy surfaces. Instead, the vibrational and rotational energies of a molecule can be computed directly from the wavefunction. From these wavefunctions a variety of molecular properties can also be computed. We will present results for several simple molecules.

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