VSCF/VCI in curvilinear coordinates: Application to the hydroxymethyl radical

Eugene Kamarchik

Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94551
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We have recently developed an algorithm to perform vibrational self-consistent field (VSCF) and vibrational configuration interaction (VCI) calculations using an arbitrary set of curvilinear coordinates. The kinetic energy operator is computed numerically and evaluated directly on a pseudospectral grid without any further approximation. Both the kinetic and potential energy terms employ separate n-mode decompositions allowing the convergence of these terms with respect to the level of mode coupling to be explored. The use of curvilinear coordinates introduces a second mean field term to the VSCF procedure which yields an effective mass as well as an effective potential. The algorithm is tested on the hydroxymethyl radical CH$_2$OH, which has a single low frequency torsional mode. Comparison is made with previous treatments using the Watson Hamiltonian in cartesian normal mode coordinates.