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Rovibrational Energies of H2+ Using Fully Nonadiabatic Wavefunctions STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, Retired — Using variational Monte Carlo methods we examined a number of fully nonadiabatic trial wavefunctions in order to determine which features best describe the lowest several rovibrational states of H_2^+ and its isotopormers. We found that vibrational states could be easily described but that rotational excited states are more complicated. We show how the energies produced by these forms compare to previous calculations and discuss how the results of this work can be applied to larger systems.

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