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Comparing the Born-Oppenheimer Approximation and Fully Nonadiabatic Calculations STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, Retired — Using Variational Monte Carlo methods we have calculated Born-Oppenheimer energies for the H2+ molecular ion at several internuclear distances. With these we then construct the potential curve and the lowest several rovibrational energies. Using the trial wavefunctions at each internuclear distance we also evaluate both the diagnonal and non-diagonal corrections to the Born-Oppenheimer approximation. These corrections are then added to the Born-Oppenheimer energies to produce more accurate estimates for the lowest several rovibrational energies. We compare the results of each level of approximation with results obtained from a fully-nonadiabatic wavefunction.

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