A FIRST PRINCIPLE EFFECTIVE HAMILTONIAN FOR INCLUDING NON-ADIABATIC EFFECTS FOR H_2^+ AND HD^+

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We compute non-adiabatic corrections for all bound and long lived quasi-bound vibrational levels of H_2^+ and HD^+ for selected rotational levels. This is done using the Bunker and Moss formalism with the correction factors computed from *ab initio* wavefunctions. The electronic wave functions are expanded in terms of nuclear centered gaussian basis functions. The agreement with accurate calculations is very good: for H_2^+, most transition frequencies are predicted to within about 0.0001 cm^{-1}. For HD^+, the results are not quite as good due to the uncertainties in the adiabatic correction. This paves the way for using these techniques to accurately predict the non-adiabatic effects for more complicated molecules.