A FIRST PRINCIPLE EFFECTIVE HAMILTONIAN FOR INCLUDING NON-ADIABATIC EFFECTS FOR H$_2^+$ AND HD$^+$

DAVID W. SCHWENKE, Mail Stop 230-3, NASA Ames Research Center, Moffett Field, CA 94035-1000.

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.