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State-of-the Art Procedure for the Calculation of Quartic Force Fields: Application to HO_2^+ TIMOTHY LEE, XINCHUAN HUANG, NASA Ames Research Center — In the 1990's, ab initio methods began to yield quartic force fields for use in the calculation of ro-vibrational spectra with an accuracy that previously had been unimaginable. The main reason for this advance was the development of efficient computer programs for calculating singles and doubles coupled-cluster energies that included an estimate for connected triple excitations, denoted CCSD(T). Thus the advent of CCSD(T) quartic force fields computed with large one-particle basis sets changed the paradigm for the ab initio calculation of ro-vibrational spectra. Small correction terms have now been successfully incorporated into these procedures, including core-correlation, scalar relativistic, and others. Previously, we investigated procedures where all of these correction terms are appended in one way or another to a base calculation. In the current work, we develop a new procedure where most of these correction terms are included from the beginning, while still minimizing the overall computational cost. Our new procedure is detailed and its application to the lowest triplet and singlet states of HO_2^+ presented.

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