GENERATING SPECTRA FROM GROUND STATE WAVE FUNCTIONS: UNRAVELING ANHARMONIC EFFECTS IN THE $OH^- \cdot H_2O$ AND $H_5O_2^+$ VIBRATIONAL PREDISSOCIATION SPECTRA

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An approach is described for calculating anharmonic spectra for polyatomic molecules using only the ground state probability amplitude.[a] The underlying theory is based on properties of harmonic oscillator wave functions and is tested for Morse Oscillators with a range of anharmonicities. More extensive tests are performed with $H_3O_2^-$, using the potential and dipole surfaces of Bowman and co-workers.[b] The resulting energies are compared to earlier studies that employed the same potential surface and the agreement is shown to be very good. The vibrational spectra are calculated for $H_3O_2^-$, $D_3O_2^-$ and $H_5O_2^+$ and its deuterated analogues. When possible, comparisons are made experimental spectra from 600 - 4500 cm^{-1}. The frequencies and intensities of the fundamentals are found to be in excellent agreement and many combination bands involving one quantum of excitation in each of two modes are also well-reproduced.

[a] A. B. McCoy, E. G. Diken and Mark A. Johnson, *J. Phys. Chem. A* in press
[b] *J. Am. Chem. Soc.* **2004**, *126*, 5042