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Influence of Combination and Overtone Vibrations on Resonant Positron Annihilation Spectra.¹ G. F. GRIBAKIN, Queen's University Belfast, J. F. STANTON, University of Florida, J. R. DANIELSON, M. R. NATISIN, C. M. SURKO, University of California, San Diego — Low-energy annihilation spectra of positrons on molecules are typically dominated by positron capture in vibrational Feshbach resonances (VFR) of dipole-coupled fundamental modes.² However, anharmonic effects can lead to a coupling of the fundamentals to multiquantum excitations (e.g., combinations and overtones) that lead to the enhancement or suppression of the VFR.³ Further, in most molecules there is a broad spectrum of enhanced annihilation between the fundamentals, presumably due to directly excited combination and overtones, where the vibrational density is typically too high to identify discrete modes. An extension of the Gribakin-Lee theory, using the calculated anharmonic vibrational spectra and dipole transition amplitudes for vibrations containing up to 3 quanta, is compared to experiments for several small molecules. This work demonstrates the effects of vibrational anharmonicity and the importance of including higher order couplings. Prospects for the use of a new high-resolution positron beam for the meaurement of VFR's due to individual multi-modes will be described.

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