PHOTOELECTRON SPECTRA FROM WAVE PACKET DYNAMICS

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Franck-Condon factors for photoelectron spectra can be computed from: (1) the overlap between initial and target vibrational wave functions; and (2) Fourier transform of a wave packet time autocorrelation function. These techniques were implemented in the new spectra modeling software using harmonic well approximation and full quantum mechanical treatment. The photoelectron spectrum of N_3 was modeled using *ab-initio* potential energy surfaces of the cation electronic states. Anharmonic effects are discussed.