MULTISTATE VIBRONIC HAMILTONIAN FOR THE NITRATE RADICAL

JOHN F. STANTON, *Department of Chemistry, The University of Texas, Austin, TX, USA*.

The quasidiabatic model of Köppel, Domcke and Cederabaum has proven to be a powerful tool for computing intensities and level positions in electronic spectra involving strong vibronic coupling effects. The model has been used, as parametrized by very high-level equation-of-motion coupled cluster (EOM-CC) calcaultions, is demonstrated by applications to the NO_3 radical.