HIGH-ACCURACY DIABATIC TREATMENT OF NO_3 ENERGY LEVELS

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Recent developments in vibronic coupling theory and quantum chemistry now allow the parametrization of vibronic Hamiltonians that are capable of achieving semi-quantitative agreement with experimental energy levels for strongly coupled systems. First applied to the HCO_2 and BNB radicals, this sophisticated parametrization has been used for the nitrate radical. Results of calculations bearing on both all electronic states of NO_3 below 2 eV will be presented.