ON THE MAGNITUDE OF THE NONADIABATIC ERROR FOR HIGHLY COUPLED RADICALS

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A review is given of recent advances in the construction of (quasi)diabatic model Hamiltonians and their application to analyzing the spectroscopy of molecules with strong vibronic coupling. A numerical application to the vibronic levels of the BNB radical below 0.6 eV is presented, together with corresponding adiabatic (quantum chemistry) calculations. The agreement with the experimental levels is nearly quantitative with the model Hamiltonian, attesting to the power of the approach. On the contrary, it is also revealed that the magnitude of the nonadiabatic contributions to the zero-point energy and the lowest fundamental frequency of the coupling mode are considerably larger than expected, at least by your narrator.