FRANCK–CONDON SPECTRAL CALCULATION ON TRANS–HYDROQUIONE USING CORRELATION FUNCTION APPROACH

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IVR in polyatomic molecules has been found to be extremely fast even at energies as low as a few hundred wavenumbers. In order to understand the IVR dynamics better one can proceed to calculate the fluorescence spectra and compare with the experimental data. However, for polyatomic molecules with large number of vibrational modes even calculating a simple Franck–Condon spectrum is not a simple task. As a first step towards this we have calculated the excitation and dispersed fluorescence spectra of hydroquinone, *ab initio*, using a correlation function approach using a quadratic Hamiltonian. Time dependent coupled cluster method was used to propogate the wavefunction in time. The comparison between the calculated and experimental spectra will be presented and the validity of the method will be discussed vis–á–vis the observed IVR behaviour.