VIBRONIC COUPLING IN ASYMMETRIC DIMERS: GENERALIZATION OF THE FULTON-GOUTERMAN APPROACH

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Fulton and Gouterman proposed a theory for the modeling of vibronic spectra of bichromophores with a symmetry operation exchanging the individual monomers.[a] This model has proven useful for computing absorbtion and emission spectra for the $S_1 \leftarrow S_0$ and $S_2 \leftarrow S_0$ electronic transitions of the dimer when there is coupling to the vibrational levels.[b] We have extended the FG model to cases where the bichromophore lacks a symmetry operation. This new model will cover systems with asymmetries arising from the environment, conformation, or composition of the dimer. Application of this theory to the spectra of the asymmetric bichromophore d5-diphenylmethane (diphenylmethane with all of the aromatic hydrogens on one phenyl group replaced by deuterium atoms) will be presented and compared to high resolution laser-induced fluorescence (LIF) and single vibronic level fluorescence (SVLF) experimental spectra.[c]

[a] R. Fulton and M. Gouterman, *J. Chem. Phys.* 25, 1059-1071 (1961).
[b] P. Ottiger, S. Leutwyler, and H. Köppel, *J. Chem. Phys.* 131, 204308 (2009).
[c] Zwier, private communication