Radiative and nonradiative electron transfer in donor-acceptor compounds

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Synthetic and spectral studies of electronic and molecular structure have been performed for a number of electron donor-acceptor (D-A) compounds, including TICT molecules. The CT character of the lowest excited singlet states has been investigated by means of the solvatochromic effects on the spectral position and profile of the stationary absorption and fluorescence spectra. The mechanism of the CT absorption and/or CT emission has been discussed in terms of the Mulliken-Murrell model of the CT complexes and the Marcus formalism of radiative electron transfer. The determination of the electronic transition dipole moments corresponding to the CT absorption and CT fluorescence and the band-shape analysis of the corresponding spectra lead to the quantities relevant for the CT→S_0 radiative charge recombination in the Marcus inverted region. Moreover, it has been shown that Marcus theory can be applied for the quantitative description of the radiationless charge recombination processes in cases when intersystem crossing to the excited triplet states may be neglected. The experimental and computational results led us to propose a simple model which allows to predict the photophysical behavior of a particular D-A compound from the properties of its donor and acceptor moieties.
