Structural aspects of the mechanism of photochemical radical pair formation in crystalline fluorene containing acridine

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In previous work [1] experiments have been reported to demonstrate that, in crystalline fluorene ($C_{13}H_{10}$) containing acridine ($C_{13}H_9N$) in small molar fraction, radiation from a mercury lamp leads to radical pair formation ($C_{13}H_9\cdot$ and $C_{13}H_9NH\cdot$) within 10^{-6} s; the acridine triplet state is concluded to be an unlikely precursor of this radical pair. We investigated the structural aspects of the acridine molecules as guests in the fluorene crystal, with acridine simulated to be in either the ground state or excited states, by the method of atom–atom potential energy functions. The results show that in either case only a relatively small distance prevails between the nitrogen atom of a guest molecule and a hydrogen atom of a methylene group in adjacent fluorene host molecules, thus facilitating the hydrogen atom transfer process. The structure of the radical pair is also being investigated.

1 R. Furrer, F. Fujara, C. Lange, D. Stehlik and W. Vollmann, *Chem. Phys. Lett.*, *76* (1980) 383 - 389, and references cited therein.

Exciton fusion simulations on binary and ternary lattices: cluster effects

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Monte Carlo simulations of exciton annihilation on random binary and ternary lattices were performed for various combinations of random excitation, random walk, trapping, decay and fusion. The variables included concentrations and excitation densities. The results are compared with the theory of homogeneous kinetics and with experiments on mixed naphthalene crystals. The emphasis is on the effects of clusters and percolation.

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