

The microscopic model of electron transfer reactions in disordered solid matrices.

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ABSTRACT

The original model of the hopping mechanism for electronic conduction in photosensitive organic materials is considered. The electron transfer (ET) in active centers of such systems proceeds via local intra- and intermolecular modes. The active modes, as a rule, operate beyond the kinetic regimes, which are usually postulated in the existing theories of the ET. Our alternative dynamic ET model for local modes immersed in the continuum harmonic medium is formulated for both classical and quantum regimes, and accounts explicitly for the mode/medium interaction. The kinetics of the energy exchange between the local ET subsystem and the surrounding environment determine essentially the total ET rate. The efficient computer code for rate computations is elaborated. The computations are available in the wide range of system parameters, such as the temperature, external field, the local mode frequency and the characteristics of the mode/medium interaction.

The computational algorithm is based on the technique elaborated earlier for treating H-atom transfer reactions but differs from it by several details. The most important amongst them is the idea of analytic continuation of the correlation function, representing the medium frequency spectrum, to the lower complex time half-plane. It assured the systematic and successful convergence of the rate integrals which is now extended down to a relatively low- temperature kinetic regimes. The relation of the present approach to the Marcus ET theory and to the underlying quantum-statistical reaction rate theory (Levich-Dogonadze, 1959; Dogonadze et al and Jortner et al, 1970-1980) is discussed and illustrated by the results of computations for practically important target systems.