Discrete-state approach to the time evolution of molecular states. Del Re, Giuseppe; Foerner, Wolfgang; Hofmann, Detlef; Ladik, Janos.

Abstract

The general formalism for determining Born probabilities assocd. with transitions between sets of coupled localized states of mols. is developed and discussed. Special emphasis has been put to the nature of the states involved and to the filtering effects of prepn. and detection in processes like redox action involving distant sites of the same redox mol. Numerical examples are given, and steps to be followed in the anal. of a concrete case are illustrated in detail on preliminary results. These were obtained in studying intramol. electron transfer in the iron-imidazole part of a heme group.