PHOTODISSOCIATION DYNAMICS OF RADICALS: THEORY AND TRAJECTORY STUDIES

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A theoretical study of the markedly nonstatistical dissociation dynamics of the ethyl radical is done by fully numerical classical trajectory calculations on a coupled-cluster-quality potential surface. Analysis of the trajectories finds long-lived quasiperiodic orbits. An analysis of the trajectories in the complete phase space was done using time-frequency analysis via a wavelet transform. Comparisons of the lifetimes to Lyapunov exponents, Kolmogorov entropy, and a scalar orbital complexity show that the lifetime against dissociation in an individual trajectory for the ethyl radical is clearly correlated to the degree of nonergodicity in that trajectory. The particular degrees-of-freedom involved in the dynamical trapping are also identified. Inverse wavelet transforms indicate that structured spectra should be seen in these cases.