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Short-time dynamics detail mechanism of Fe(CO)5 dissociation

The sub-picosecond dynamics of gas-phase Fe(CO)5 have been simulated by the fewest switches surface hopping method based on TDDFT (CAM-B3LYP) forces. The dynamics simulations were initiated in the S6 1MLCT state corresponding to the optically bright transition in the UV absorption spectrum centered at 266 nm. We show that in-phase oscillations of predominantly axially coordinated carbonyl leads to periodic population transfer to the dissociative 1MC states. On a similar timescale, large amplitude angular distortions analogous to the established ground state pseudorotation give changes in bonding that are explained in terms of frontier molecular orbitals. The analysis of the dynamics reveals periodic bursts of CO occurring on 90 fs intervals that correspond to the period of axial C-C stretching. Fluctuations in the electronic structure are also discussed for iron-complexes in solution, including simulations of spectroscopic observables.

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