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Title:Femtosecond transient absorption, nanosecond time-resolved resonance Raman, and density functional theory study of fenofibric acid in acetonitrile and isopropyl alcohol solvents
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Abstract:Hydrogen abstraction reaction of fenofibric acid (FA) in acetonitrile and isopropyl alcohol solvents was studied by femtosecond transient absorption (fs-TA) and nanosecond time-resolved resonance Raman (ns-TR3) spectroscopy experiments. The singlet excite state (1FA) (nΠ*) with a maximum transient absorption at 352 nm observed in the fs-TA experiments undergoes efficient intersystem crossing (ISC) to convert into a nΠ* triplet state FA (3FA) that exhibits two transient absorption bands at 345 and 542 nm. The nΠ* 3FA species does not decay obviously within 3000 ps. In the ns-TR3 experiments, the nΠ* 3FA is also observed and completely decays by 120 ns. Compared with the triplet states of benzophenone (BP) and ketoprofen (KP), the nΠ* 3FA species seems to have a much higher hydrogen abstraction reactivity so that 3FA decays fast and generates a FA ketyl radical like species. In isopropyl alcohol solvent, the nΠ* 3FA exhibits similar reactivity and promptly abstracts a hydrogen from the strong hydrogen donor isopropyl alcohol solvent to generate a ketyl radical intermediate. With the decay of the FA ketyl radical, no light absorption transient (LAT) intermediate is observed in isopropyl alcohol solvent although such a LAT species was observed after similar experiments for BP and KP. Comparison of the ns-TR3 spectra for the species of interest with results from density functional theory calculations were used to elucidate the identity, structure, properties, and major spectral features of the intermediates observed in the ns-TR3 spectra. This comparison provides insight into the structure and hydrogen abstraction reactivity of the triplet states of BP derivatives.
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