TIME-RESOLVED RAMAN STUDIES OF THE ELECTRON ADDUCTS OF BENZOATE ANION IN WATER

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Benzoate anion, a widely used food preservative, undergoes redox reactions, particularly in soft drinks, to produce benzene, a well known carcinogen. We are currently examining the structure and kinetic properties of the radical intermediates derived from this molecule for a better understanding of the reaction pathways that would allow controlling the end product. In this study, the reaction of benzoate anion with the solvated electron was induced by electron pulse irradiation of oxygen-free water. The chemical transients produced in the reaction were studied by time-resolved resonance Raman spectroscopy. The electron addition to the benzoate anion initially produces a dianion radical which absorbs at 440nm. The dianion radical reacts with water, with a reaction period of about 10 ns, to form the protonated monoanion radical with a small blue shift of approximately 10 nm in the absorption maximum. However, the resonance Raman spectra of the two transients differ greatly. Also, the overall enhancement of the resonance Raman signals was orders of magnitude lesser than that of other transient species having comparable extinction coefficients. This observation suggests that these radicals undergo very fast photochemistry that competes with the Raman scattering process. The details of the vibrational spectroscopic and kinetic findings of this ongoing study will be discussed in this presentation.