

Abstract Submitted  
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**Vibrational Coherences and Proton-Transfer Dynamics of Ionized Phenoxide in Aqueous Solution Observed by Few-Femtosecond Transient Absorption Spectroscopy.** TUSHAR DEBNATH, MUHAMMAD SHAFIQ MOHD YUSOF, PEI JIANG LOW, ZHI HENG LOH, Nanyang Tech Univ — Optical transient absorption spectroscopy with few-cycle (6-fs) pulses elucidates ionization-induced vibrational coherences and proton-transfer dynamics of small molecules in aqueous solution. Strong-field ionization of sodium phenoxide ( $\text{C}_6\text{H}_5\text{O}^- \text{Na}^+$ ) yields the phenoxyl radical ( $\text{C}_6\text{H}_5\text{O}^{\circ-}$ ) and the hydrated electron. The former appears as an absorption band at 400 nm atop the broad absorption feature of the hydrated electron. The phenoxyl radical absorption band exhibits pronounced amplitude and energy modulations in the time domain, which upon Fourier transformation, yields its vibrational frequencies. These frequencies are assigned with the aid of density-functional theory calculations and are comparable to those obtained from gas-phase and argon matrix measurements. Time-domain analysis of the vibrational coherences furnishes Huang-Rhys factors and dephasing times for the vibrational modes that are coupled to the ionization transition. Finally, the transient absorption spectrum reveals a feature at 428 nm that is assigned to the phenol radical cation ( $\text{C}_6\text{H}_5\text{OH}^{\circ+}$ ). The formation of the radical cation species within the instrument response of our experiment suggests that ionization-induced proton transfer (IIPT) from the solvent (water) to the phenoxyl radical occurs on the sub-10-fs timescale. Our results shed light on the elementary ultrafast dynamics that accompany the interaction of ionizing radiation with molecules of biological relevance.

Tushar Debnath  
Nanyang Tech Univ

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