PHOTOELECTRON-PHOTOFRAGMENT COINCIDENCE SPECTROSCOPY OF TERT-BUTOXIDE AND THE CARBANION ISOMER

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The photodetachment dynamics of the $C_4H_9O^-$ anion, produced by proton abstraction from tert-butanol has been studied using a cryogenically-cooled linear electrostatic ion trap to store a fast ion beam[b]. The ion trap is coupled with a Photoelectron-Photofragment Coincidence spectrometer for a kinematically complete experiment in which dissociative neutral intermediates of known internal energy are created by photodetachment of a stable molecular anion. By collecting all resultant neutral fragments from the dissociation event in coincidence with the detached electron using time- and position-sensitive detectors, the correlated momenta and energies of all products can be determined. At 388, 537, and 600nm, both stable and dissociative photodeatchment processes of $C_4H_9O^-$ are observed. The stable channel is consistent with previous photodetachment spectrum from *tert*-butoxide anion[c] as well as a Franck-Condon simulation of the photoelectron spectrum. The dissociative channel is consistent with a methyl loss from an alkylhydroxy radical. Results will be analyzed in the context of calculations employing MP2/6-311++G(d,p) and CBSQ level of theory.

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