ELECRONIC STRUCTURE OF ALKOXY RADICAL ISOMERS FROM ANION PEI SPECTROSCOPY

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Anion photoelectron imaging spectra of two butenoxyl (3-buten-1-oxyl and 3-buten-2-oxyl) radical isomers are presented. The neutral electron affinities are comparable to those measured for saturated alkoxy radicals [Ramond et al., J. Chem. Phys. 112, 1158 (2000)], and the measured term energies for the à ²A state of both isomers is approximately 0.1 eV. However, spectra of the two isomers exhibit distinct differences, particularly in the low electron binding energy signal that may be due to the presence of structural isomers. The experimental spectra are analyzed with supporting MP2 calculations and Franck-Condon simulations. Overall, the results underscore how the electronic properties vary with subtle changes in alkoxy radical structure, which may have implications for atmospheric photochemistry, as alkoxy radicals are key intermediates of the tropospheric oxidation of volatile organic compounds.

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