A FIVE-CARBON UNSATURATED CRIEGEE INTERMEDIATE: SYNTHESIS, SPECTROSCOPIC IDENTIFICATION, AND THEORETICAL STUDY OF 3-PENTEN-2-ONE OXIDE

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Biogenic alkenes, such as isoprene and α-pinene are the prominent source of volatile organic compounds (VOCs) emitted into the atmosphere. Atmospheric processing of alkene molecules via reaction with ozone leads to formation of zwitterionic reactive intermediates with a carbonyl oxide functional group, known as Criegee intermediates (CIs).[c] CIs exhibit strong absorption $\pi^* \leftarrow \pi$ in the near ultraviolet and visible (UV-vis) region due to the carbonyl oxide moiety. Previously, this laboratory reported the electronic spectra of the four-carbon CIs with unsaturated substituents derived from isoprene ozonolysis, methyl vinyl ketone oxide (MVK-oxide) and methacrolein oxide (MACR-oxide), on the first $\pi^* \leftarrow \pi$ to transition under jet-cooled conditions.[d,e] In the present study, we focus on the laboratory identification of a five-carbon, unsaturated Criegee intermediate 3-penten-2-one oxide, which can be produced upon atmospheric ozonolysis of substituted isoprenes. The UV–vis induced depletion spectrum of 3-penten-2-one oxide was recorded via depletion of the VUV photoionization signal (at 10.5 eV) on the m/z 100 mass channel using a time-of-flight mass spectrometer (TOF-MS). The effects of an additional methyl group in the stability of the CI and its associated electronic properties are revealed by comparing the experimentally observed UV–vis spectrum of the 3-penten-2-one oxide with isoprene-derived CI, MVK-oxide.

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