INFRARED SPECTRA OF GASEOUS (Z)-3-IODO-BUT-2-EN-1-YL [C$_2$H$_3$C(CH$_3$)I] RADICAL, METHYL VINYL KETONE OXIDE [C$_2$H$_3$(CH$_3$)OO] CRIEGEE INTERMEDIATE, AND C$_2$H$_3$C(=C(CH$_3$))OO PEROXY RADICAL PRODUCED UPON PHOTODISSOCIATION OF (Z)-1,3-DIODO-BUT-2-ENE [(CH$_2$I)HC=C(CH$_3$)I] IN OXYGEN

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Methyl vinyl ketone oxide [MVKO, C$_2$H$_3$C(CH$_3$)OO], an important Criegee intermediate in ozonolysis of isoprene, was recently identified in laboratories with near infrared action spectrum (to produce OH) using photolysis of a gaseous mixture of 1,3-diiodo-but-2-ene [(CH$_2$I)HC=C(CH$_3$)I] and O$_2$ , but its mid-infrared spectrum and the detailed mechanism of its formation remains unexplored. We employed a step-scan Fourier-transform infrared spectrometer to investigate the reaction intermediates. Upon irradiation at 248 nm of gaseous (Z)-1,3-diiodo-but-2-ene, the (Z)-3-iodo-but-2-en-1-yl [C$_2$H$_3$C(CH$_3$)I] radical was observed, indicating the fission of the terminal allylic C-I bond, not the central vinylic C-I bond. This radical is characterized by infrared absorption bands at 1406, 1261, 1109, 1019, 924, and 902 cm$^{-1}$. Upon irradiation at 248 nm of a gaseous mixture of (Z)-1,3-diiodo-but-2-ene and O$_2$ at 35 Torr, the Criegee intermediate MVKO, characterized by infrared absorption bands at 1416, 1383, 1346, 1060, 987, 948, and 908 cm$^{-1}$, was observed. At pressure 236 Torr, the reaction adduct 3-iodo-but-1-en-1-yl-peroxy [C$_2$H$_3$C(=C(CH$_3$))OO] radical, characterized by infrared absorption bands at 1375, 1296, 1213, 1161, 1108, 1063, 986, 934, and 885 cm$^{-1}$, was observed. These new spectra of C$_2$H$_3$C(CH$_3$)I, C$_2$H$_3$C(=C(CH$_3$))OO, and C$_2$H$_3$C(=C(CH$_3$))OO provide valuable information for the understanding of the formation mechanism of the Criegee intermediate MVKO from the source reaction of photolysis of (CH$_2$I)HC=C(CH$_3$)I in O$_2$ in laboratories.

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