

SUPPLEMENTARY INFORMATION

Tracking the reaction networks of acetaldehyde oxide and glyoxal oxide Criegee intermediates in the ozone-assisted oxidation reaction of crotonaldehyde

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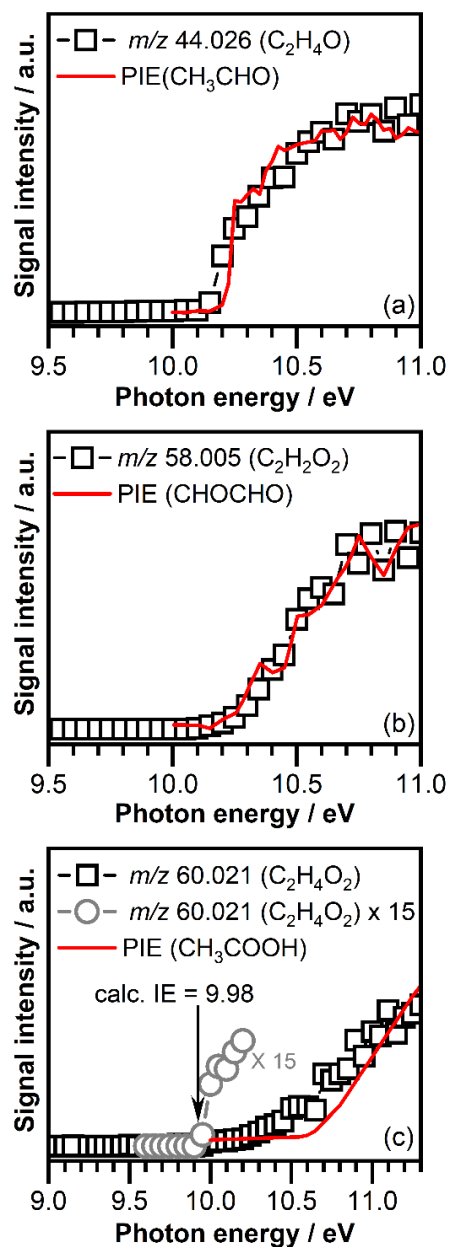


Figure S1: Photoionization identification of the oxidation products recorded at (a) m/z 44.026 (C_2H_4O), (b) m/z 58.005 ($C_2H_2O_2$), and (c) m/z 60.021 ($C_2H_4O_2$) in the JSR experiment at a temperature of 390 K (open symbols). Solid read lines correspond to the measured photoionization spectra of (a) acetaldehyde,¹ (b) glyoxal,² and (c) acetic acid.³ Indicated by an arrow in panel (c) is the calculated adiabatic ionization energy of glycolaldehyde.⁴

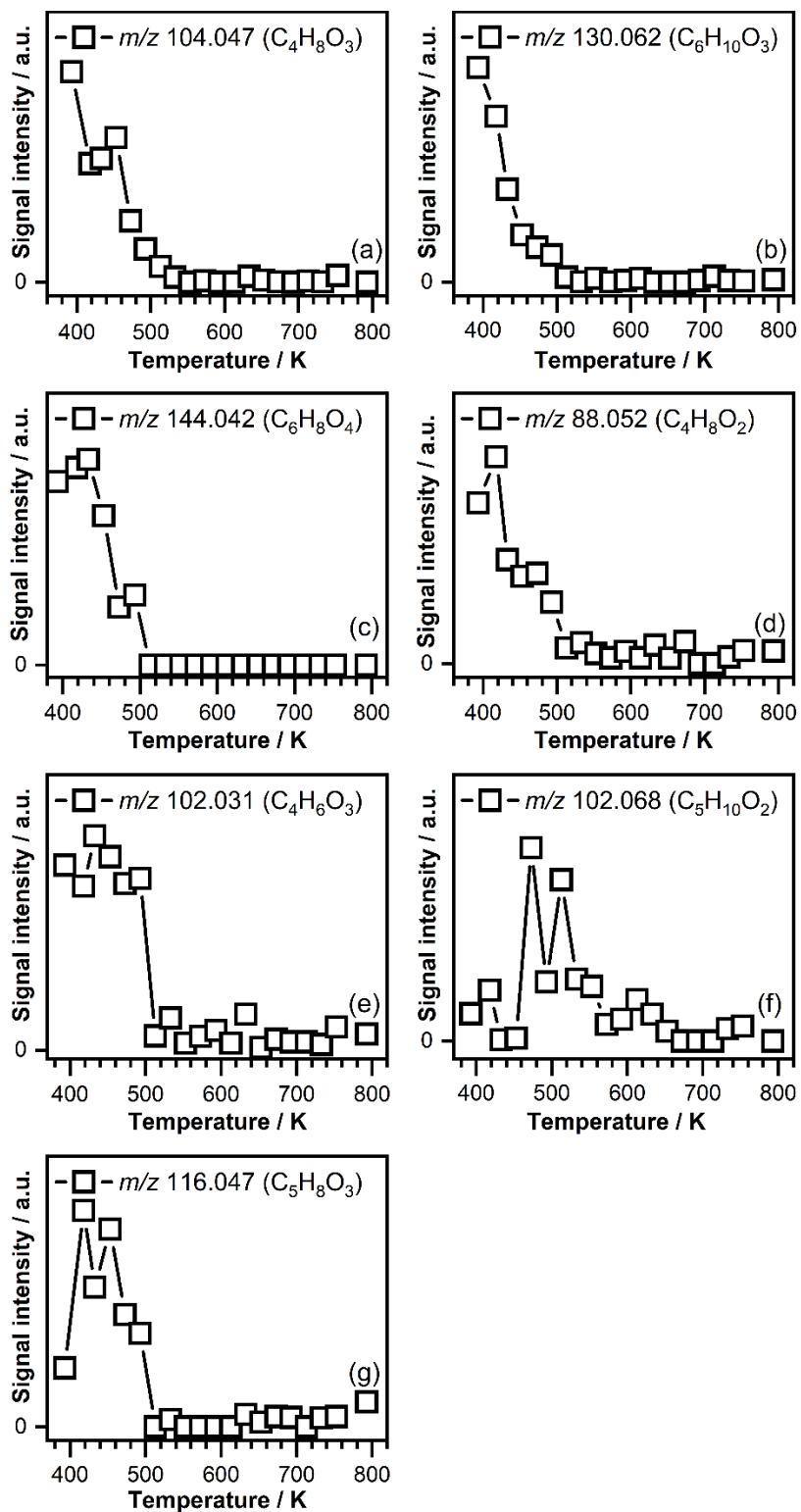


Figure S2: Temperature profiles recorded at a photon energy of 10.50 eV at (a) m/z 104.047, (b) m/z 130.062 (c) m/z 144.042, (d) m/z 88.052, (e) m/z 102.031, (f) m/z 102.068, and (g) m/z 116.047 corresponding to bimolecular reaction products of CI-1 and CI-2.

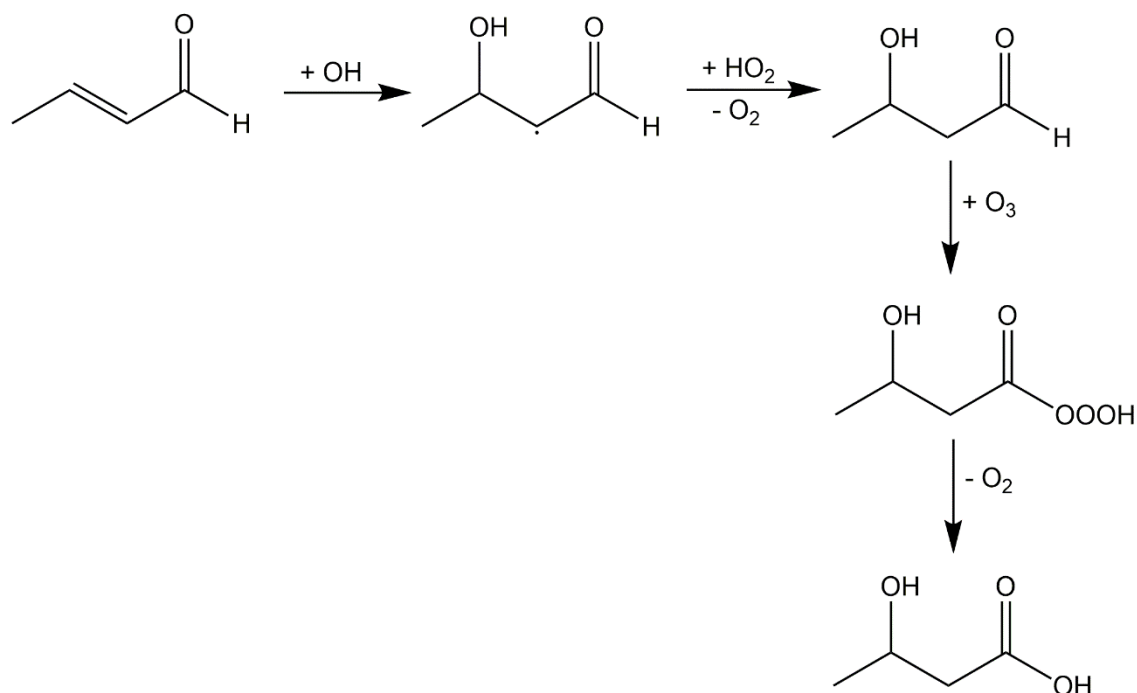


Figure S3: The formation channel of the 3-hydroxybutanoic acid. The 1,3-dipolar insertion of ozone into the C-H bond of 3-hydroxybutanal to form 3-hydroxy-1-trioxidaneylbutan-1-one, and its subsequent decomposition involving intramolecular H transfer to form 3-hydroxybutanoic acid and molecular oxygen has been adopted from literature.^{5,6}

References:

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