Supplementary Information

for

Effect of NOx on product yields and Arrhenius parameters of gas-phase oxidation of β-ocimene initiated by OH· radicals

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Content Summary

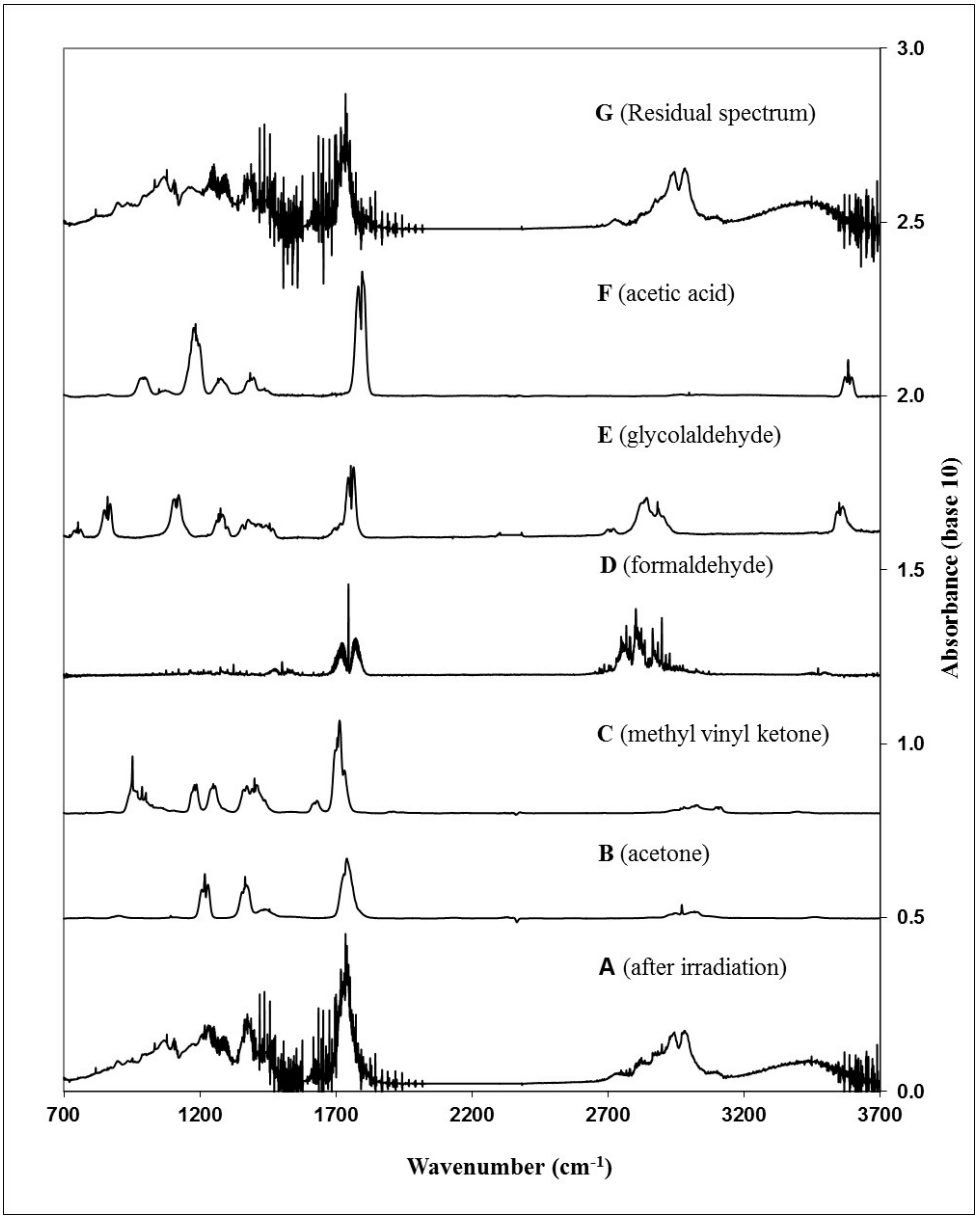

Figure S1: Panel A shows the infrared spectrum of a β-ocimene/H_2O_2/air reaction mixture after irradiation and subtraction of residual β-ocimene. Panels B, C, D, E and F show reference spectra of acetone, methyl vinyl ketone, formaldehyde, glycolaldehyde, and acetic acid, respectively. Panel G shows the residual product spectrum obtained after subtraction of features due to the reference spectra from the spectrum in panel A.

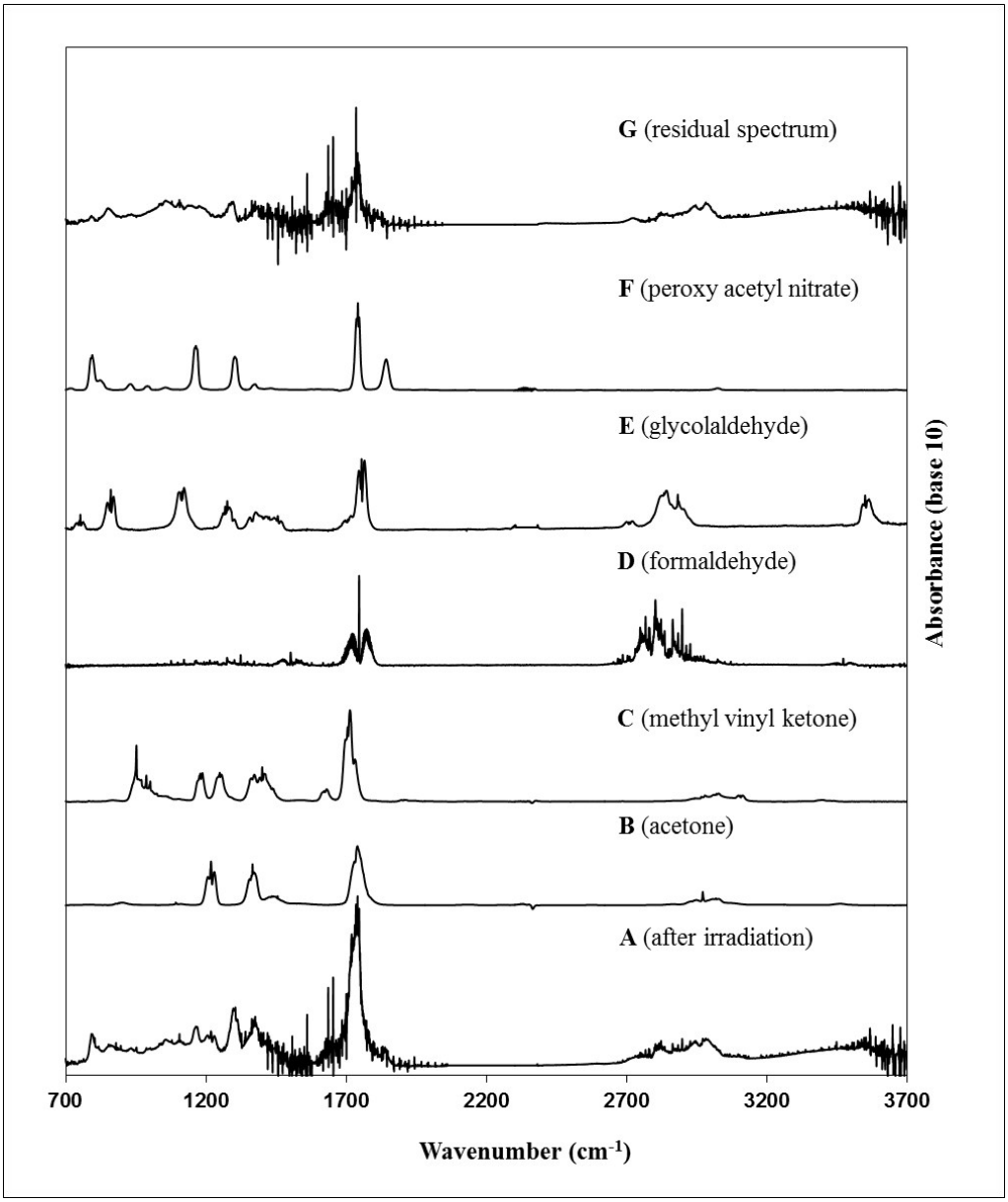

Figure S2: Panel A shows the infrared spectrum of a β-ocimene/H_2O_2/NO_X/air reaction mixture after irradiation and subtraction of residual β-ocimene. Panel B, C, D, E and F show reference spectra of acetone, methyl vinyl ketone, formaldehyde, glycolaldehyde, and peroxy acetyl nitrate, respectively. Panel G shows the residual product spectrum obtained after subtraction of features due to the reference spectra from the spectrum in panel A.

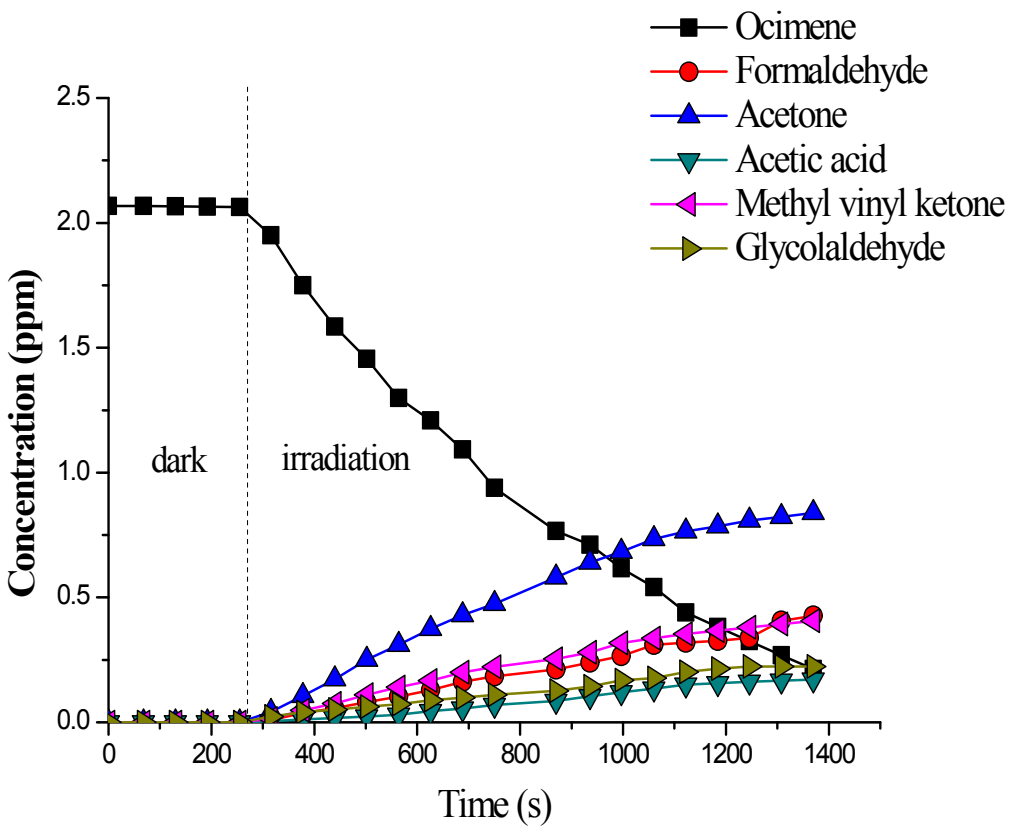

Figure S3: Concentration-time profiles of ocimene and the reaction products formaldehyde, acetone, methyl vinyl ketone, glycolaldehyde and acetic acid **(in the absence of NO_x)** obtained from the irradiation of a β-ocimene/H_2O_2/air reaction mixture.

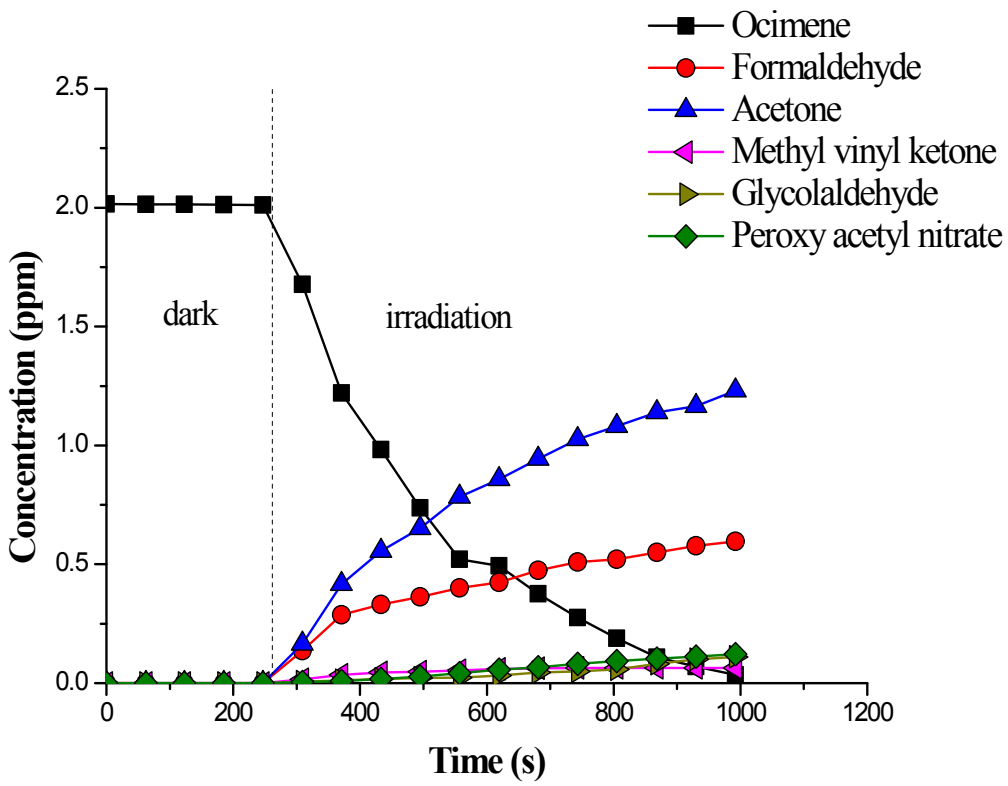

Figure S4: Concentration-time profiles of ocimene and the reaction products formaldehyde, acetone, methyl vinyl ketone, glycolaldehyde and peroxy acetyl nitrate **(in the presence of NO_x)** obtained from the irradiation of a β-ocimene/H_2O_2/NO_x/air reaction mixture.

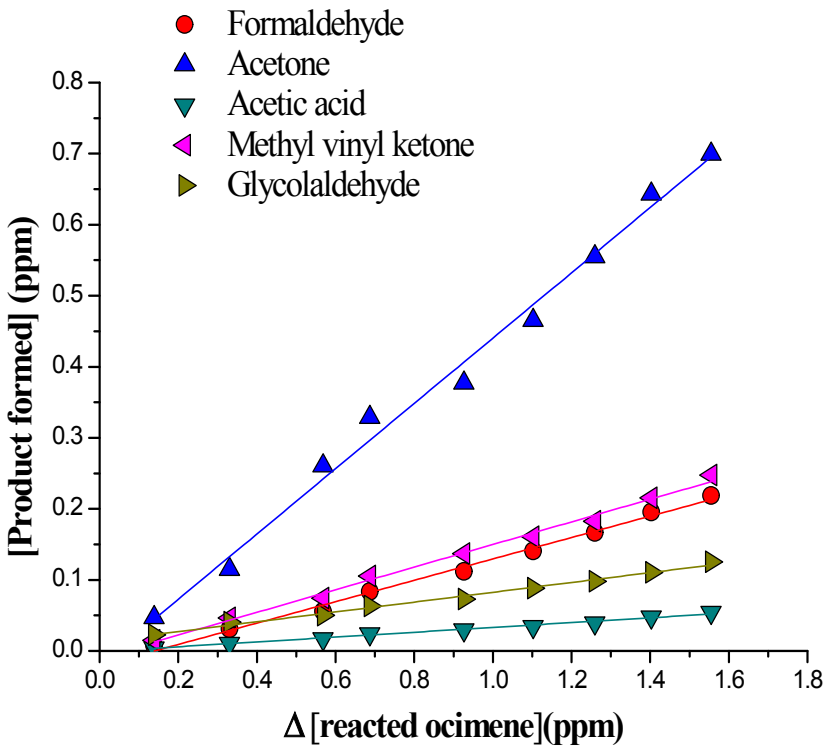

Figure S5: Plots of the concentrations of the reaction products formaldehyde (○), acetone (△), acetic acid (▽), methyl vinyl ketone (◁) and glycolaldehyde (▷) as a function of reacted β-ocimene obtained from the irradiation of a β-ocimene/H_2O_2/air reaction mixture in the absence of NO_x.

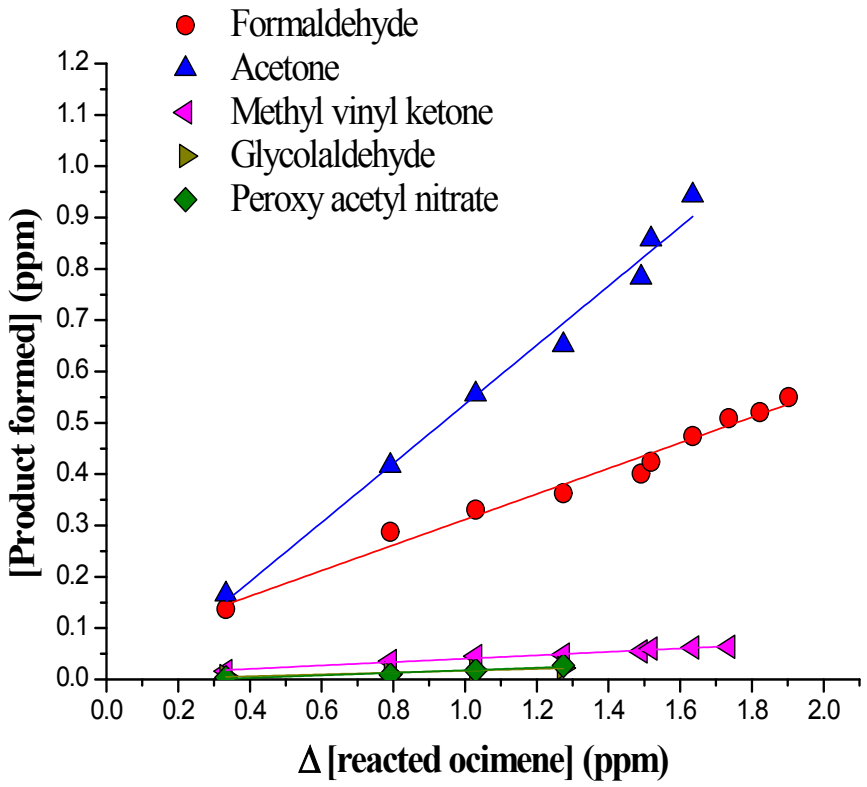

Figure S6: Plots of the concentrations of the reaction products formaldehyde (○), acetone (Δ), methyl vinyl ketone (◁), glycolaldehyde (▷) and peroxy acetyl nitrate (◇) as a function of reacted β-ocimene obtained from the irradiation of a β-ocimene/H_2O_2/air reaction mixture in the presence of NO_x.

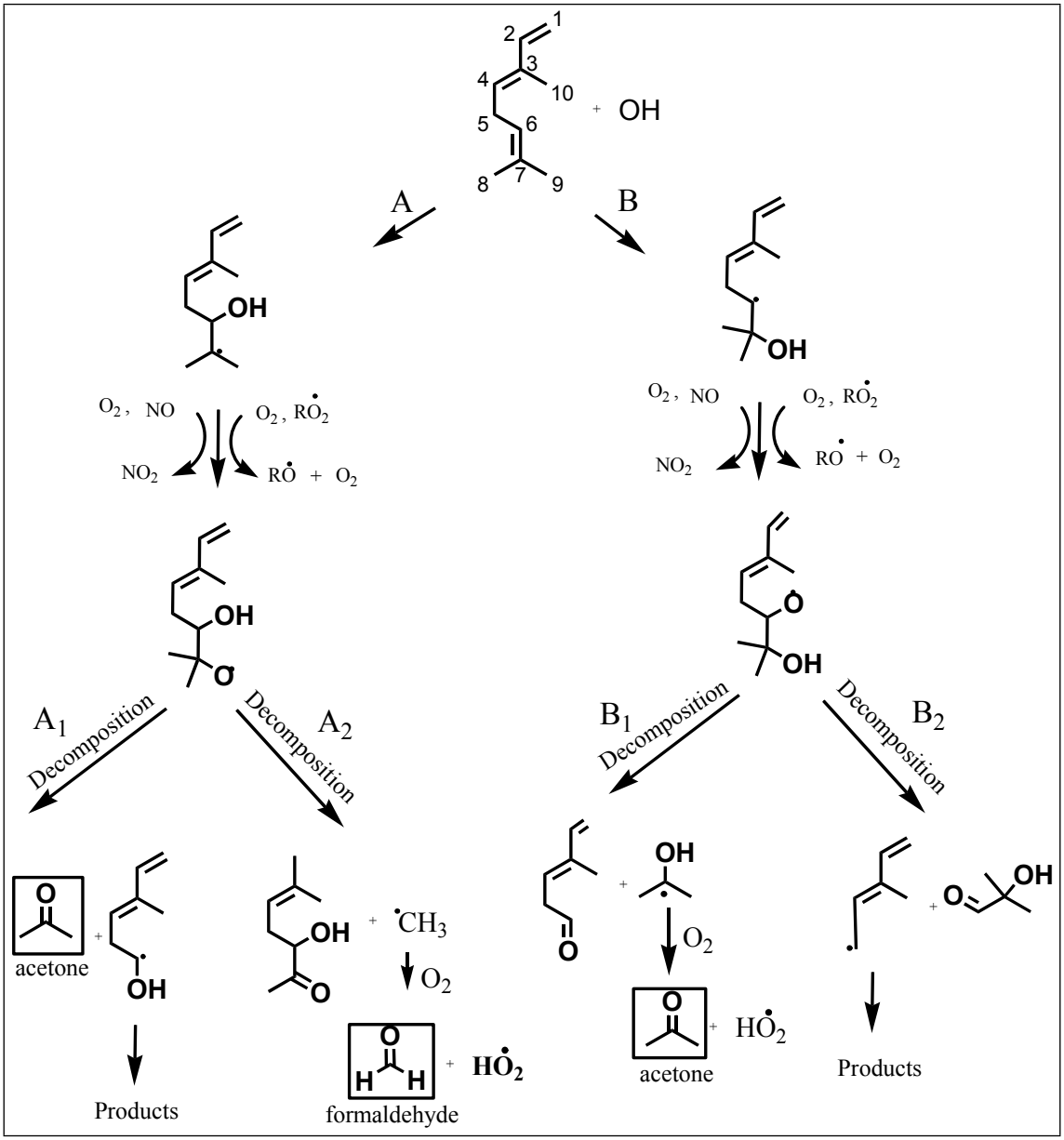

Figure S7. Simplified mechanism for the OH·-radical initiated oxidation of β-ocimene via addition of OH· to the double bond binding C_6 and C_7.

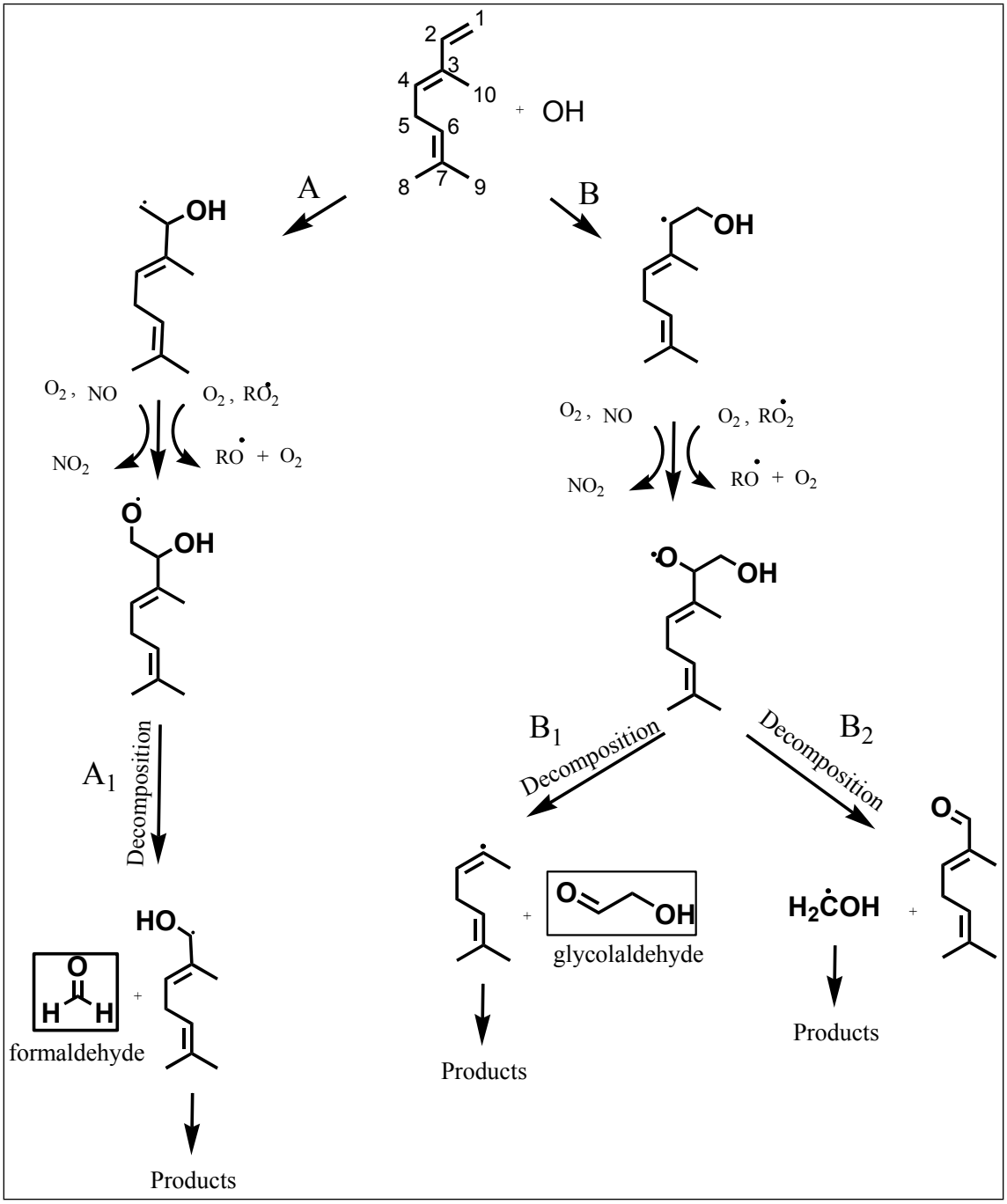

Figure S8. Simplified mechanism for the OH·-radical initiated oxidation of β-ocimene via addition of OH· to the double bond binding C_1 and C_2.

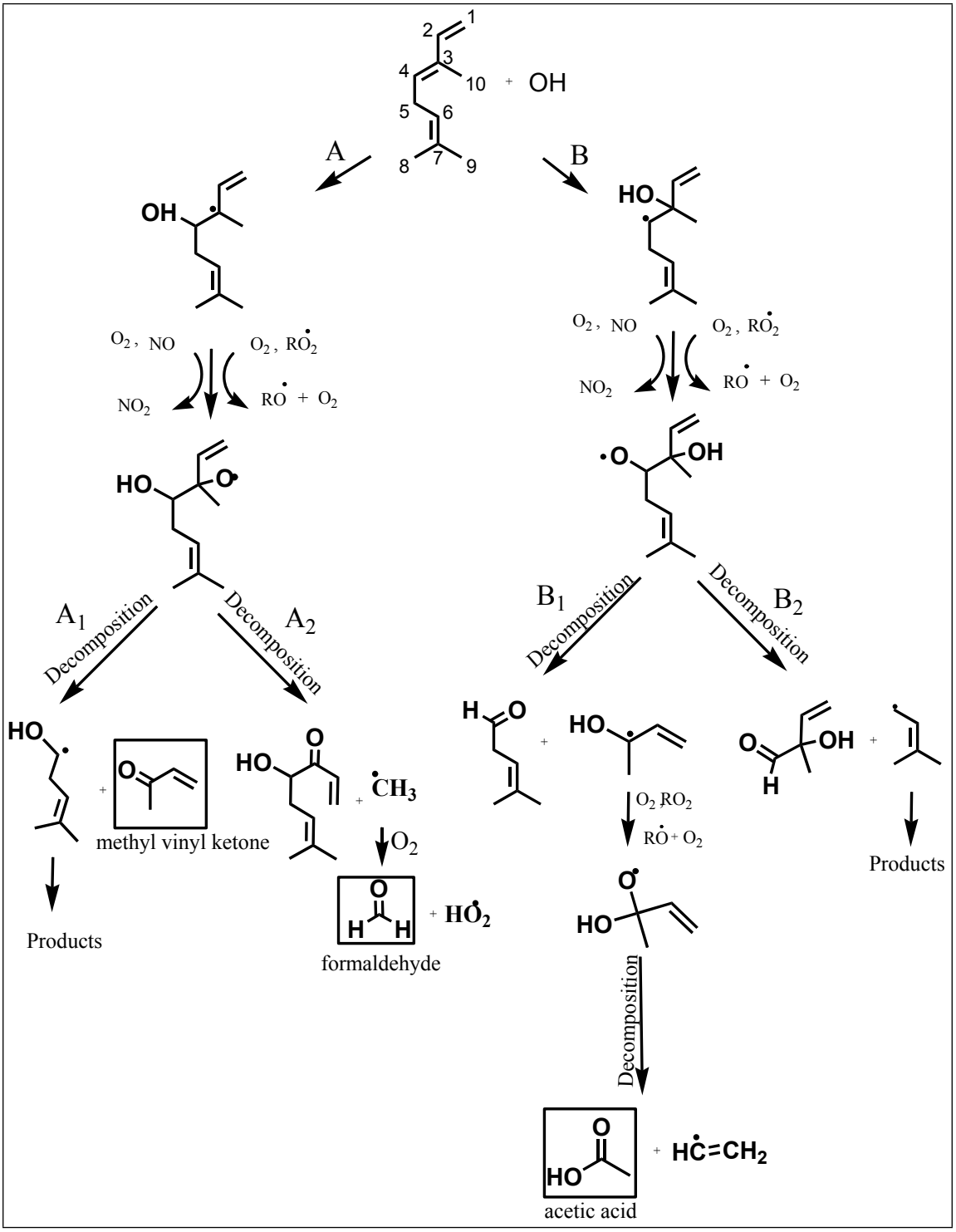

Figure S9. Simplified mechanism for the OH·-radical initiated oxidation of β-ocimene via addition of OH· to the double bond binding C_3 and C_4.