Electronic Supplementary Information (ESI)

Gas-Phase Degradation of 2-butanethiol Initiated by OH Radicals and Cl Atoms. Kinetics, Product Yields and Mechanism at 298K and Atmospheric Pressure

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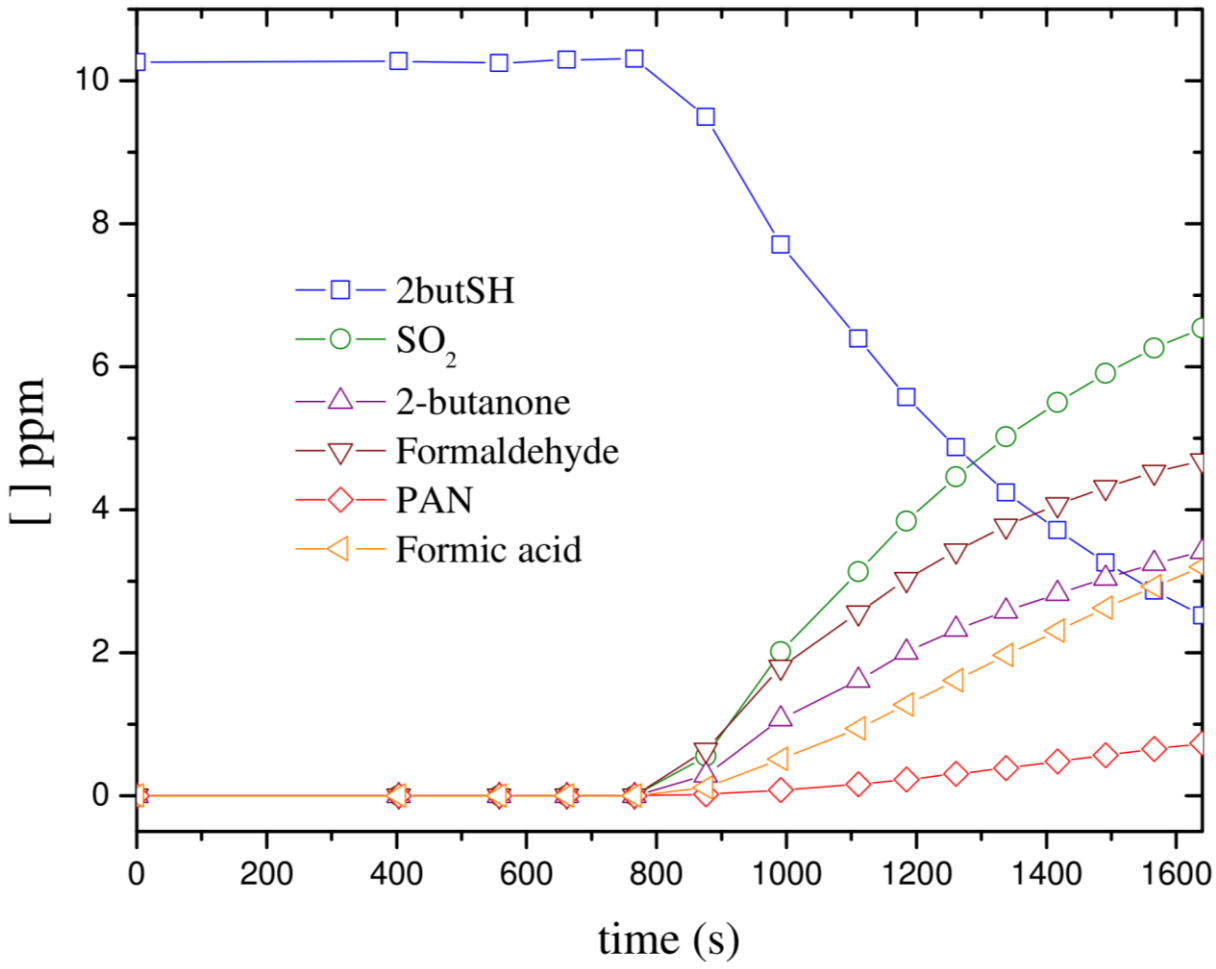

Figure S 1. Plots of Concentration-time profile of products arising from reactions of 2butSH with OH radicals at atmospheric pressure of synthetic air and 298 K.

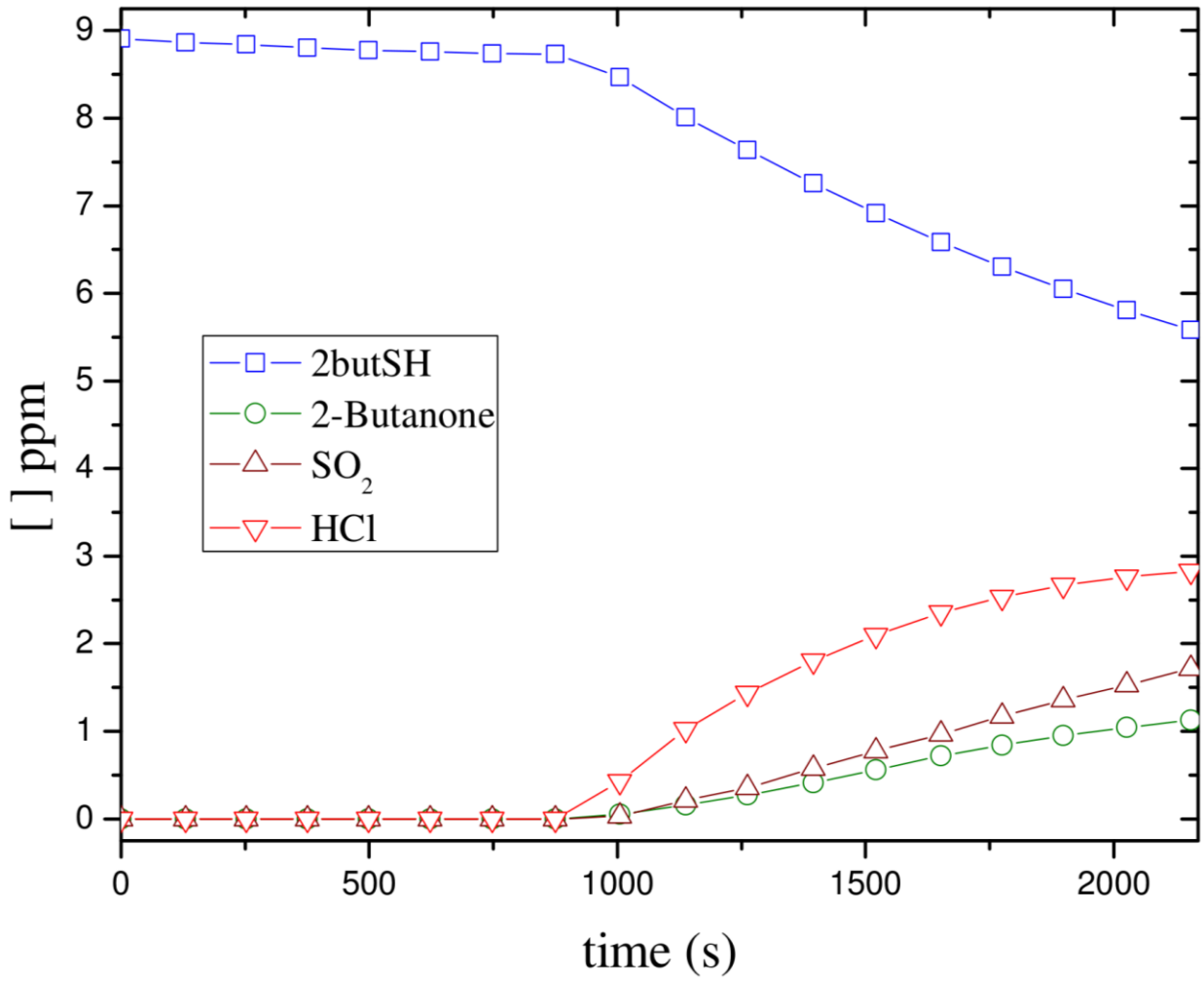

Figure S 2. Plots of Concentration-time profile of products arising from reactions of 2butSH with Cl atoms at atmospheric pressure of synthetic air and 298 K.

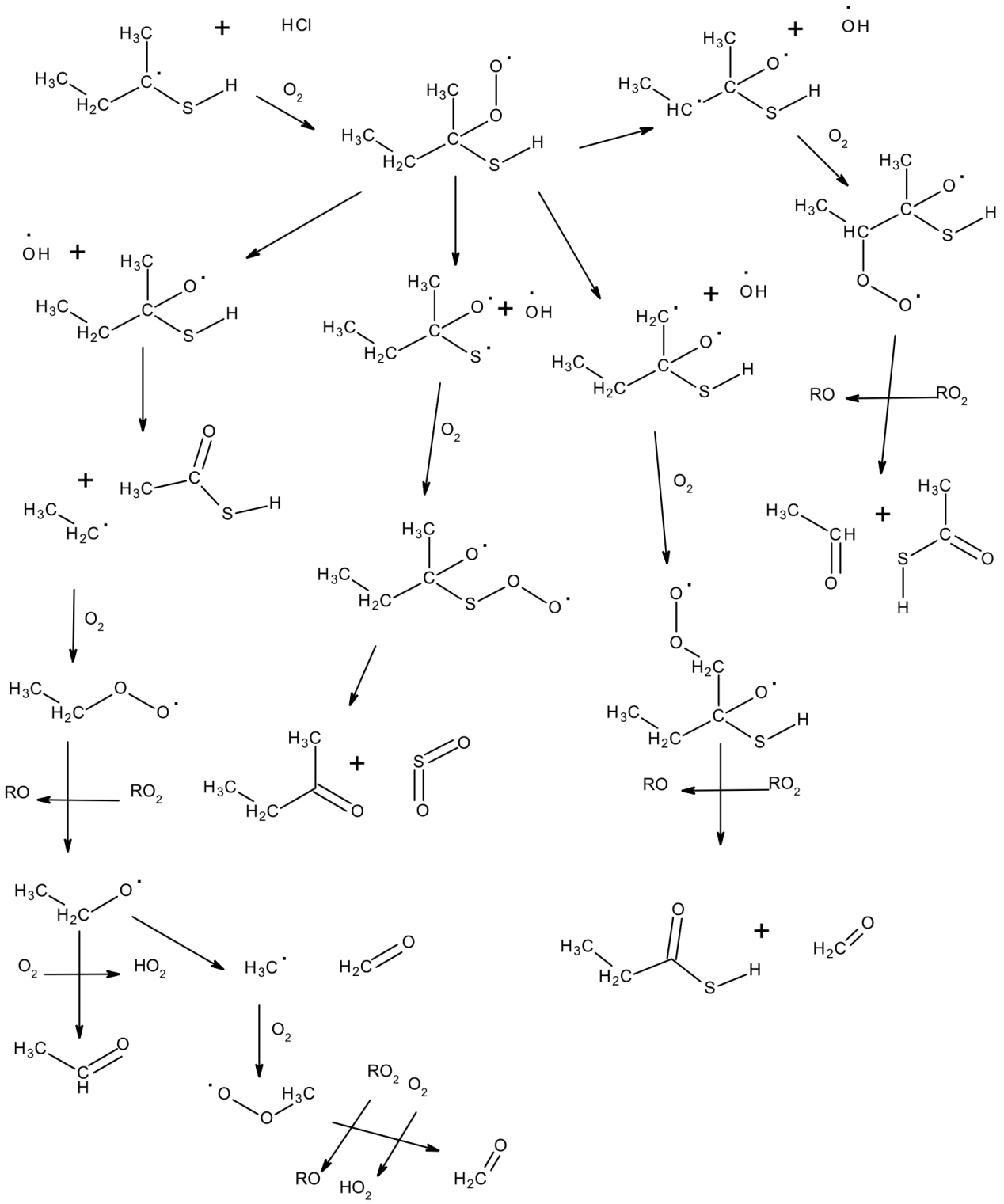

Figure S 3. Proposed mechanism for the OH radical and Cl atoms oxidation of 2butSH at 298 K and atmospheric pressure of synthetic air. The mechanism show the possible pathways for H-abstraction on the C-H groups of the alkyl chain of the 2butSH.

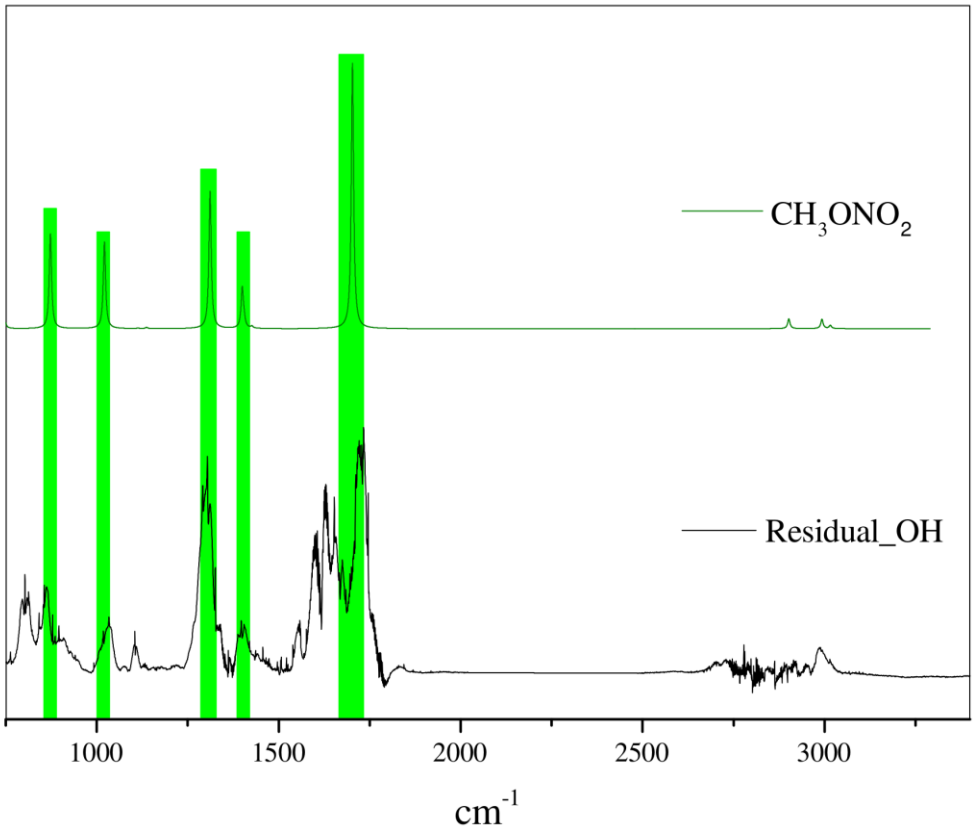

Figure S 4. Comparison between the calculated spectrum of methyl nitrate (CH_3ONO_2) with the residual spectra of OH initiated oxidation experiment (trace H). Black line shows the residual spectrum after of subtract the spectrum of the identified compounds and green line shows the theoretical spectrum calculated at wB97X-D[1]/6-31G(d,p)[2] level of theory using g09[3] software package. scaling factor of 0.949 was used. Good agreement was obtained between the spectra, especially in the IR features at 1311 cm and 1702 cm

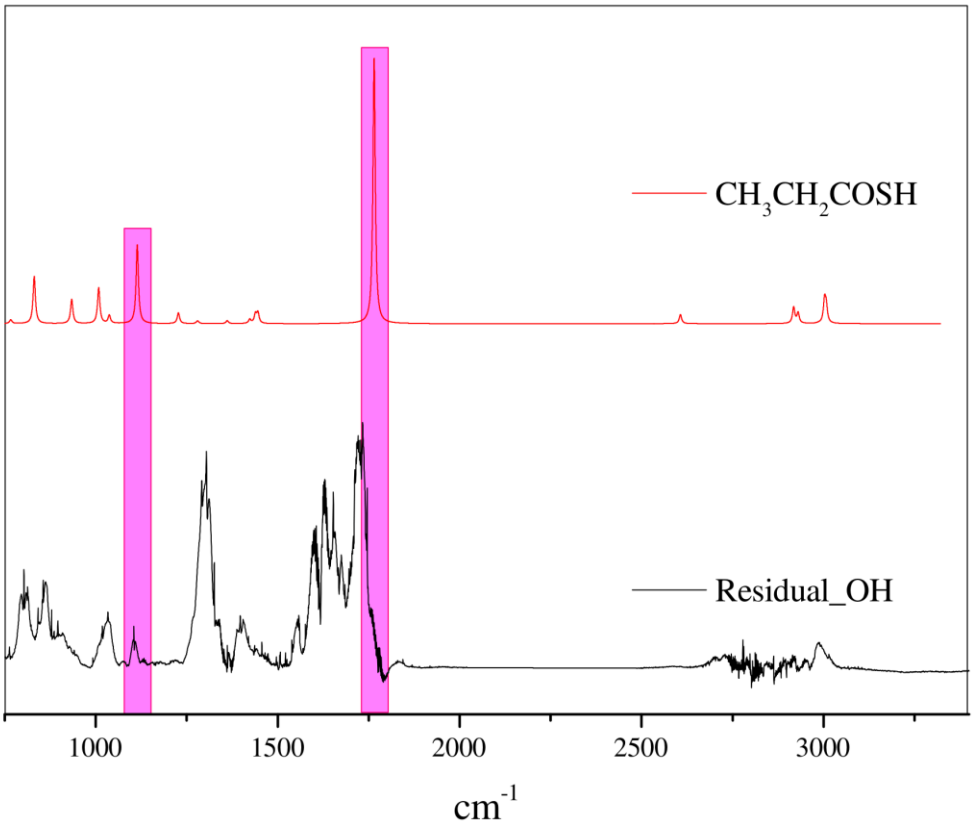

Figure S 5. Comparison between the calculated spectrum of ethanethioic S-acid (CH_3COSH) with the residual spectra of OH initiated oxidation experiment (trace H). Black line shows the residual spectrum after of subtract the spectrum of the identified compounds and red line shows the theoretical spectrum calculated at wB97X-D[1]/6-31G(d,p)[2] level of theory using g09[3] software package. scaling factor of 0.949 was used.

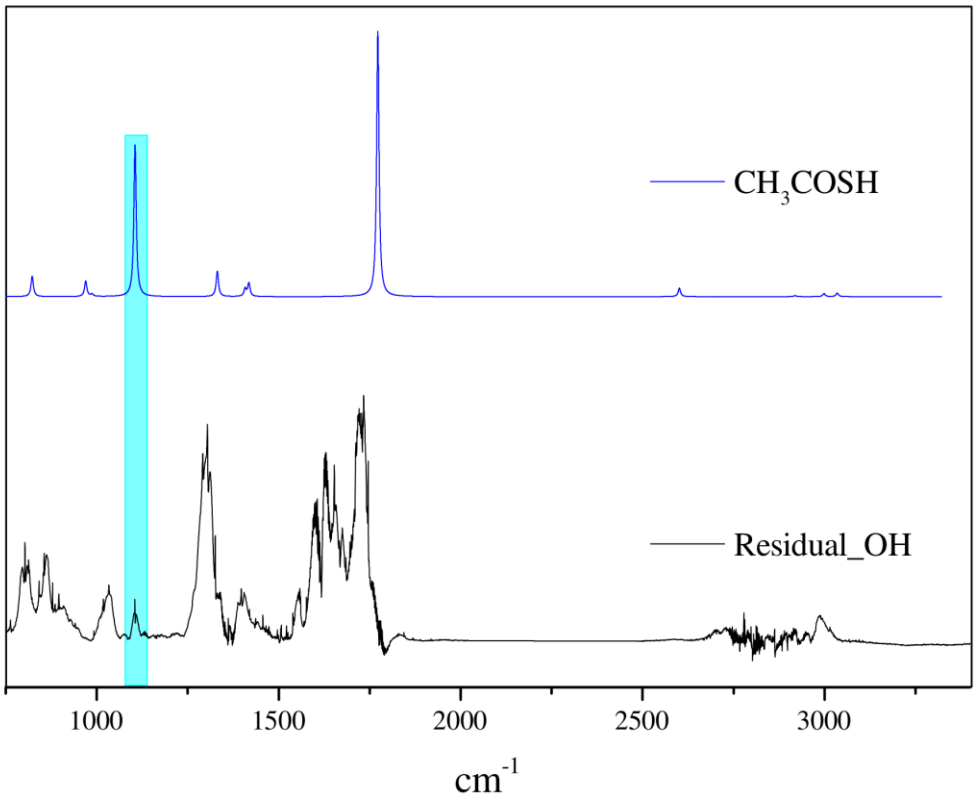

Figure S 6. Comparison between the calculated spectrum of propanethioic S-acid (CH_3CH_2COSH) with the residual spectra of OH initiated oxidation experiment (trace H). Black line shows the residual spectrum after of subtract the spectrum of the identified compounds and blue line shows the theoretical spectrum calculated at wB97X-D[1]/6-31G(d,p)[2] level of theory using g09[3] software package. scaling factor of 0.949 was used.

References.

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