Supporting Information: Different Chlorine and Hydroxyl Radical Environments Impact *m*-xylene Oxidation Products

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Modeled chamber spectra and potential model error

The blacklight spectrum used in the SAPRC model in this study is shown in Figure S1 alongside literature absorption cross sections¹ for radical precursors. Absorption spectra for CINO₂ and H_2O_2 fall in the tail of the blacklight emissions spectrum and small differences in the spectra would substantially alter the anticipated photolysis rate.



Figure S1: UV blacklight spectrum and relevant absorption cross sections. Inset shows small overlap between UV blacklight spectrum and H_2O_2 absorption cross section.

Experimental time series

Time series of radical precursors and key gas phase species are shown here for Experiments 3, 8, 9 and 10 in Figures S2-5.



Figure S2: Experiment 3 ($Cl_2 + NO$) precursor consumption and selected product formation. Dashed vertical line indicates end of illumination period.



Figure S3: Experiment 8 ($Cl_2 + CINO_2$) precursor consumption and selected product formation. Dashed vertical line indicates end of illumination period.



Figure S4: Experiment 10 ($CI_2 + CINO_2 + H_2O_2$) precursor consumption and selected product formation. Dashed vertical line indicates end of illumination period.



Figure S5: Experiment 9 ($CI_2 + H_2O_2$) precursor consumption and selected product formation. Dashed vertical line indicates end of illumination period.



Figure S6: Experiment 1 (CINO₂) consumption of CINO₂ and nocturnal formation of CINO₂ and N_2O_5

Modeled and measured m-xylene consumption

Chamber modeling and measured decay of *m*-xylene normalized to maximum concentration.



Figure S7: Experiment 4 consumption of m-xylene and chamber modeled consumption.



Figure S8: Experiment 2 consumption of m-xylene and chamber modeled consumption.



Figure S9: Experiment 6 consumption of m-xylene and chamber modeled consumption

Modeled oxidant exposures



Figure S10: Modeled CI and OH exposures for CI radical precursor experiments.

References

S. P. Sander, R. R. Friedl, D. M. Golden, M. J. Kurylo, G. K. Moortgat, P. H. Wine, a R. Ravishankara, C. E. Kolb, M. J. Molina, S. Diego, L. Jolla, R. E. Huie and V. L. Orkin, Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies Evaluation Number 15, *Cross Sect.*, 2006, California, 1–153.