

Supplementary material

Glyoxal SOA chemistry: effects of dilute nitrate and ammonium and support for organic radical-radical oligomer formation

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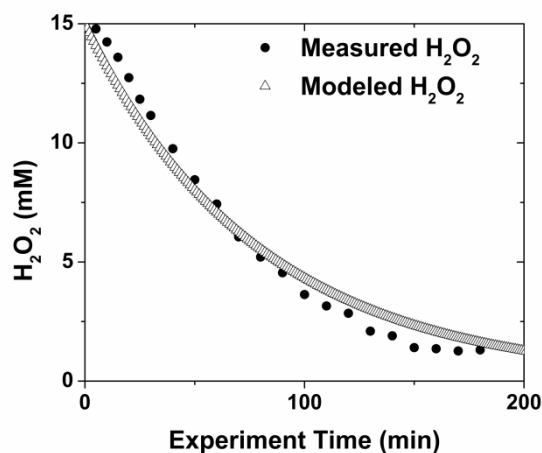
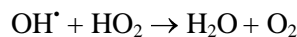
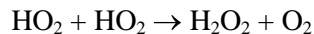
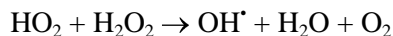
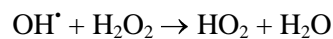
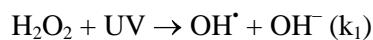


Fig. S1. Measured and modelled H_2O_2 concentration in H_2O_2 + UV control experiment. The concentration of H_2O_2 as a function of time in the H_2O_2 + UV control experiments was modelled (FACSIMILE for Windows Version 4.1.45) using the following reactions and rate constants provided by Lim et al.^[1] with the exception of k_1 .



The H_2O_2 photolysis rate constant, $k_1 = 1.0 \times 10^{-4}$ was determined by fitting the model to measured H_2O_2 concentrations. This value of k_1 was then used in the FACSIMILE model for glyoxal to estimate the concentration of OH^\bullet (M; $[\text{OH}^\bullet]_{\text{initial}} = 7.8 \times 10^{-13}$, $[\text{OH}^\bullet]_{\text{final}} = 6.0 \times 10^{-12}$, $[\text{OH}^\bullet]_{\text{average}} = (1 \pm 2) \times 10^{-12}$) during glyoxal experiments from initial precursor concentrations (e.g., 5 mM H_2O_2 , 1 mM GLY).^[1]

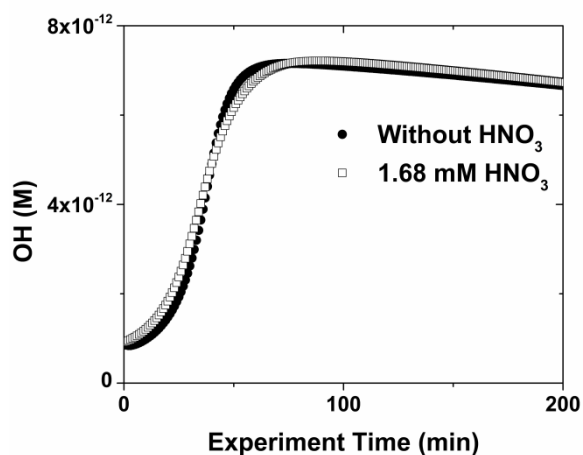


Fig. S2. Modelled OH[•] concentration in GLY + OH[•] in the presence and absence of HNO₃. Note OH[•] is formed from H₂O₂ photolysis and reacts with GLY and its reaction products. Inclusion of HNO₃ reactions discussed in the methods does not change [OH[•]] prediction.

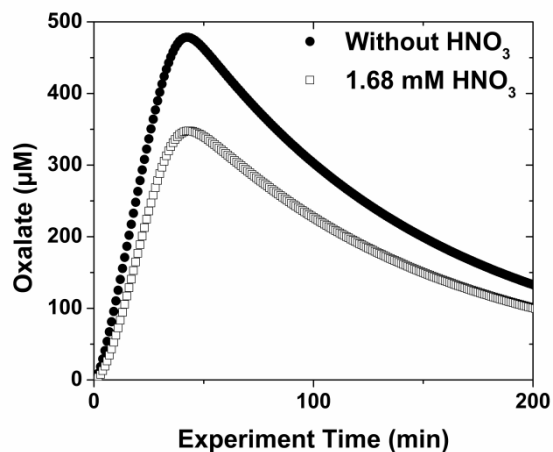


Fig. S3. Modelled oxalate concentrations from GLY + OH[•] with and without HNO₃.

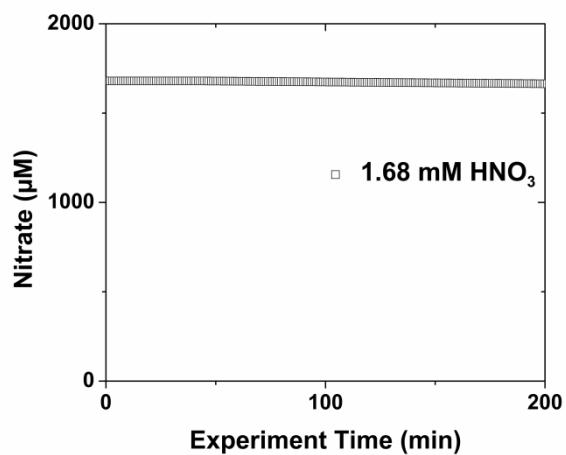


Fig. S4. Modelled nitrate concentration in $\text{GLY} + \text{OH}^\bullet + \text{HNO}_3$ experiment.

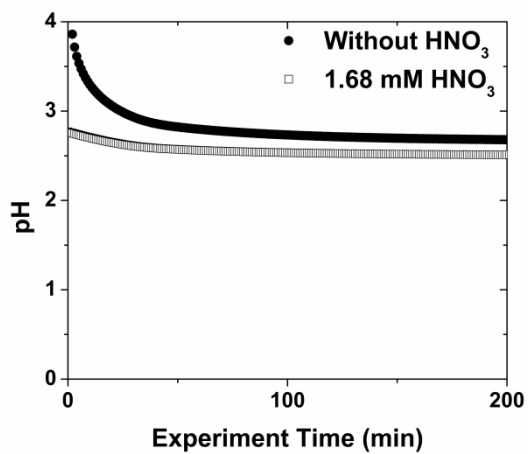


Fig. S5. Modelled pH in $\text{GLY} + \text{OH}^\bullet$ experiments conducted in the presence and absence of HNO_3 .

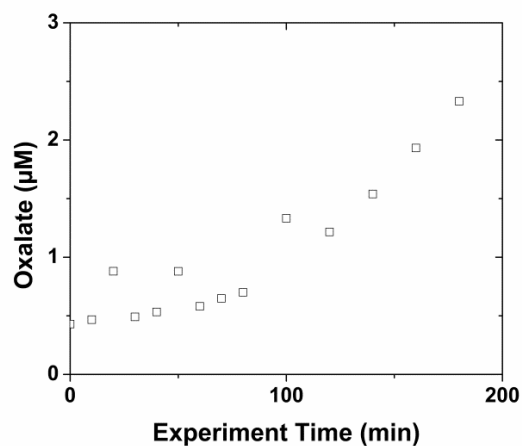


Fig. S6. Oxalate concentration measured by IC in GLY + HNO₃ + UV control experiment. Some oxalate formation is seen, but concentrations are much lower and formation is much slower than in GLY + OH[•] + HNO₃ experiments. OH[•] production from HNO₃ + UV is modest.

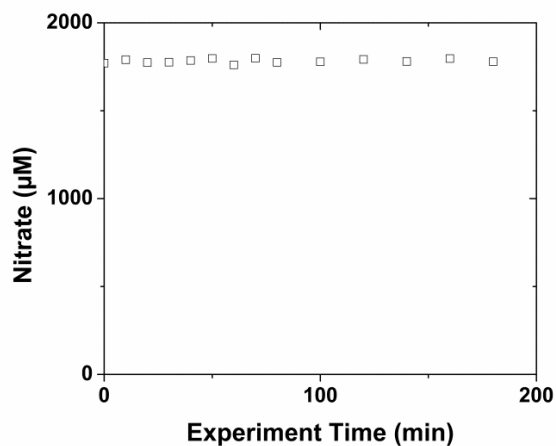


Fig. S7. Nitrate concentration measured by IC in GLY + HNO₃ + UV control experiment.

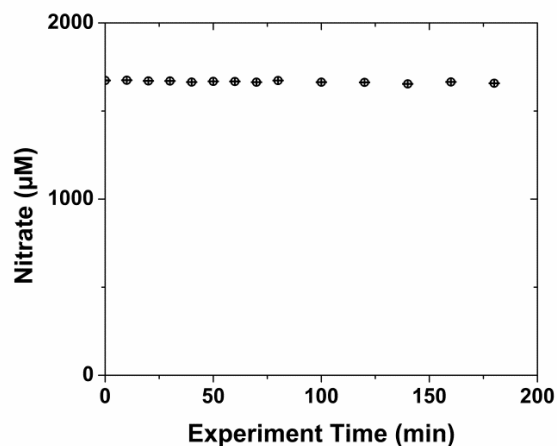


Fig. S8. Nitrate concentration measured by IC in GLY + OH[•] + HNO₃ experiment. Error bars represent the coefficient of variation (<1 %) across three experiments.

References

- [1] Y. B. Lim, Y. Tan, M. J. Perri, S. P. Seitzinger, B. J. Turpin, Aqueous chemistry and its role in secondary organic aerosol (SOA) formation. *Atmos. Chem. Phys.* **2010**, *10*, 10521–0539. [doi:10.5194/acp-10-10521-2010](https://doi.org/10.5194/acp-10-10521-2010)