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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Kinetics of dimethyl sulfide (DMS) reactions with isoprene-derived Criegee intermediates studied with direct UV absorption" *by* Mei-Tsan Kuo et al.

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Dear colleagues,

During and after the publication of the Newland et al. (2015) paper on the impact of DMS in the isoprene + O3 system, quantum chemical and theoretical kinetic calculations on CI + DMS reactions were performed, prompted by the Newland et al. observations that show a fast reaction. These theoretical results were not published yet, but could be a useful addition to the Kuo et al. 2020 paper. The authors of the Kuo et al. paper have been contacted regarding a possible merging of the theoretical work.

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Discussion paper

The calculations explore the CH2OO + DMS reaction at a reasonable level of theory, finding only reaction pathways with an energy barrier of several kcal/mol. The rate coefficient derived was very low, k(298 K) = 5.6×10-19 cm3 molecule-1 s-1, indicating that DMS is apparently not consumed by CI. Calculations to investigate the role of DMS as a potential catalyst were also performed. For small CI, it was found that DMS does not react as an efficient catalyst. This matches the results of Kuo et al. (2020), as well as those of Newland et al (2015) who saw no nett DMS consumption. Exploratory calculations also showed that DMS does not catalyze redissociation of the cyc-CH2OOS(O)O- cyclo-adduct formed in the CI + SO2 reaction, which would have reduced the efficacy of the reference CI+SO2 reaction used by Newland et al. No other catalytic effects of DMS were investigated.

Reference

Newland, M. J., Rickard, A. R., Vereecken, L., Muñoz, A., Ródenas, M. and Bloss, W. J.: Atmospheric isoprene ozonolysis: impacts of stabilised Criegee intermediate reactions with SO2, H2O and dimethyl sulfide, Atmospheric Chem. Phys., 15(16), 9521–9536, doi:10.5194/acp-15-9521-2015, 2015.

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