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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Atmospheric Chemistry, Sources, and Sinks of Carbon Suboxide, C_3O_2" *by* Stephan Keßel et al.

Anonymous Referee #2

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General Comments: This is a thorough study of the atmospheric chemistry of carbon suboxide (C3O2) combining experimental and theoretical results with atmospheric modelling. The experimental results are in qualitative agreement with the previous determination of the rate constant for reaction with OH, and present a new determination of the rate constant for reaction with ozone. The theoretical results roughly support the experimentally determined rate constants and suggest some interesting species for future study. The paper is well written and the results are clearly presented.

Specific Comments: On line 16 of page 4 in the description of the theoretical calculations, it is stated without reference that the energies are expected to be accurate to within ∼2 kcal/mol. Is this true for the barrier heights for ozonolysis as well? Can you include a reference supporting the statement that the M05-2X geometries will be sufficient for future single point calculations? On line 11 of page 7 in the description of the

relative rate study, it is stated that significant reaction with surfaces, CH3ONO, NO, or radicals formed in the dark can be ruled out. Is reaction with HO2 accounted for? Or is it assumed to be slower that R3?

Technical Corrections: Page 8, line 25, "addiction"; SI page 1, at the top of the 2nd paragraph, the acronym "CI" is defined in the text but not in the supplemental information; Figure S2, the caption for the fourth image is somewhat confusing and in the caption for the fifth image "C-C bond is strongly elongates".

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