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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Atmospheric chemistry of trans-CF_3CH=CHF: products and mechanisms of hydroxyl radical and chlorine atom initiated oxidation" *by* M. S. Javadi et al.

Anonymous Referee #1

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The authors present an FTIR product study of the oxidation of trans-CF3CH=CHF, a potential replacement compound for CFC/HFCs. The studies are conducted using either OH or Cl atoms to initiate the oxidation. The methods used are certainly well-established, and the senior authors are certainly expert in this type of study. The work conducted using Cl-atoms seems thorough and complete. Effects of oxygen partial pressure on product yields are examined, and a quantitative explanation of the results (in terms of competing alkoxy radical reactions) is clearly presented. However, it is my opinion that more work on the OH system is required before publication in ACP can be recommended, for reasons described below.

The OH data presented indicate 100% yields of the two expected products, HCOF and CF3CHO, in the initial phases of the oxidation, with a noticeable decline in the yields of these species as the oxidation progresses. The authors present a possible explanation for this observation, the reaction of the relevant alkoxy radicals with NO2 to produce nitrates, but this hypothesis is not fully developed or tested - e.g., were any nitrate absorption bands evident in the spectra? Were any experiments conducted with small amounts of added NO2 to test the hypothesis? How much NO2 was present at the onset of the curvature, and what does this say about the reactivity of the alkoxy radicals? With respect to this last question, the decomposition of hydroxy-alkoxy radicals is usually quite rapid, and is at least sufficiently rapid in this case to render reaction with O2 negligible. I would suspect that only a few mTorr of NO2 are present at the onset of curvature? If this is sufficient NO2 to compete with alkoxy decomposition, this would be a significant finding. In summary, it seems to me that more experiments and analysis can and should be done to answer these and related questions.

There are also a couple of minor points that require clarification: 1) The text refers to 2-14% conversion of the parent compound, but Figure 2 shows larger conversions (more than 2 mTorr lost out of initial 8-10 mTorr mentioned in the figure caption). 2) The caption to Figure 2 refers to data "obtained in the absence of NO". Does this refer to experiments conducted without any NO added initially? These experiments are not talked about in the text, I don't think.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 1069, 2008.