Warming Refrigerants?

P. Sebastianelli^{1*}, C. Griffith², M. C. P. Taylor³, S.H. Kable³, C. S. Hansen³, M.J.T. Jordan²

¹ School of Earth, Atmospheric and Life Science, University of Wollongong, Wollongong, Australia ² School of Chemistry, University of Sydney, Sydney, Australia ³ School of Chemistry, University of New South Wales, Sydney, Australia

* Corresponding author: Paolo Sebastianelli [paolos@uow.edu.au]

Abstract

Hydrofluoroolefins (HFOs) are used as fourth-generation refrigerants. They have been thought to be promising chemical replacements for previous refrigerants due to their zero ozone-depleting potential (ODP) and assumed low global warming potential (GWP) [Arora et al. 2018]. However, there has been recent evidence that HFOs could decompose under atmospheric conditions into hydrofluorocarbons (HFCs) [Campbell et al. 2021]. In this work, we explored theoretically the possible tropospheric photolysis pathways of one of the most important HFO breakdown products: fluorinated acetaldehydes. Three HFOs were considered: HFO-1234ze, HFO-1243ze, and HFO-1252ze, producing CF₃CHO, CHF₂CHO, and CH₂FCHO, respectively [Javadi et al. 2008]. Here, we show how their major tropospheric photolysis channels have been characterised by an accurate simulation protocol. A comparative analysis of the results reveals that HFO-1234ze has the highest likelihood of HFC production.

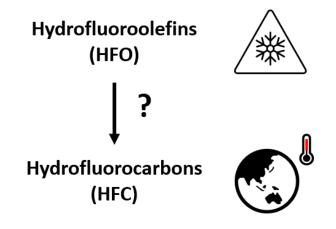


Fig. 1 - Are HFOs source of HFCs?

References

P. Arora, G. Seshadri, A.K. Tyagi (2018). Fourth-generation refrigerant: HFO-1234yf. *Current Science* 115, 1497-1503. https://www.jstor.org/stable/26978441

J. S. Campbell, K. Nauta, S. H. Kable, and C. S. Hansen (2021). Photodissociation dynamics of CF3CHO: C-C bond cleavage. *J. Chem. Phys.* 155, doi: 10.1063/5.0073974

M. S. Javadi, R. Søndergaard, O. J. Nielsen, M. D. Hurley, and T. J. Wallington (2008). Atmospheric chemistry of trans-CF3CH=CHF: Products and mechanisms of hydroxyl radical and chlorine atom-initiated oxidation. *Atmos. Chem. Phys.* 8, 3141–3147 doi: 10.5194/acp-8-3141-2008