Goldschmidt 2023 Abstract 31–38.
https://doi.org/10.7185/gold2023.20416

# Multiphase atmospheric fate of muconaldehyde

**NICOLAS BRUN**[1,2], JUAN MIGUEL GONZALEZ-SANCHEZ[2,3], SYLVAIN RAVIER[3], BRICE TEMIME ROUSSEL[3], SERGIO HARB[4], MANUELA CIRTOG[4], BÉNÉDICTE PICQUET-VARRAULT[4], MARCELLO BRIGANTE[5], GILLES MAILHOT[5], JEAN-LOUIS CLÉMENT[2] AND ANNE MONOD[6]

[1]Aix Marseille Univ, CNRS, LCE, Marseille

[2]Aix Marseille Univ, CNRS, ICR, Marseille, France

[3]Aix Marseille Univ, CNRS, LCE, Marseille, France

[4]Univ Paris Est Creteil and Université Paris Cité, CNRS, LISA, F-94010, Créteil, France

[5]Institut de Chimie de Clermont-Ferrand, Université Clermont Auvergne, CNRS, Clermont Auvergne INP, F-63000 Clermont-Ferrand, France

[6]Aix Marseille University, CNRS, LCE

Presenting Author: nicolas.brun@univ-amu.fr

The atmospheric reactivity of muconaldehyde, a non-commercial ring-opening product detected during the oxidation of aromatic species [1,2], has been scarcely studied.

Unsaturated dicarbonyl compounds such as muconaldehyde can easily partition into the atmospheric aqueous phase due to their high effective Henry's law constant driven by a fast hydration of the carbonyl functions and the salting in effect [3]. It is essential to study the atmospheric multiphase reactivity of these compounds since these polyfunctional compounds and their reaction products can contribute to secondary organic aerosol, ozone and radical formation in the boundary layer, and thus have direct implications for human health and climate.

In this work muconaldehyde was synthesized and purified using 3 different pathways. Its effective Henry's law constant was determined using a new simple and fast method. Its hydration was investigated using NMR spectroscopy. A set of kinetic experiments was performed on muconaldehyde to determine its aqueous photolysis, oxidation by ·OH and $SO_4^{\cdot-}$ as well as its gas phase oxidation by $NO_3$· and $O_3$, in complement to previous studies [4,5,6]. Kinetics results and investigation of products formation will be presented, and the inferred multiphase atmospheric fate of muconaldehyde will be discussed under various atmospheric conditions.

[1] Ghigo, & Tonachini (1999), *Journal of the American Chemical Society*, *121*(36), 8366–8372.

[2] Sato, Takami, Kato, Seta, Fujitani, Hikida, Shimono, & Imamura (2012), *Atmospheric Chemistry and Physics*, *12*(10), 4667–4682.

[3] Shen, Chen, Li, Qian, Qin, & Shi (2018), *Environmental Science and Technology*, *52*(19), 10997–11006.

[4] Klotz, Bierbach, Barnes & Becker (1995), *Environmental science & technology*, *29*(9), 2322-2332

[5] Klotz, Barnes, & Becker (1999), *International Journal of Chemical Kinetics*, *31*(10), 689–697.

[6] Xiang & Zhu (2007), *Chemical Physics Letters*, *450*(1–3),