Data for: Characterization of organic nitrate constituents of secondary organic aerosol (SOA) from nitrate-radical-initiated oxidation of limonene using high-resolution chemical

SND-ID: snd1047-1. **Version**: 1.0. **DOI**: https://doi.org/10.5878/002984

Citation

Hallquist, M. (2018) Data for: Characterization of organic nitrate constituents of secondary organic aerosol (SOA) from nitrate-radical-initiated oxidation of limonene using high-resolution chemical (Version 1.0) [Data set]. University of Gothenburg. Available at: https://doi.org/10.5878/002984

Alternative title

Iodide-HR-ToF-CIMS Data from NO3-initiated Oxidation of Limonene

Creator/Principal investigator(s)

Mattias Hallquist - University of Gothenburg, Department of Chemistry & Molecular Biology

Research principal

University of Gothenburg - Department of Chemistry & Molecular Biology

Description

The gas-phase nitrate radical (NO3*) initiated oxidation of limonene can produce organic nitrate species with varying physical properties. Low-volatility products can contribute to secondary organic aerosol (SOA) formation and organic nitrates may serve as a NOx reservoir, which could be especially important in regions with high biogenic emissions. This work presents the measurement results from flow reactor studies on the reaction of NO3 with limonene using a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer (HR-ToF-CIMS) combined with a Filter Inlet for Gases and AEROsols (FIGAERO). Major condensed-phase species were compared to those in the Master Chemical Mechanism (MCM) limonene mechanism, and many non-listed species were identified. The volatility properties of the most prevalent organic nitrates in the produced SOA were determined. Analysis of multiple experiments resulted in the identification of several dominant species (including C10H15NO6, C10H17NO6, C8H11NO6, C10H17NO7, and C9H13NO7) that occurred in the SOA under all conditions considered. Additionally, the formation of dimers was consistently observed and these species resided almost completely in the particle phase. The identities of these species are discussed, and formation mechanisms are proposed. Cluster analysis of the desorption temperatures corresponding to the analyzed particle phase species yielded at least five distinct groupings based on a combination of molecular weight and desorption profile. Overall, the results indicate that the oxidation of limonene by NO3 produces a complex mixture of highly oxygenated monomer and dimer products that contribute to SOA formation.

Purpose:
To explore the chemical composition of low-volatility gas and aerosol-phase species, formed from mixtures of N2O5 and limonene, as measured by a High Resolution Time-of-Flight Chemical Ionization Mass spectrometer (HR-ToF-CIMS) coupled to a Filter Inlet for Gases and AEROsols (FIGAERO) inlet.

The objectives of this work were three-fold namely, to: (i) determine the molecular formula of major nitrate species, produced from the reaction of limonene with NO3, that could contribute significantly to SOA formation and growth, (ii) compare the distribution of measured products to that of the expected products (formed via the Master Chemical Mechanism (MCM)) to identify any discrepancies in the mechanistic understanding of nitrate formation from limonene, and (iii) categorize, via cluster analysis, the thermodynamic desorption data measured for selected condensed-phase species.

Language

English

Study design

Experimental study

Data format / data structure

Numeric

Geographic spread

Geographic location: Sweden

Responsible department/unit

Department of Chemistry & Molecular Biology

Funding 1

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2015-04123

Funding 2

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2014-05332

Funding 3

- Funding agency: The Swedish Research Council Formas
- Funding agency's reference number: 2015-1537

Funding 4

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2013-06917

Research area

Science and technology (CESSDA Topic Classification)

Natural sciences (Standard för svensk indelning av forskningsämnen 2011)

Chemical sciences (Standard för svensk indelning av forskningsämnen 2011)

Keywords

Nitrates, Mass spectrometry, Aerosols, Nitrate particles, Organic particles, Oxidation/reduction

Publications

Faxon, C., Hammes, J., Pathak, R. K., and Hallquist, M.: Characterization of organic nitrate constituents of secondary organic aerosol (SOA) from nitrate-radical-initiated oxidation of limonene using High-Resolution Chemical Ionization Mass Spectrometry, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2017-584, in review, 2017.

Accessibility level

Access to data through SND
Data are accessible by order

Use of data

Things to consider when using data shared through SND

Versions

Version 1.0. 2018-04-04

Homepage

https://www.gu.se/en/chemistry-molecular-biology/our-research/atmospheric-science

Download metadata

DataCite

DDI 2.5

DDI 3.3

DCAT-AP-SE 2.0

JSON-LD

PDF

Citation (CSL)

Published: 2018-04-04
Last updated: 2024-07-08