A four carbon organonitrate as a significant product of secondary isoprene chemistry

SND-ID: 2021-330-1. **Version**: 1. **DOI**: https://doi.org/10.5878/wfv9-a491

Download data

Br-CIMS_12Aug.tsv *(19.31 KB)*
Br-CIMS_16Aug.tsv *(19.33 KB)*
Br-CIMS_9Aug.tsv *(21.28 KB)*
I-CIMS_12Aug.tsv *(64.75 KB)*
I-CIMS_13Aug.tsv *(58.04 KB)*
I-CIMS_16Aug.tsv *(14.68 KB)*
I-CIMS_9Aug.tsv *(68.57 KB)*
I-CIMS_Amazon.tsv *(74.05 KB)*
I-CIMS_Changping.tsv *(589.91 KB)*
I-CIMS_Gbg.tsv *(5.52 KB)*
I-CIMS_HK.tsv *(49.12 KB)*
I-CIMS_Jülich.tsv *(900.78 KB)*
NO2_Amazon.tsv *(98.19 KB)*
NOx_Changping.tsv *(95.74 KB)*
NOx_Gbg.tsv *(5.46 KB)*
NOx_HK.tsv *(2.35 MB)*
NOx_Jülich.tsv *(484.36 KB)*
TD-CRDS_12Aug.tsv *(3.91 KB)*
TD-CRDS_13Aug.tsv *(1.26 KB)*
TD-CRDS_16Aug.tsv *(1.82 KB)*
TD-CRDS_9Aug.tsv *(1.36 KB)*

Download all files

2021-330-1-1.zip *(~4.86 MB)*

Citation

Hallquist, M., & Tsiligiannis, E. (2021) A four carbon organonitrate as a significant product of secondary isoprene chemistry (Version 1) [Data set]. University of Gothenburg. Available at: https://doi.org/10.5878/wfv9-a491

Creator/Principal investigator(s)

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Description

Oxidation of isoprene by nitrate radicals (NO3) or by hydroxyl radicals (OH) under high NOx conditions forms a substantial amount of organonitrates (ONs). ONs impact NOx concentrations and consequently ozone formation while also contributing to secondary organic aerosol. Here we show that the ONs with the chemical formula C4H7NO5 are a significant fraction of isoprene-derived ONs, based on chamber experiments and ambient measurements from different sites around the globe. From chamber experiments we found that C4H7NO5 isomers contribute 5-17% of all ONs formed during nighttime and constitute more than 40% of the ONs after further daytime oxidation. In ambient measurements C4H7NO5 isomers usually dominate both nighttime and daytime, implying a long residence time compared to C5 ONs which are removed more rapidly. We propose potential nighttime sources and secondary formation pathways, and test them using a box model with an updated isoprene oxidation scheme.

This dataset is based on oxidation experiments of isoprene + NO3 radicals at the atmospheric chamber SAPHIR, in Jülich, Germany and ambient data from five different locations. More specifically, this dataset is provided in order for users to be able to replicate the results from the Tsiligiannis et al. publication. It includes time-series of gaseous species.

The files called I-CIMS contain compounds that measured using a chemical ionization mass spectrometer (CIMS) with iodide as the reagent ion. The files called Br-CIMS contain compounds that measured using a chemical ionization mass spectrometer (CIMS) with bromide as the reagent ion. The files called TD-CRDS contain the total alkyl nitrates measured using a thermal dissociation−cavity ring-down spectrometer.
The chamber data are indicated by the date of the experiment (e.g. 9Aug). The ambient data are indicated by the location where they collected (e.g. Amazon).

All the date & time data corresponds to local time. For each column, the naming e.g. "BrC4H7NO5_ncps" or "C4H7INO5_ppt", corresponds to the chemical formula of the compound (C4H7NO5) clustering with either bromide or iodide, and the measurement units (ncps=normalized counts per second) or (ppt=parts per trillion by volume). File delimiter is the tabstop.

The data from the SOAS campaign can be found here:
https://csl.noaa.gov/groups/csl7/measurements/2013senex/Ground/DataDownload/index.php?page=/groups/csl7/measurements/2013senex/Ground/DataDownload/

Data contains personal data

No

Language

English

Time period(s) investigated

2013 – 2019

Data format / data structure

Numeric

Geographic spread

Geographic location: Sweden, Brazil, Hong Kong, China, Germany

Geographic description:
The ambient data are indicated by the location where they collected (e.g. Amazon).

The exact locations are:
"Gbg" = Gothenburg city's port, Sweden.
"Jülich" = Forschungszentrum Jülich (FZJ), Germany.
"Changping" = 40km north-east of downtown Beijing, China close to Changping town.
"HK" = Hok Tsui Tsuen area, south-east on the Hong Kong island, China.
"Amazon" = Central Amazonia, at a site located 60 km northwest of Manaus, Brazil (0.235680° S, 60.12560° W, 110 m above sea level) facing a huge area (1600 km2) of nearly pristine forest to the east.

Responsible department/unit

Department of Chemistry and Molecular Biology

Research area

Environmental sciences (Standard för svensk indelning av forskningsämnen 2011)

Meteorology and atmospheric sciences (Standard för svensk indelning av forskningsämnen 2011)

Geoscientific information (INSPIRE topic categories)

Environment (INSPIRE topic categories)

Keywords

Nitrogen oxides, Atmospheric ozone, Atmospheric conditions, Organonitrate, Isoprene

Publications

Epameinondas Tsiligiannis, Rongrong Wu, Ben H. Lee, Christian Mark Garcia Salvador, Michael Priestley, Philip T.M. Carlsson, Sungah Kang, Anna Novelli, Luc Vereecken, Hendrik Fuchs, Alfred W. Mayhew, Jacqueline F. Hamilton, Peter M. Edwards, Juliane L. Fry, Bellamy Brownwood, Steven S. Brown, Robert J Wild, Thomas J. Bannan, Hugh Coe, James Allan, Jason D. Surrat, Asan Bacak, Paul Artaxo, Carl Percival, Song Guo, Min Hu, Tao Wang, Thomas F. Mentel, Joel A. Thornton, and Mattias Hallquist. (2021). A four carbon organonitrate as a significant product of secondary isoprene chemistry (submitted manuscript).

Accessibility level

Access to data through SND
Data are freely accessible

Use of data

Things to consider when using data shared through SND

Versions

Version 1. 2021-12-06

Download metadata

DataCite

DDI 2.5

DDI 3.3

DCAT-AP-SE 2.0

JSON-LD

PDF

Citation (CSL)

File overview (CSV)

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