ATom: L2 Measurements from NOAA ToF Chemical Ionization Mass Spectrometer, Version 2

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Documentation Revision Date: 2021-08-13

Dataset Version: 2

Summary

This dataset provides the mixing ratios of reactive nitrogen and halogen species measured by the NOAA Iodide Ion Time-of-Flight Chemical Ionization Mass Spectrometer (NOAA CIMS) during airborne campaigns conducted by NASA's Atmospheric Tomography (ATom) mission for ATom-3 and ATom-4 campaigns. The NOAA CIMS uses chemical ionization mass spectrometric detection of gas phase organic and inorganic analytes via I- adduct formation. Measurements for ATom include N2O5 (dinitrogen pentoxide), ClNO2 (chloro nitrite), Cl2 (Chlorine), HCOOH (formic acid), C2H4O3S (hydroperoxymethyl thioformate), BrCl (bromine monochloride), BrCN (cyanogen bromide), and BrO (bromine monoxide). ATom deploys an extensive gas and aerosol payload on the NASA DC-8 aircraft for systematic, global-scale sampling of the atmosphere, profiling continuously from 0.2-13 km altitude. This comprehensive dataset will be used to improve the representation of chemically reactive gases and short-lived climate forcers in global models of atmospheric chemistry and climate.

In this version, the calibration method used to determine the instrument sensitivity to $C_2H_4O_3S$ utilizes more accurate actinometry of chlorine radicals, which are used to produce known quantities of $C_2H_4O_3S$ from dimethyl sulfide. To correct for an overestimation in Version 1, $C_2H_4O_3S$ mixing ratios have been reduced by an ATom mission average of 38% ± 17% (1 sigma). Updated precision and accuracy for $C_2H_4O_3S$ measurements are also provided. No other data have changed.

This dataset includes 200 data files in ICARTT (*ict.) format, with eight data files per flight date.

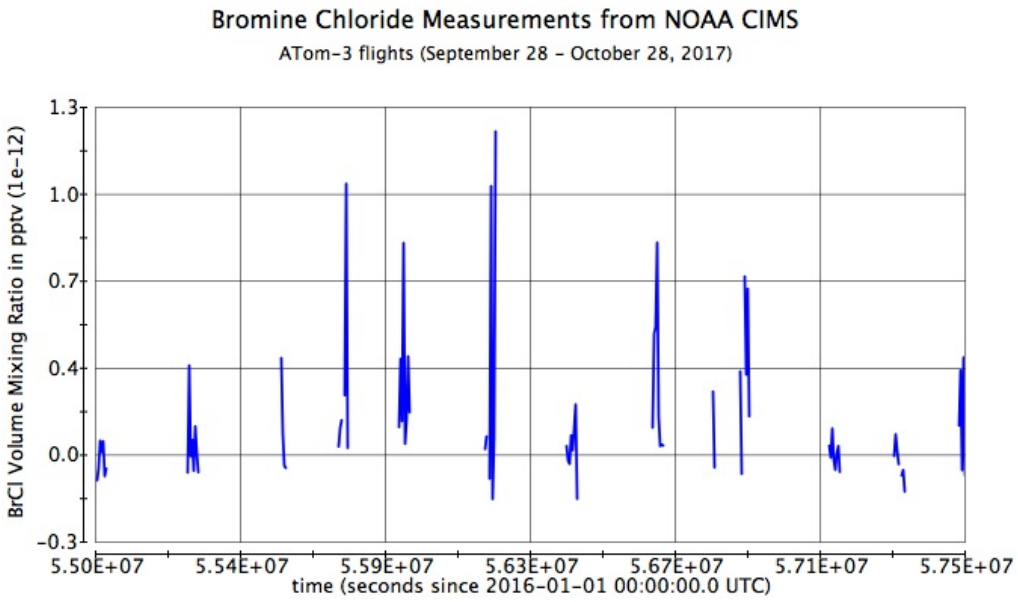

Figure 1. Bromine chloride measurements from the NOAA CIMS instrument during the ATom-3 campaign.

Citation

Veres, P.R., J.A. Neuman, and T.B. Ryerson. 2021. ATom: L2 Measurements from NOAA ToF Chemical Ionization Mass Spectrometer, Version 2. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1921

Table of Contents

1. Dataset Overview

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Project: Atmospheric Tomography Mission

The Atmospheric Tomography Mission (ATom) was a NASA Earth Venture Suborbital-2 mission. It studied the impact of human-produced air pollution on greenhouse gases and on chemically reactive gases in the atmosphere. ATom deployed an extensive gas and aerosol payload on the NASA DC-8 aircraft for a systematic, global-scale sampling of the atmosphere, profiling continuously from 0.2 to 12 km altitude. Flights occurred in each of four seasons over a 4-year period.

Related Publication

Veres, P. R., J. A. Neuman, T. H. Bertram, E. Assaf, G. M. Wolfe, C. J. Williamson, B. Weinzierl, S. Tilmes, C. R. Thompson, A. B. Thames, J. C. Schroder, A. Saiz-Lopez, A. W. Rollins, J. M. Roberts, D. Price, J. Peischl, B. A. Nault, K. H. Møller, D. O. Miller, S. Meinardi, Q. Li, J.-F. Lamarque, A. Kupc, H. G. Kjaergaard, D. Kinnison, J. L. Jimenez, C. M. Jernigan, R. S. Hornbrook, A. Hills, M. Dollner, D. A. Day, C. A. Cuevas, P. Campuzano-Jost, J. Burkholder, T. P. Bui, W. H. Brune, S. S. Brown, C. A. Brock, I. Bourgeois, D. R. Blake, E. C. Apel, and T. B. Ryerson. 2020. Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere. Proceedings of the National Academy of Sciences 117:4505–4510. https://doi.org/10.1073/pnas.1919344117

Related Datasets

Veres, P.R., J.A. Neuman, and T.B. Ryerson. 2019. ATom: L2 Measurements from the NOAA ToF Chemical Ionization Mass Spectrometer (CIMS). ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1745

- Version 1 of the current dataset and is now superseded.

Wofsy, S.C., et al. 2018. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1581

- Data from all ATom instruments and all four flight campaigns, including aircraft location and navigation data, merged to several different time bases.

Wofsy, S.C., and ATom Science Team. 2018. ATom: Aircraft Flight Track and Navigational Data. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1613

- Flight path (i.e., location and altitude) data for each of the four campaigns provided in KML and CSV formats.

2. Data Characteristics

Spatial Coverage: Global; flights circumnavigate the globe, primarily over the oceans

Spatial Resolution: Point measurements

Temporal Coverage: Periodic flights occurred during the ATom-3 and ATom-4 campaigns only.

Deployment	Date Range
ATom-1	July 29 - August 23, 2016
ATom-2	January 26 - February 21, 2017
ATom-3	**September 28 - October 28, 2017**
ATom-4	**April 24 - May 21, 2018**

Temporal Resolution: 1 second

Data File Information

This dataset includes 200 data files in ICARTT (*ict.) format, with eight data files per flight date. Data files conform to the ICARTT File Format Standards V1.1. File are named NOAACIMS-**X**_DC8_**YYYYMMDD**_R#.ict, where **X** is the species abbreviation (BrCl, BrCN, BrO, C2H4O3S, Cl2, ClNO2, HCOOH, N2O5; with 25 files each), **YYYYMMDD** is the start date (in UTC time) of the flight, and R# is the file version or revision number.

Table 1. File names and descriptions.

File Name	Units	Description
NOAACIMS-BrCl_DC8_YYYYMMDD_R#.ict	pptv	Bromine monochloride volume mixing ratio
NOAACIMS-BrCN_DC8_YYYYMMDD_R#.ict	pptv	Cyanogen bromide volume mixing ratio
NOAACIMS-BrO_DC8_YYYYMMDD_R#.ict	pptv	Bromine monoxide volume mixing ratio
NOAACIMS-C2H4O3S_DC8_YYYYMMDD_R#.ict ***	ppt	Hydroperoxymethyl thioformate volume mixing ratio

NOAACIMS-Cl2_DC8_YYYYMMDD_R#.ict	pptv	Chlorine volume mixing ratio
NOAACIMS-ClNO2_DC8_YYYYMMDD_R#.ict	ppt	Chloro nitrite volume mixing ratio
NOAACIMS-HCOOH_DC8_YYYYMMDD_R#.ict	pptv	Formic acid volume mixing ratio
NOAACIMS-N2O5_DC8_YYYYMMDD_R#.ict	ppt	Dinitrogen pentoxide volume mixing ratio

*** Updated in Version 2. See Section 8: Dataset Revisions for details.

Data File Details

For all files,

- Missing data are indicated by -9999.000.
- UTC_NOAACIMS are in "seconds since 000 UTC" on the day of flight.

3. Application and Derivation

ATom builds the scientific foundation for mitigation of short-lived climate forcers, in particular, methane (CH_4), tropospheric ozone (O_3), and Black Carbon aerosols (BC).

ATom Science Questions

Tier 1

- What are chemical processes that control the short-lived climate forcing agents CH_4, O_3, and BC in the atmosphere? How is the chemical reactivity of the atmosphere on a global scale affected by anthropogenic emissions? How can we improve chemistry-climate modeling of these processes?

Tier 2

- Over large, remote regions, what are the distributions of BC and other aerosols important as short-lived climate forcers? What are the sources of new particles? How rapidly do aerosols grow to CCN-active sizes? How well are these processes represented in models?
- What type of variability and spatial gradients occurs over remote ocean regions for greenhouse gases (GHGs) and ozone-depleting substances (ODSs)? How do the variations among air parcels help identify anthropogenic influences on photochemical reactivity, validate satellite data for these gases, and refine knowledge of sources and sinks?

Significance

ATom delivers unique data and analysis to address the Science Mission Directorate objectives of acquiring “datasets that identify and characterize important phenomena in the changing Earth system” and “measurements that address weaknesses in current Earth system models leading to improvement in modeling capabilities.” ATom will provide unprecedented challenges to the CCMs used as policy tools for climate change assessments, with comprehensive data on atmospheric chemical reactivity at global scales, and will work closely with modeling teams to translate ATom data to better, more reliable CCMs. ATom provides extraordinary validation data for remote sensing.

4. Quality Assessment

Table 2. Uncertainty measurements.

Species	Precision	Accuracy
BrCl	0.2 pptv per second	25% + 0.4 pptv
BrCN	5 pptv per second	25% + 0.4 pptv
BrO	0.3 pptv per second	25% + 0.2 pptv
C2H4O3S ***	0.4 ppt (1 sigma)	17% + 0.4 ppt
Cl2	0.2 pptv per second	15% + 0.4 pptv
ClNO2	0.1 ppt (1 sigma)	15% + 0.05 ppt
HCOOH<	15 pptv per second	15% + 100 pptv
N2O5	0.1 ppt (1 sigma)	15% + 0.03 ppt

******* Updated in Version 2. See Section 8: Dataset Revisions for details.

5. Data Acquisition, Materials, and Methods

Project Overview

ATom made global-scale measurements of the chemistry of the atmosphere using the NASA DC-8 aircraft. Flights spanned the Pacific and Atlantic Oceans, nearly pole-to-pole, in continuous profiling mode, covering remote regions that receive long-range inputs of pollution from expanding industrial economies. The payload had proven instruments for in situ measurements of reactive and long-lived gases, diagnostic chemical tracers, and aerosol size, number, and composition, plus spectrally resolved solar radiation and meteorological parameters.

Combining distributions of aerosols and reactive gases with long-lived GHGs and ODSs enables disentangling of the processes that regulate atmospheric chemistry: emissions, transport, cloud processes, and chemical transformations. ATom analyzes measurements using customized modeling tools to derive daily averaged chemical rates for key atmospheric processes and to critically evaluate Chemistry-Climate Models (CCMs). ATom also differentiates between hypotheses for the formation and growth of aerosols over the remote oceans.

National Oceanic and Atmospheric Administration Iodide Ion Time-of-Flight Chemical Ionization Mass Spectrometer

Instrument	Full Name	Contact Person	Type	Measurements	Data Variables
NOAA	National Oceanic and Atmospheric Administration	J. Andy		gas phase organic and	HCOOH, ClNO2, N2O5, BrO, Cl2,

CIMS	Spectrometer	Neuman		inorganic analytes	BrCN, BrCl, C2H4O3S

The NOAA CIMS uses chemical ionization mass spectrometric to detect gas-phase organic and inorganic analytes via I- adduct formation with an instrumental response of <1 second.

6. Data Access

These data are available through the Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC).

ATom: L2 Measurements from NOAA ToF Chemical Ionization Mass Spectrometer, Version 2

Contact for Data Center Access Information:

- E-mail: uso@daac.ornl.gov
- Telephone: +1 (865) 241-3952

7. References

Veres, P. R., J. A. Neuman, T. H. Bertram, E. Assaf, G. M. Wolfe, C. J. Williamson, B. Weinzierl, S. Tilmes, C. R. Thompson, A. B. Thames, J. C. Schroder, A. Saiz-Lopez, A. W. Rollins, J. M. Roberts, D. Price, J. Peischl, B. A. Nault, K. H. Møller, D. O. Miller, S. Meinardi, Q. Li, J.-F. Lamarque, A. Kupc, H. G. Kjaergaard, D. Kinnison, J. L. Jimenez, C. M. Jernigan, R. S. Hornbrook, A. Hills, M. Dollner, D. A. Day, C. A. Cuevas, P. Campuzano-Jost, J. Burkholder, T. P. Bui, W. H. Brune, S. S. Brown, C. A. Brock, I. Bourgeois, D. R. Blake, E. C. Apel, and T. B. Ryerson. 2020. Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere. Proceedings of the National Academy of Sciences 117:4505–4510. https://doi.org/10.1073/pnas.1919344117

8. Dataset Revisions

Version	Release Date	Revision Notes	DOI
2.0	2021-08-13	The calibration method for calculating $C_2H_4O_3S$ was updated to address an underestimation in the determination of instrument sensitivity as a result of an experiment contaminant. $C_2H_4O_3S$ mixing ratios in Version 2 have been reduced relative to Version 1 by an average of 38% ± 17% (1 sigma). Precision and accuracy for $C_2H_4O_3S$ measurements (Table 4) have also been updated (previously: 0.1 ppt (1 sigma) and 55% + 0.06 ppt). No other data were altered.	https://doi.org/10.3334/ORNLDAAC/1921
1.0	2020-01-23	Initial data release. Now supersedes by Version 2, and available upon request only.	https://doi.org/10.3334/ORNLDAAC/1745