

1. Dataset Overview
2. Data Characteristics
3. Application and Derivation
4. Quality Assessment
5. Data Acquisition, Materials, and Methods
6. Data Access
7. References
8. Dataset Revisions

1. Dataset Overview

This dataset provides the concentrations of gas-phase organic and inorganic analytes measured by the California Institute of Technology (CIT) Chemical Ionization Mass Spectrometer (CIMS), or CIT-CIMS, flown on the NASA DC-8 aircraft during the four ATom campaigns. The CIT-CIMS employs CF₃O⁻ ion chemistry with two independent mass spectrometers (compact time-of-flight and triple quadrupole) to enable sensitive and specific measurements of atmospheric trace gases. The measurements include hydrogen peroxide (H₂O₂), hydrogen cyanide (HCN), nitric acid (HNO₃), methyl hydrogen peroxide (CH₃OOH), peroxyacetic acid (C₂O₃H₄), peroxyxynitric acid (HO₂NO₂), and sulfur dioxide (SO₂), in units of parts-per-trillion-by-volume.

This is Version 2 of this dataset. Version 2 contains the initial release of files for the ATom-4 campaign and CIT-SO₂ files for the ATom-3 campaign. Additional details can be found in Section 8. Dataset Revisions.

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 Datasets

Allen, H.M., J.D. Crouse, M.J. Kim, A.P. Teng, and P.O. Wennberg. 2019. ATom: L2 In Situ Data from Caltech Chemical Ionization Mass Spectrometer (CIT-CIMS). ORNL DAAC, Oak Ridge, Tennessee, USA. <https://doi.org/10.3334/ORNLDAAC/1713>

- This is Version 1 of this dataset. Now superseded and available only upon request.

Wofsy, S.C., S. Afshar, H.M. Allen, E.C. Apel, E.C. Asher, B. Barletta, et al. 2021. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols, Version 2. ORNL DAAC, Oak Ridge, Tennessee, USA. <https://doi.org/10.3334/ORNLDAAC/1925>

- 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>

- Flightpath (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 each campaign

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

There are 294 data files in ICARTT (*.ict) format included in this dataset. Data files conform to the [ICARTT File Format Standards V1.1](#). Files are named **group_DC8_YYYYMMDD_R#.ict**, where **group** is the data file group (Table 1), **YYYYMMDD** is the start date (in UTC time) of the flight, and **R#** is the file version or revision number

Table 1. Data file groups and descriptions.

Group	Number of Files	Description
CIT-H2O2	45	Contain concentrations of hydrogen peroxide in part per trillion by volume
CIT-HCN	48	Contain concentrations of hydrogen cyanide in parts per trillion by volume
CIT-HNO3	48	Contain concentrations of nitric acid in parts per trillion by volume
CIT-MHP	48	Contain concentrations of methyl hydrogen peroxide in parts per trillion by volume from the triple quadrupole instrument
CIT-MHP-ToF	13	Contain methyl hydrogen peroxide uncertainties in parts per trillion by volume from the compact time of flight instrument
CIT-PAA	22	Contain concentrations of peroxyacetic acid in parts per trillion by volume
CIT-PNA	22	Contain concentrations of peroxyxynitric acid in parts per trillion by volume

Data File Details

No data values are represented by -9999.0.

All files contain the time variable *UTC_start* which is the "Start time in seconds since 0000 UTC".

3. Application and Derivation

ATom builds the scientific foundation for mitigation of short-lived climate forcers, in particular, methane (CH₄), tropospheric ozone (O₃), and Black Carbon aerosols (BC).

ATom Science Questions

Tier 1

- What are chemical processes that control the short-lived climate forcing agents CH₄, O₃, 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 the 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. Uncertainties of variables.

Variable	File Grouping	Uncertainty
H2O2_CIT	CIT-H2O2	±(30% of measurement value + 50 pptv)
HCN_CIT	CIT-HCN	±(50% of measurement value + 50 pptv)
HNO3_CIT	CIT-HNO3	±(30% of measurement value + 50 pptv)
MHP_CIT	CIT-MHP	±(30% of measurement value + 25 pptv)
MHP-ToF_CIT	CIT-MHP-ToF	±(30% of measurement value + 50 pptv)
PAA_CIT	CIT-PAA	±(50% of measurement value + 30 pptv)
PNA_CIT	CIT-PNA	±(30% of measurement value + 100 pptv)
SO2_CIT	CIT-SO2	±(25% of measurement value + 134 pptv) *

* Improved from ±(30% of measurement value + 250 pptv) in Version 1

5. Data Acquisition, Materials, and Methods

Project Overview

ATom makes global-scale measurements of the chemistry of the atmosphere using the NASA DC-8 aircraft. Flights span 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 has 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 greenhouse gases (GHG) and ozone-depleting substances (ODS) 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 CCMs. ATom also differentiates between hypotheses for the formation and growth of aerosols over the remote oceans.

Caltech Chemical Ionization Mass Spectrometers

The Caltech Chemical Ionization Mass Spectrometers (CIT-CIMS) instrument as deployed during ATom uses two mass spectrometers, a compact time-of-flight, and a triple quadrupole, to detect trace gases in the atmosphere. Analytes react with the CF₃O-reagent ion to form specific product ions which are subsequently detected by the mass analyzers. The triple quadrupole mass spectrometer enables collisional induced fragmentation (CID) of product ions, and subsequent analysis of fragment ions. These methods allow for distinguishing certain mass analogs and reducing instrumental backgrounds. For ATom, CH₃OOH data is derived from the triple quadrupole instrument, and the remainder of the data files are from the compact time-of-flight instrument. For additional information, see Crouse et al. (2006), St. Clair et al. (2010), and the [ESPO CIT-CIMS Instrument](#) page.

6. Data Access

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

ATom: In Situ Data from Caltech Chemical Ionization Mass Spectrometer (CIT-CIMS), V2

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

7. References

Crouse, J.D., K.A. McKinney, A.J. Kwan, and P.O. Wennberg. 2006. Measurement of gas-phase hydroperoxides by chemical ionization mass spectrometry. *Analytical Chemistry* 78:6726–6732. <https://doi.org/10.1021/ac0604235>

St. Clair, J.M., D.C. McCabe, J.D. Crouse, U. Steiner, and P.O. Wennberg. 2010. Chemical ionization tandem mass spectrometer for the in situ measurement of methyl hydrogen peroxide. *Review of Scientific Instruments* 81:094102. <https://doi.org/10.1063/1.3480552>

8. Dataset Revisions

Version	Release Date	Description
2.0	2021-12-20	Initial release of files for the ATom-4 campaign and CIT-SO2 files for the ATom-3 campaign. All other files were updated to their most current revision.
1.0	2019-09-30	Initial release of files for the ATom-1, ATom-2, and ATom-3 campaigns and CIT-SO2 files for the ATom-1 and ATom-2 campaigns. Now superseded and available only upon request.



[Privacy Policy](#) | [Feedback](#) | [Help](#)

Home

About Us

Mission
Data Use and Citation
Policy
User Working Group
Partners

Get Data

Science Themes
NASA Projects
All Datasets

Submit Data

Submit Data Form
Data Scope and
Acceptance
Data Authorship Policy
Data Publication Timeline
Detailed Submission
Guidelines

Tools

MODIS
THREDDS
SDAT
Daymet
Airborne Data Visualizer
Soil Moisture Visualizer
Land - Water Checker

Resources

Learning
Data Management
News
Earthdata Forum

Contact Us