Latest Revision: **27 September 2025**
MetaData File provided: June 2015

Data Set Description:

PI:	Kimberly Strong University of Toronto, Department of Physics Toronto, Ontario, Canada
Instrument:	Fourier Transform Infrared Spectrometer (FTIR)
Site(s):	NDACC Station "toronto.tao" University of Toronto Atmospheric Observatory (TAO) Toronto, Ontario, Canada 43.66°N, 79.40°W, 174 m above sea level
Measurement Quantities:	Vertical column densities above Toronto (0-120 km) in units of [molecules/cm^2] Vertical volume mixing ratio profiles above Toronto (0-120 km) in units of [ppbv]
Data License:	CC-BY-NC-SA license (Attribution-NonCommercial-ShareAlike)
Location of L0/L1 data:	University of Toronto servers
DOI:	No DOI has been assigned to data archived on NDACC.

DOIs for papers using Toronto NDACC FTIR data:

- S. Yamanouchi, S. Conway, K. Strong, O. Colebatch, E. Lutsch, S. Roche, J. Taylor, C.H. Whaley, and A. Wiacek. "Replication Data for: NDACC FTIR trace gas measurements at the University of Toronto Atmospheric Observatory from 2002 - 2020", https://doi.org/10.5683/SP2/VC8JMC, Borealis, V1, 2022.

- E. Mahieu, M. De Mazière, D.W.T. Griffith, J.W. Hannigan, N. Jones, E. Lutsch, I. Ortega, C. Paton-Walsh, K. Strong, and C. Vigouroux. FTIR measurements of formic acid (2010-2012) (Version v1.0) [Data set]. Zenodo, 2021. http://doi.org/10.5281/zenodo.4321349

- S. Yamanouchi, K. Strong, E. Lutsch, D.B.A. Jones, N. Gervasi, and R. Sandrin. Detection of HCOOH, CH3OH, CO, HCN and C2H6 in Wildfire Plumes Transported over Toronto Using Ground-based FTIR Measurements from 2002-2018, https://doi.org/10.5683/SP2/LLIOJW, Scholars Portal Dataverse, V1, 2020.

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Instrument Description:

An ABB Bomem DA8 Fourier Transform Infrared (FTIR) spectrometer has been operated at the University of Toronto Atmospheric Observatory (TAO) on a continuous basis since May 2002 (following installation in October 2001), with a solar tracker manufactured by Aim Controls. The FTS is operated in solar absorption geometry at its maximum optical path difference of 250 cm corresponding to a spectral resolution of 0.004 cm^{-1}. The DA8 is equipped with both InSb and MCT detectors and a KBr beamsplitter. Combined, these resources cover the mid-infrared from about 650 to 6600 cm^{-1}. The optical filters used are those recommended by the NDACC Infrared Working Group and are listed in the table below. Filter 7 is not standard and was acquired to enable near-IR measurements. There are significant coverage gaps in F6 measurements in 2002-2003. No data were recorded in Aug-Sep 2004 and Dec 2006-Jan 2007 due to a suntracker failure. Also no data were recorded in Mar-Jun 2009 due to an alignment issue.

The Toronto measurements from December 6, 2007 to March 30, 2009 are affected by an instrument artifact, which appears to be due to instrument misalignment and gives rise to anomalous retrievals for some gases, including CH4 and OCS. Any measurements used during this period should be treated with caution.

NDACC filter	approx. range in cm^{-1}	before June 2003	after June 2003
Filter 1	4000 to 4300	routine	routine
Filter 2	2900 to 3500	routine	routine
Filter 3	2400 to 3100	routine	routine
Filter 4	2000 to 2700	routine	routine
Filter 5	1500 to 2200	not available	routine
Filter 6	750 to 1350	routine	routine
Filter 7	5800 to 6600	not available	not available

Algorithm Description:

Vertical profiles of volume mixing ratios of trace gases are derived using the Optimal Estimation Method, as implemented in SFIT4 and distributed through https://wiki.ucar.edu/display/sfit4/Infrared+Working+Group+Retrieval+Code%2C+SFIT. The most recently updated species, CHF_2Cl, and O_3, were retrieved using SFIT4 version 1.0.18, while all other species were retrieved using version 0.9.4.4 with full error analysis.

Vertical profiles of volume mixing ratios are weighted by the airmasses in each retrieval layer and integrated to give the total or partial columns in molecules/cm^2. We report total columns and profiles.

The retrieval results reported here use the Signal-to-Noise-Ratio (SNR) calculated from the spectrum for each target gas to define the measurement noise covariance matrix, with the a priori covariance matrix S_a adjusted to optimize the retrievals.

The microwindows and interfering species follow the NDACC IRWG recommendations.

Spectra used in the retrievals were recorded at 250 cm maximum optical path difference (OPD), except for filter 6 measurements, which are recorded at 200 cm OPD. Prior to 2006, filter 6 measurements were made at both 200 cm and 250 cm OPD. Typically, four scans are co-added, with five co-added for filter 6.

An optimized quality criterion has been applied using a threshold for the ratio of the spectral RMS residual (goodness of fit) and degrees-of-freedom for signal (DOFS). The thresholds were determined by a trade-off curve of the number of filtered measurements for the entire time series versus the RMS/DOFS ratio. The threshold was selected as the elbow of the trade-off curve, where the absolute second derivative is maximum. New retrievals using SFIT4 v1.0.1.8 instead use individual thresholds for RMS and DOFs. The threshold values are listed below:

Standard NDACC IRWG Species

C_2H_6	4.75 % RMS/DOFS
CH_4	0.25 % RMS/DOFS (for CAMS consolidated data product)
CO	1.00 % RMS/DOFS (for CAMS consolidated data product)
HCl	2.95 % RMS/DOFS
HCN	1.40 % RMS/DOFS
HF	4.50 % RMS/DOFS
HNO_3	4.00 % RMS/DOFS
N_2O	0.30 % RMS/DOFS
O_3	4.5 % max RMS, min DOFS = 0.6, max DOFS = 7 (for irwg2023 data product)

Non-standard NDACC IRWG Species

C_2H_2	7.50 % RMS/DOFS
CH_3OH	5.50 % RMS/DOFS

HCOOH 9.50 % RMS/DOFS
HCHO 3.50 % RMS/DOFS (for CAMS consolidated data product)
NH_3 5.40 % RMS/DOFS
OCS 4.00 % RMS/DOFS
CHF2Cl (HCFC-22) 1.3 % max RMS, min DOFS = 0.9, max DOFS = 10 (for irwg2023 data product)

In addition, a few random outliers are removed based on a qualitative assessment of the residuals.

Current Data Versions:

Standard NDACC IRWG Species

C_2H_6	version 002
CH_4	version 004 (CAMS consolidated product), version 003 (CAMS Rapid Delivery)
CO	version 005 (CAMS consolidated product), version 004 (CAMS Rapid Delivery)
HCl	version 002
HCN	version 002
HF	version 002
HNO_3	version 002
N_2O	version 003
O_3	version irwg2023_001 (and version 003 for CAMS Rapid Delivery)

Non-standard NDACC IRWG Species

C_2H_2	version 002
CH_3OH	version 002
HCOOH	version 003
HCHO	version 005 (CAMS consolidated product), version 004 (CAMS Rapid Delivery)
NH_3	version 002
OCS	version 001
CHF2Cl (HCFC-22)	version 001

Ancillary Data:

July 2024 – O_3 retrievals were updated to new microwindows using a Tikhonov regularization as suggested by the IRWG ozone strategy working group (irwg2023 retrieval).

January 2021 – Began submitting HCHO to the CAMS Rapid Delivery service.

March 2018 – Began submitting CO, CH_4, and O_3 to CAMS Rapid Delivery service. These species are processed using the CAMS consolidated retrieval procedure, which features a hard-coded error analysis routine and more stringent QA requirements via the additional CAMS-QC checker. Additionally, the archived versions of these species are processed using the CAMS consolidated retrieval procedure as well.

October 2016 – for the QA4ECV CO data product (CO data version 003):

The ATM line list (http://mark4sun.jpl.nasa.gov/toon/linelist/linelist.html) is used in the forward calculation. For interfering species, the HITRAN 2008 line list with additional pseudo-line parameters is used.

Line compilation: For retrievals using SFIT4 v0.9.4.4, the HITRAN 2008 line list with additional pseudo-line parameters is used in the forward calculation. Details regarding the C2H6 pseudo line list can be found in Franco et al., 2015. For retrievals using SFIT4 v1.0.18, the HITRAN 2020 line list is used.

Physical models: Temperature and pressure profiles are derived from NCEP analyses for each day to approx. 1.0 mbar and WACCM monthly mean above.

A priori profiles of trace gas volume mixing ratios are from the WACCM v4/v6 model (WACCM/IRWG version numbers), where possible and/or appropriate, while some updated strategies using SFIT4 1.0.18 use the newer WACCM v6/v7 model (WACCM/IRWG version numbers). HALOE climatologies, MkIV balloon flight results (http://mark4sun.jpl.nasa.gov/science.html) and "Standard Profiles" used in MIPAS retrievals (http://www.atm.ox.ac.uk/group/mipas/species) have been used as a priori information for some species when no WACCM profiles are available or where their use improves the retrievals

The Instrumental Line Shape (ILS) is monitored with HBr cell spectra (and since 2016 also with an N2O cell) on a quasi-regular basis. The cell spectra are analysed with LINEFIT [Hase, Applied Optics, 1999].

A local weather station (Davis VP+) was installed in October 2001 and records surface temperature, pressure, humidity, solar radiation, UV intensity and winds. The Davis VP+ was replaced with a Davis VP2+ on 5 February 2013. A Vaisala PTB300 was installed on 27 February 2013 and records air pressure with a Class A precision. The PTB300 was then replaced with a Vaisala PTB330 on 17 April 2020.

Expected Precision/Accuracy of Instrument:

The error calculations are based on the methodology of Rodgers [1,2]. In addition to the measurement (S_m) errors calculated as described in those papers, random forward model parameter errors have been calculated as described by Rodgers [3] the K_b values calculated by SFIT4 and our best estimate of the uncertainties in temperature (S_{temp}) and solar zenith angle (S_{sza}). Systematic forward model errors, i.e. errors due to uncertainties in line intensity and line widths, are calculated based HITRAN 2008 errors. Interference errors, as described by Rodgers and Connor [4] have also been calculated to account for uncertainties in retrieval parameters (wavelength shift, instrument line shape, background slope and curvature, phase error) and in interfering gases simultaneously retrieved. These interference errors are included in the random uncertainty estimate. The error budget calculation is described in depth by Batchelor et al. [5]. The total error (S_{total}) has been determined by adding all components in quadrature:

$$S_{total} = \sqrt{S^2_{random} + S^2_{systematic}}$$
$$= \sqrt{\left(S^2_m + S^2_{temp} + S^2_{int\,spec} + S^2_{int\,ret} + S^2_{sza}\right) + \left(S^2_{line\,int} + S^2_{airbroad} + S^2_{temp}\right)}$$

where S_m is the measurement error, S_{temp} is the temperature error (both a random and systematic component), $S_{int\,spec}$ is the error due to interfering species, $S_{int\,ret}$ is the interference error due to retrieval parameters, S_{sza} is the error due to uncertainty in the solar zenith angle, $S_{line\,int}$ is the error due to line intensity, and $S_{airbroad}$ is the error due to pressure and temperature broadening of the spectroscopic lines. The smoothing error is not included in the total error budget.

The data user is referred to a careful discussion of error analysis for ground-based FTIR observations presented in:

[1] C.D. Rodgers. Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation. Rev Geophys, 14(4), 609-624, 1976.

[2] C.D. Rodgers. Characterization and error analysis of profiles retrieved from remote sounding measurements. J Geophys Res, 95, 5587-5595, 1990.

[3] C.D. Rodgers. Inverse Methods for Atmospheric Sounding: Theory and Practice. Series on Atmospheric, Oceanic and Planetary Physics, vol. 2. New Jersey: World Scientific Publishing Co Pte Ltd, 2000.

[4] C.D. Rodgers and B.J. Connor. Intercomparison of remote sounding instruments. J Geophys Res, 108, doi:10.1029/2002JD002299, 2003.

[5] R.L. Batchelor, K. Strong, R. Lindenmaier, R.L. Mittermeier, H. Fast, J.R. Drummond, and P.F. Fogal. A new Bruker IFS 125HR FTIR spectrometer for the Polar Environment Atmospheric Research Laboratory at Eureka, Canada - measurements and comparison with the existing Bomem DA8 spectrometer. J. Atmos. Oceanic Technology, 26 (7), 1328-1340, 2009. https://doi.org/10.1175/2009JTECHA1215.1

Instrument History:

- December 2000: Installation of the DA8.
- 2001: Installation of the suntracker and commissioning of the complete FTIR system.
- Early 2002: Additional work by Bomem to improve the alignment.
- Summer 2002: Exit apertures installed on MCT and InSb detectors.
- November 2002: MCT detector replaced (to improve sensitivity).
- August-September 2004 and Dec 2006-Jan 2007: No data due to suntracker failure.
- November 2007: Bomem service visit: laser beam and mirror alignment optimized.

- December 6, 2007 to March 30, 2009: Measurements are affected by an instrument artifact and should be treated with caution.
- March-June 2009: No data were recorded due to DA8 alignment issues.
- July 2009 and September 2009: Bomem service visits: instrument alignment.
- April 2011: Scanning mirror motor on the DA8 was replaced.
- September 2012: Bomem service visit: metrology laser replaced by Bomem service engineer.
- August 2013: Bomem service visit: instrument alignment improved.
- March-May 2014: No measurements due to computer failure.
- August 12, 2014: Began operations with a "Community Solar Tracker" suntracker. This uses the same mirrors as the previous Aim Controls heliostat but provides active tracking with a CCD camera rather than four photodiodes.
- March-May 2015: DA8 electronics issues. Vector Processing computer and IEM33 power board replaced. IEK0100L back plane electronics board repaired.
- June 2015: Suntracker cover automated, allowing increase in measurement time.
- July 2015: DA8 white light replaced.
- October-November 2015: New scan motor bearing and instrument alignment.
- February 2016: First N2O cell tests.
- 7 June 2016: DA8 internal source mirror motor failed. Replaced July 25.
- November 2018: DA8 source motor and beam selector solenoid failure. Both replaced.
- 23 November 2018: Internal aperture failure.
- 20 February 2019: Source mirror repaired.
- July-September 2019 – ABB service visit July 22-26, including alignment to obtain ILS from emission input (solar beam). Followed by extensive realignment of the DA8, no measurements.
- October 2019: Started recording ILS measurements though DA8 emission point using the sun as the source.
- April 2020: Vaisala PTB330 replaced PTB300.
- April 2021: Azimuth stepper motor replaced on AIMS heliostat.
- March 2020 to March 2022 - Building access restricted at the University of Toronto due to COVID-19, but we were able to continue TAO DA8 FTIR measurements, as well as OP-FTIR boundary-layer measurements following the University’s research protocols.
- 1-27 November 2020 – No measurements due to instrument issues and lack of on-site personnel support due to COVID-19.
- 1-18 April 2022: No measurements due to scan motor maintenance.
- 30 March 2022 – 31 October 2023: Currently having intermittent scan motor issues and alignment issues that cause some loss of measurements.
- 19 July 2023: Beam selector solenoid having issues, sample chamber flaps deactivated to remedy solenoid problem
- 13 September 2023: TAO DA8 MCT Pre-Amp Z10 changed to 30 Kohm to improve signal.
- 24 November 2023: DA8 scan motor replaced and scan motor issues appear fixed.
- 25 November 2025: DA8 folding mirror adjusted for IR retro and improvement of ILS
- 26 June 2025: InSb and MCT detector dewars re-evacuated.

Reference Articles:

PhD Theses

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Victoria A. Flood, Using ground-based infrared spectroscopy, satellite measurements, and models to understand short-lived climate forcers and wildfire emissions over Canada, PhD Thesis, Department of Physics, University of Toronto, 2025. https://hdl.handle.net/1807/145088

Shoma Yamanouchi, Long-term Analysis of Toronto-Area Atmospheric Composition, PhD Thesis, Department of Physics, University of Toronto, 2021. http://hdl.handle.net/1807/106479

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Jeffrey R. Taylor, Assessment of Trace Gas Observations from the Toronto Atmospheric Observatory, PhD Thesis, Department of Physics, University of Toronto, 2008. http://hdl.handle.net/1807/17305

Aldona Wiacek, First Trace Gas Measurements Using Fourier Transform Infrared Solar Absorption Spectroscopy at the University of Toronto Atmospheric Observatory, PhD Thesis, Department of Physics, University of Toronto, 2006. https://librarysearch.library.utoronto.ca/permalink/01UTORONTO_INST/14bjeso/alma991106405283106196

Selected Articles

For a complete list, see: https://www.atmosp.physics.utoronto.ca/people/strong/papers.html

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