MetaData File provided: June 2015
Latest Revision: 15 August 2023

**Data Set Description:**

PI: Kimberly Strong
University of Toronto, Department of Physics
Toronto, Ontario, Canada

Instrument: Fourier Transform Infrared Spectrometer (FTIR)

Site(s): Eureka, Nunavut (CANDAC PEARL facility)
NDACC Station Eureka
80.05 N, 86.42 W, 610 m above sea level

Measurement Quantities: Vertical column densities above Eureka (0-120 km) in units of [molecules/cm$^2$]
Vertical volume mixing ratio profiles above Eureka (0-120 km) in units of [ppbv]

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DOI: No DOI has been assigned to data archived on NDACC.

DOIs for papers using Eureka NDACC FTIR data:

S. Barthlott, M. Schneider, F. Hase, T. Blumenstock, G. Mengistu Tsidu, M. Grutter de la Mora, K. Strong, J. Notholt, E. Mahieu, N. Jones, and D. Smale. The ground-based MUSICA dataset: Tropospheric water vapour isotopologues (H216O, H218O and HD16O) as obtained from NDACC/FTIR solar absorption spectra, [Data set]. Zenodo, 2016. http://doi.org/10.5281/zenodo.48902

K. Bognar, R. Alwarda, K. Strong, M.P. Chipperfield, S.S. Dhomse, J.R. Drummond, W. Feng, V. Fioletov, B. Herrera, E.M. McCullough, T. Wizenberg, and X. Zhao. Replication data for: Unprecedented spring 2020 ozone depletion in the context of 20 years of measurements at Eureka, Canada, https://doi.org/10.5683/SP2/OLZ4PK, Scholars Portal Dataverse, V1, 2020.

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

E. Mahieu, L. Clarisse, Lieven, P.-F. Coheur, B. Franco, J. Notholt, M. Palm, K. Strong, and T. Wizenberg. Remote-sensing measurements and model simulations of peroxyacetyl nitrate (PAN) [Data set]. In Elem Sci Anth (v1.0, Vol. 9). Zenodo, 2021. https://doi.org/10.5281/zenodo.5111613

K. Strong, S. Roche, E. McGee, A. Jalali, K.A. Walker, and D. Wunch. "Replication Data for: A comparison of carbon monoxide retrievals between the MOPITT satellite and Canadian High-Arctic ground-based NDACC and TCCON FTIR measurements", https://doi.org/10.5683/SP3/1GBGMY, Borealis, V1, 2022.

T. Wizenberg, K. Strong, D. Jones, E. Lutsch, E. Mahieu, B. Franco, and L. Clarisse. Replication Data for: Exceptional Wildfire Enhancements of PAN, C2H4, CH3OH, and HCOOH Over the Canadian High Arctic During August 2017, https://doi.org/10.5683/SP3/6PBAHK, Borealis, V1, 2022.

**Contact Information:**

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| Name: | Kimberly Strong |
| Address: | University of Toronto<br>Department of Physics<br>60 St. George Street<br>Toronto, Ontario, Canada |
| Phone: | +001-416-946-3217 |
| FAX: | +001-416-978-8905 |
| Email: | strong@atmosp.physics.utoronto.ca |
| WEB: | http://www.atmosp.physics.utoronto.ca/people/strong/strong.html<br>https://www.pearl-candac.ca |

**Instrument Description:**

A Bruker IFS 125HR Fourier Transform Infra-red (FTIR) spectrometer has been operated at the CANDAC Polar Environment Atmospheric Research Laboratory (PEARL) at Eureka during the sunlit part of the year (late February to late October) since August 2006. The FTS is operated in solar absorption geometry at its maximum optical path difference of 257 cm corresponding to a spectral resolution of 0.0035 $cm^{-1}$. The Bruker 125HR is equipped with three detectors: InSb and MCT for the middle infrared, and an InGaAs detector for the near infrared. It is also equipped with KBr and $CaF_2$ beamsplitters. Combined, these resources cover the middle infrared from about 650 to 6600 $cm^{-1}$ and the near infrared from 5000 to 15000 $cm^{-1}$. The mid-IR optical filters used are those recommended by the NDACC Infrared Working Group and are listed in the table below. The near-infrared measurements are made as part of the Total Carbon Column Observing Network.

| NDACC filter | approx. range in $cm^{-1}$ | before July/2007 | after July/2007 |
|---|---|---|---|
| Filter 1 | 3950 to 4300 | routine | routine |
| Filter 2 | 2700 to 3600 | not available | routine |
| Filter 3 | 2400 to 3100 | routine | routine |
| Filter 4 | 1900 to 2700 | routine | routine |
| Filter 5 | 1800 to 2200 | routine | routine |
| Filter 6 | 650 to 1400 | routine | routine |
| Filter 7 | 600 to 1050 | not available | routine |

**Algorithm Description:**

Vertical profiles of volume mixing ratios of trace gases are derived using the Optimal Estimation Method, as implemented in SFIT4 (SFIT4:V0.9.4.4 with full error analysis) and distributed through https://wiki.ucar.edu/display/sfit4/Infrared+Working+Group+Retrieval+Code%2C+SFIT. 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.

All the spectra used in the retrievals were recorded at 257 cm maximum Optical Path Difference (OPD).

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. The threshold values are listed below:

Standard NDACC IRWG Species

| | |
|---|---|
| $C_2H_6$ | 1.50 % RMS/DOFS |
| $CH_4$ | 2.50 % RMS/DOFS (for CAMS consolidated data product) |
| $ClONO_2$ | 4.00 % RMS/DOFS |
| CO | 2.50 % RMS/DOFS (for CAMS consolidated data product) |
| HCl | 0.60 % RMS/DOFS |
| HCN | 0.22 % RMS/DOFS |

| | |
|---|---|
| HF | 0.75 % RMS/DOFS |
| $HNO_3$ | 2.20 % RMS/DOFS |
| $N_2O$ | 3.00 % RMS/DOFS |
| $O_3$ | N/A % RMS/DOFS (for CAMS consolidated data product, no max RMS/DOFS specified) |

Non-standard NDACC IRWG Species

| | |
|---|---|
| $C_2H_2$ | 2.00 % RMS/DOFS |
| $C_2H_4$ | 2.00 % RMS/DOFS |
| $CH_3OH$ | 5.00 % RMS/DOFS |
| HCOOH | 2.50 % RMS/DOFS |
| HCHO | 3.00 % RMS/DOFS |
| $NH_3$ | 3.50 % RMS/DOFS |
| $NO_2$ | 1.50 % RMS/DOFS |
| OCS | 4.00 % RMS/DOFS |
| PAN | 3.50 % RMS/DOFS |

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 004 |
| $CH_4$ | version 004 (CAMS consolidated product), version 003 (CAMS rapid delivery) |
| $ClONO_2$ | version 003 |
| CO | version 005 (CAMS consolidated product), version 004 (CAMS rapid delivery) |
| HCl | version 003 |
| HCN | version 003 |
| HF | version 003 |
| $HNO_3$ | version 003 |
| $N_2O$ | version 003 |
| $O_3$ | version 004 (CAMS consolidated product), version 003 (CAMS rapid delivery) |

Non-standard NDACC IRWG Species

| | |
|---|---|
| $C_2H_2$ | version 003 |
| $C_2H_4$ | version 001 |
| $CH_3OH$ | version 003 |
| HCOOH | version 004 |
| HCHO | version 003 |
| $NH_3$ | version 003 |
| $NO_2$ | version 002 |
| OCS | version 001 |
| PAN | version 003 |

**Ancillary Data:**

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 QA4ECV CO data product (data version 003):
Line compilation: The ATM line list (http://mark4sun.jpl.nasa.gov/toon/linelist/linelist.html) is used in the forward calculation. For interferring species, the HITRAN 2008 line list with additional pseudo-line parameters is used.

Line compilation: 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.

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

A priori profiles of trace gas volume mixing ratios are from the WACCM v4 model, where possible and/or appropriate. 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) are also 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].

**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:**

- July 2006: Installation by Bruker engineers Gregor Surawicz and Tony Eng.
- February – April 2007 and 2008: Intercomparison with existing Bomem DA8 FTIR and the Portable Atmospheric Research Interferometric Spectrometer for the Infrared (PARIS-IR)
- July 2007: intercomparison with existing Bomem DA8 Fourier transform spectrometer
- July 2007: Filter wheel moved in the front of the detectors and filters 2 and 7 installed.

- 15 August – 15 Sept 2007: Intensive measurements for NDACC IRWG Aura validation exercise
- 8 April 2008: Near-IR measurements during ARCTAS NASA DC-8 and ER-2 spirals
- August 2009: InGaAs detector installed, enabling NIR measurements. Alternating NIR and MIR operation began thereafter, involving alternating use of the $CaF_2$ and KBr beamsplitters.
- July 2010: First Bruker service visit, for instrument relocation nearer to the suntracker and solar beam, made possible by the removal of the former NDACC Bomem DA8 FTIR in spring 2009.
- 2012-2013: Due to funding issues, PEARL changed from continuous year-round operations to a campaign mode.
- 25 June – 4 July 2012: On-site visit and data acquisition
- 21 June – 4 July 2013: Installation of new custom-built "Community Solar Tracker" suntracker and Robodome, replacing the previous Environment Canada photodiode suntracker and enabling remote control from Toronto
- March 2014: PEARL resumed nearly continuous year-round operations.
- February 2015: New computer installed.
- July 2015: Metrology laser replaced with SIOS model.
- February 2016: First N2O cell tests.
- March 2017: Alignment of 125HR by on-site team: near-IR modulation efficiency improved, mid-IR modulation efficiency decreased.
- March 2018: Small adjustment of the flat mirror before the exit aperture in the interferometer. Increased modulation efficiency at max OPD for mid-IR tests by ~10%. ME for near-IR tests was unaffected.
- February 2019: Installation of two new aperture wheels (to remedy a misalignment issue when changing aperture sizes), as well as a new entrance window. This was followed by realignment that improved modulation efficiency in the near and mid-IR.
- April 2019: Mirror adjustment to center the solar beam on the internal aperture.
- 22 June – 31 July 2019: Mid-IR NDACC measurements were suspended as we did not have an operator on site for beamsplitter swaps and LN2 filling. Near-IR TCCON measurements continued during this time via remote operation from Toronto.
- March 2020: Vaisala PTU30T pressure sensor used for NIR measurements installed in the suntracker dome, along with a Raspberry Pi computer for data logging from the sensor.
- 28 March 2020: Mid-IR measurements were suspended at the end of March 2020 as we did not have a CANDAC/PEARL operator on site after 28 March 2020 due to the COVID-19 pandemic and the associated travel restrictions. Near-IR measurements continued remotely from Toronto until 6 July 2020, after which a laser failure caused measurements to be halted.
- October – November 2021: On-site visit. SIOS laser replaced. Repairs made on the heliostat dome to replace a worn-out track for the dome shutter that failed in early 2021 and prevented the dome from opening properly.
- August 2022: On-site visit. External alignment of the solar beam partially corrected, enabling some remote near-IR TCCON measurements after the visit.

- March – April 2023: On-site visit. The suntracker became misaligned during winter 2023, causing the solar beam to no longer be focused on the input aperture nor to fill the input OAP mirror. On-site team re-leveled the suntracker and made minor adjustments to the input mirrors to get the solar beam back onto the input aperture and fill the mirrors. HBr, N2O, and HCl cell tests were conducted and measurements were analyzed to ensure FTIR alignment was maintained. Issues with the suntracker dome persisted after the team left, and it would intermittently not respond to open/close commands.
- June – July 2023: On-site visit. Some solar measurements were made but repairs to the Robodome were unsuccessful. Remote measurements are not currently possible due to the uncertain nature of the dome status. An upwards-facing webcam was installed in the suntracker dome in July 2023 to aid in remote measurements.

**<u>Reference Articles:</u>**

<u>PhD Theses</u>

Sébastien Roche, Measurements of Greenhouse Gases from Near-Infrared Solar Absorption Spectra, PhD Thesis, Department of Physics, University of Toronto, 2021. https://www.atmosp.physics.utoronto.ca/people/strong/Roche_PhD_thesis_July2021.pdf

Erik M. Lutsch, The Influence of Biomass Burning on the Arctic Atmosphere, PhD Thesis, Department of Physics, University of Toronto, 2019. https://tspace.library.utoronto.ca/handle/1807/97562

Daniel Weaver, Water Vapour Measurements in the Canadian High Arctic, PhD Thesis, Department of Physics, University of Toronto, 2019. https://tspace.library.utoronto.ca/handle/1807/95942

Joseph Mendonca, Improving the Retrievals of Greenhouse Gases from Ground-Based Solar Absorption Spectra, PhD Thesis, Department of Physics, University of Toronto, 2017. https://tspace.library.utoronto.ca/handle/1807/80207

Rodica Lindenmaier, Studies of Arctic Middle Atmosphere Chemistry using Infrared Absorption Spectroscopy, PhD Thesis, Department of Physics, University of Toronto, 2012. https://tspace.library.utoronto.ca/handle/1807/32814

<u>Selected Articles</u>

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

I. Ortega, B. Gaubert, J.W. Hannigan, G. Brasseur, H.M. Worden, T. Blumenstock, H. Fu, F. Hase, P. Jeseck, N. Jones, C. Liu, E. Mahieu, I. Morino, I. Murata, J. Notholt, M. Palm, A. Röhling, Y. Té, K. Strong, Y. Sun, and S. Yamanouchi. Anomalies of O3, CO, C2H2, H2CO, and C2H6 detected with multiple ground-based Fourier-transform infrared spectrometers and assessed with model simulation in 2020: COVID-19 lockdowns versus natural variability. Elementa: Science of the Anthropocene, 11(1), 00015, 2023. https://doi.org/10.1525/elementa.2023.00015

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S. Vandenbussche, B. Langerock, C. Vigouroux, M. Buschmann, N.M. Deutscher, D.G. Feist, O. García, J.W. Hannigan, F. Hase, R. Kivi, N. Kumps, M. Makarova, D.B. Millet, I. Morino, T. Nagahama, J. Notholt, H. Ohyama, I. Ortega, C. Petri, M. Rettinger, M. Schneider, C.P. Servais, M.K. Sha, K. Shiomi, D. Smale, K. Strong, R. Sussmann, Y. Té, V.A. Velazco, M. Vrekoussis, T. Warneke, K.C. Wells, D. Wunch, M. Zhou, and M. De Mazière. Nitrous Oxide Profiling from Infrared Radiances (NOPIR): Algorithm Description, Application to 10 Years of IASI Observations and Quality Assessment. Remote Sensing, 14, 1810, 2022. https://doi.org/10.3390/rs14081810

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