

MetaData File provided: June 2015.
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Data Set Description:

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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/cm²]
Vertical volume mixing ratio profiles above Eureka (0-120 km)
in units of [ppbv]

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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 CaF₂ 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 ₂ O	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 ₂ H ₂	2.00 % RMS/DOFS
CH ₃ OH	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

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

Current Data Versions:

Standard NDACC IRWG Species

C ₂ H 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 ₂ O	version 003
O ₃	version 004 (CAMS consolidated product), version 003 (CAMS rapid delivery)

Non-standard NDACC IRWG Species

C ₂ H ₂	version 003
CH ₃ OH	version 003
HCOOH	version 004
HCHO	version 003
NH ₃	version 003
NO ₂	version 002
OCS	version 001

Ancillary Data:

March 2018 – Began submitting CO, CH₄, and O₃ 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 interfering 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:

$$S_{\text{total}} = \text{square root of } \{(S_m^2 + S_{\text{temp}}^2 + S_{\text{int1}}^2 + S_{\text{int2}}^2 + S_{\text{sza}}^2) + S_{\text{lint}}^2 + S_{\text{width}}^2\}$$

N.B. Smoothing error is not included in the error estimate.

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.
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Instrument History:

- July 2006: Installation by Bruker engineers Gregor Surawicz and Tony Eng.
- July 2007: Filter wheel moved in the front of the detectors and filters 2 and 7 installed.
- August 2009: InGaAs detector installed, enabling NIR measurements. Alternating NIR and MIR operation began thereafter, involving alternating use of the CaF₂ and KBr beamsplitters.
- July 2010: First Bruker service visit, for instrument relocation nearer to the 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.
- August 2013: "Community Solar Tracker" suntracker and Robodome were installed, replacing the previous Environment Canada photodiode suntracker.
- 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.
- 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 – Present: Mid-IR measurements were suspended as we have not had a CANDAC/PEARL Operator on site since the end of 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.

Reference Articles:

PhD Theses

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.

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Rodica Lindenmaier, Studies of Arctic Middle Atmosphere Chemistry using Infrared Absorption Spectroscopy, PhD Thesis, Department of Physics, University of Toronto, 2012.

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Selected Articles

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

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