MetaData File provided: June 2015.
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Data Set Description:

PI: Kimberly Strong
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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 Total Column Abundances above Eureka (0-120 km) in units of [molecules/cm^2]
Vertical profiles above Eureka (0-120 km) in units of [molecules/cm^2]

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Reference Articles:

D. Weaver, K. Strong, M. Schneider, P.M. Rowe, C. Sioris, K.A. Walker, Z. Mariani, T. Uttal, C.T. McElroy, H. Vömel, A. Spassiani, and J.R. Drummond. Intercomparison of atmospheric water vapour measurements at a Canadian High Arctic site. Atmos. Meas. Tech., 10, 2851-2880, https://doi.org/10.5194/amt-10-2851-2017, 2017.

E. Lutsch, E. Dammers, S. Conway, and K. Strong. Long-range Transport of NH3, CO, HCN and C2H6 from the 2014 Canadian Wildfires. Geophys. Res. Lett., 43, 8286–8297, doi:10.1002/2016GL070114, 2016.

C. Viatte, K. Strong, J. Hannigan, E. Nussbaumer, L. Emmons, S. Conway, C. Paton-Walsh, J. Hartley, J. Benmergui, and J. Lin. Identifying fire plumes in the Arctic with tropospheric FTIR measurements and transport models, Atmos. Chem. Phys, 15, 2227-2246, doi:10.5194/acp-15-2227-2015, 2015.

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C. Viatte, K. Strong, C. Paton-Walsh, J. Mendonca, N. T. O'Neill, and J. R. Drummond. Measurements of CO, HCN, and C2H6 total columns in smoke plumes transported from the 2010 Russian boreal forest fires to the Canadian High Arctic. Atmos.-Ocean, 51 (5), 522-531, doi:10.1080/07055900.2013.823373, 2013.

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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, doi: 10.1175/2009JTECHA1215.1, 2009.

See also: http://www.atmosp.physics.utoronto.ca/people/strong/papers.html

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 midlle 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.

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

<u>Algorithm Description:</u>
November 2017 (data version 002):

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 selcted as the elbow of the trade-off curve, where the absolute second derivative is maximum. The threshold values are listed below:

C2H2:	2.00 %-rms/dofs
C2H6:	1.50 %-rms/dofs
CH3OH:	5.00 %-rms/dofs
CH4:	0.35 %-rms/dofs
ClONO2:	4.00 %-rms/dofs
CO:	2.50 %-rms/dofs (for QA4ECV CO data product)
HCl:	0.60 %-rms/dofs
HCN:	0.22 %-rms/dofs
HCOO :	4.00 %-rms/dofs
HF:	0.75 %-rms/dofs
HNO3:	2.20 %-rms/dofs
N2O:	3.70 %-rms/dofs
O3:	3.50 %-rms/dofs

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

<u>Ancillary Data:</u>
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.

June 2015:

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 v6 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 v6 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].

<u>Expected Precision/Accuracy of Instrument:</u>
June 2015:

The error calculations in this work are based on the methodology of Rodgers [1,2]. In addition to the measurement (Sm) errors calculated as described in those papers, random forward model parameter errors have been calculated as described by Rodgers [3] the Kb values calculated by SFIT4 and our best estimate of the uncertainties in temperature (Stemp) and solar zenith angle (Ssza). Systematic forward model errors, i.e. errors due to uncertainties in line intensity and line widths, are calculated based HITRAN 2008 errore. 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 (Stotal) has been determined by adding all components in quadrature:

Stotal={(Sm^2+Stemp^2+Sint1^2+Sint2^2+Ssza^2)+Slint^2+Slwdth^2}^1/2

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] Rodgers CD. Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation. Rev Geophys 1976;14(4):609-624.

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

[3] Rodgers CD. 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] Rodgers CD, Connor BJ. Intercomparison of remote sounding instruments. J Geophys Res 2003;108, doi:10.1029/2002JD002299.

[5] Batchelor RL, Strong K, Lindenmaier R, Mittermeier RL, Fast H, Drummond JR, Fogal PF. 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 Technol 2009;26(7), doi:10.1175/2009JTECHA12151.

<u>Instrument History:</u>

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.