Latest Revision: 14-Aug-2023.
MetaData File provided: September 1999.

Data Set Description:

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Co-PI:	David Griffith, Clare Paton-Walsh (Murphy) University of Wollongong, School of Chemistry Wollongong, NSW, Australia
Instrument:	Fourier Transform Infrared Spectrometer (FTIR)
Site(s):	University of Wollongong NDACC Complementary Station Australia 34.45 S, 150.88 E, 30m above sea level

Measurement Quantities:
Profile and Total Vertical Column Abundances above Wollongong
(profile: volume mixing ratio. total column: number of molecules per sq. cm)

Data License:

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Instrument Description:
Bomem: 1996-2007

A commercial Bomem DA-8 Fourier Transform Infra-red (FTIR) spectrometer has been operated at the Wollongong site on a continuous basis since May 1996.

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. (A medium resolution Bomem DA-2 had been operated at the same site before May 1996.)
The DA-8 is equipped with both InSb and MCT detectors. Combined these detectors cover the middle infrared from about 650 to 4500 cm-1. The solar beam is provided by a home-made solar tracker.

Bruker 125HR: 2007-present

A commercial Bruker IFS 125 HR was installed in August 2007. This instrument has both MIR (MCT and InSb) and NIR (Si diode and InGas) channels and an OPD of 258 cm. The Bruker was purchased to replace the Bomem. The two spectrometers ran side-by-side til April 2008, when the Bomem was decommissioned. The Bruker FTIR uses a Bruker solar tracker.

The optical filters used are those recommended by the NDACC and are listed in the table below.

NDSC filter	spectral range in cm-1	before 28/Apr/97	28/Apr/97 to 11/Aug/99	since 12/Aug/99
Filter 1	3960 to 4400	routine	routine	routine
Filter 2	2800 to 3500	not used	routine	routine
Filter 3	2380 to 3260	routine	routine	routine
Filter 4	2000 to 2650	routine	routine	routine
Filter 5	1860 to 2240	routine	routine	routine
Filter 6	700 to 1340	routine	routine	not since 2007
Filter 7	950 to 1340	not available	not available	routine
Filter 8	700 to 1060	not available	not available	routine

The splitting of the Filter 6 region into filters 7 and 8 improved our ability to quantify HNO3 and other trace gases in the spectral region below 1000 cm-1 significantly.

<u>Algorithm Description:</u>
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) 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 in HDF4 format. The molecules reported so far to the NDACC ncep data base in HDF format from SFIT4 include C2H6, CH4, CO, HCl, HCN, N2O, and O3.

The microwindows and interfering species follow the NDACC IRWG recommendations. The apriori profile used for all gases is based on WACCM version 6, except for H2O which uses the reported humidity from NCEP met data, while for CO the profiles are based on data from aircraft and other ancillary data.

The retrieval results reported here use the Signal-to-Noise-Ratio (SNR) calculated from the spectrum for each target gas to define the diagonal elements of the measurement noise covariance matrix, with the a priori covariance matrix Sa initially computed from the 50 year reported 1-sigma results from WACCM and then adjusted to optimize the retrievals for DOFS and stability (that is smooth profiles as a function of altitude).

Older ASCII Ames files from the Bomem co-exist on this database. For the period 1996 to 2001 the fitting algorithm in use is version 1.09e of SFIT, distributed and provided by C.P. Rinsland (NASA). From 2002 to 2008 the algorithm GFIT was used (Toon, JPL) version 4.4.2.

<u>Ancillary data:</u>

- Line compilation: HITRAN 2008 forms the basis. ClONO2, CFC-11, CFC-12, CFC-22, CCl4, CF4, F-113, and F-142b are from the pseudoline compilation of Geoffrey Toon (JPL).
- Physical models: PT profiles are derived from daily nmc data(NDACC data base) and those again are splined into a climatology for 35 deg lat using the tools from GFIT version 4.4.2 (mod_maker version 9) which includes the calculation of water vapor profiles from the relative humidity.

The Instrumental Line Shape (ILS) is monitored with HBr and N2O cell spectra on an approximately monthly basis since Sep 1998. The cell spectra are analysed with Linefit version 14.5 (F. Hase, 1999).

Hase, F., T. Blumenstock, and C. Paton-Walsh, 'Analysis of the instrumental line shape of high-resolution Fourier transform IR spectrometers with gascell measurements and new retrieval software', Appl. Optics, 38, 3417-3422, 1999.

<u>Expected Precision/Accuracy of Instrument:</u>
April 2017: (reference metadata file from University from Toronto)

The error calculations for this data 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 (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 computations are carried out using the off-line IDL tool errcalc_s4v0_v3.pro, written by D Smale (NIWA, 2017), based on earlier code by a number of authors (B Connor, S Wood, N Jones, J Hannigan, R bachelor).

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.

<u>Instrument History:</u>
Bomem: The fixed aperture stops were changed on day 170, 1996, day 133, 1997, and day 331, 1998. Two different MCT detectors have been used, with namely a 1 mm and a quarter mm active area - with the quarter-mm-detector in place (with a new xyz-vernier mounting) since June 1999. The FTS was moved to another wing of the building in year 2000 due to a scheduled building refurbishment. A new dynamic alignment system installed 15 August 2001.

Bruker: The FTS has not been moved from its current location since installation in 2007.

March 2009	B/S assembly locking mechanism found to be loose.
29 April 2009	Gold tracker mirrors replaced
21 July 2009	Major realignment from visit of J Robinson (NIWA) A telescopic system for fringe viewing setup to fix shear offset of the fixed cube corner. This misalignment may have been introduced in March 2009 due to loose B/S locking mechanism.
2 October 2012	Optics Re-alignment: Telescope and Haidinger Fringes Method
19 August 2014	Replace HeNe laser (SpectraPhysics) with an REO laser
30 April 2015	Laser replaced (SIOS)
19 October 2015	Minor realignment and ghost measurements
25 September 2017	Solar tracker failure, sent to Bruker, no data for 6 months

<u>NDSC retrieval exercises:</u>

Wollongong has regularly participated in all
retrieval exercises of the NDACC IRWG in recent years.

Recent Peer reviewed reference articles:

Vigouroux, C., et al. (2018), NDACC harmonized formaldehyde time-series from 21 FTIR stations covering a wide range of column abundances, Atmospheric Measurement Techniques Discussions, 2018, 1-30, doi:10.5194/amt-2018-22.

Gaudel, A., et al. (2018), Tropospheric Ozone Assessment Report: Present-day distribution and trends of tropospheric ozone relevant to climate and global atmospheric chemistry model evaluation, Elem Sci Anth., 6(1), 39, doi:http://doi.org/10.1525/elementa.2

Steinbrecht, W., et al. (2017), An update on ozone profile trends for the period 2000 to 2016, Atmos. Chem. Phys. Discuss., 2017, 1-24, doi:10.5194/acp-2017-391.

Olsen, K. S., et al. (2017), Comparison of the GOSAT TANSO-FTS TIR CH volume mixing ratio vertical profiles with those measured by ACE-FTS, ESA MIPAS, IMK-IAA MIPAS, and 16 NDACC stations, Atmos. Meas. Tech., 10(10), 3697-3718, doi:10.5194/amt-10-3697-2017.

Dammers, E., et al. (2017), Validation of the CrIS fast physical NH3 retrieval with ground-based FTIR, Atmos. Meas. Tech., 10(7), 2645-2667, doi:10.5194/amt-10-2645-2017.

Buchholz, R. R., et al. (2017), Validation of MOPITT carbon monoxide using ground-based Fourier transform infrared spectrometer data from NDACC, Atmos. Meas. Tech., 10(5), 1927-1956, doi:10.5194/amt-10-1927-2017.

Bader, W., et al. (2017), The recent increase of atmospheric methane from 10 years of ground-based NDACC FTIR observations since 2005, Atmos. Chem. Phys., 17(3), 2255-2277, doi:10.5194/acp-17-2255-2017.

Wang, Y., et al. (2016), Towards understanding the variability in biospheric CO2 fluxes: using FTIR spectrometry and a chemical transport model to investigate the sources and sinks of carbonyl sulfide and its link to CO2, Atmos. Chem. Phys., 16(4), 2123-2138, doi:10.5194/acp-16-2123-2016.

Té, Y., et al. (2016), Seasonal variability of surface and column carbon monoxide over the megacity Paris, high-altitude Jungfraujoch and Southern Hemispheric Wollongong stations, Atmos. Chem. Phys., 16(17), 10911-10925, doi:10.5194/acp-16-10911-2016.

Gaubert, B., et al. (2016), Toward a chemical reanalysis in a coupled chemistry-climate model: An evaluation of MOPITT CO assimilation and its impact on tropospheric composition, Journal of Geophysical Research: Atmospheres, 121(12), 7310-7343, doi:10.1002/2016JD024863.

Dammers, E., et al. (2016), An evaluation of IASI-NH3 with ground-based Fourier transform infrared spectroscopy measurements, Atmos. Chem. Phys., 16(16), 10351-10368, doi:10.5194/acp-16-10351-2016.

Barthlott S., M. S., F. Hase, T. Blumenstock, M. Kiel, D. Dubravica, O. E. Garcia, E. Sepulveda, G. Mengistu Tsidu, S. Takele Kenea, M. Grutter, E. F. Plaza, W. Stremme, K. Strong, D. Weaver, M. Palm, T. Warneke, J. Notholt, E. Mahieu, C. Servais, N. Jones, D. W. T. Griffith, D. Smale, and J. Robinson (2016), Tropospheric water vapour isotopologue data (H216O, H218O and HD16O) as obtained from NDACC/FTIR solar absorption spectra, ESSD:Special Issue: Twenty-five years of operations of the Network for the Detection of Atmospheric Composition Change (NDACC)

Zeng, G., et al. (2015), Multi-model simulation of CO and HCHO in the Southern Hemisphere: comparison with observations and impact of biogenic emissions, Atmos. Chem. Phys., 15(13), 7217-7245, doi:10.5194/acp-15-7217-2015.

Vigouroux, C., et al. (2015), Trends of ozone total columns and vertical distribution from FTIR observations at eight NDACC stations around the globe, Atmos. Chem. Phys., 15(6), 2915-2933, doi:10.5194/acp-15-2915-2015.

Scheepmaker, R. A., et al. (2015), Validation of SCIAMACHY HDO/H2O measurements using the TCCON and NDACC-MUSICA networks, Atmos. Meas. Tech., 8(4), 1799-1818, doi:10.5194/amt-8-1799-2015.

Kremser, S., et al. (2015), Positive trends in Southern Hemisphere carbonyl sulfide, Geophysical Research Letters, 42(21), 9473-9480.

Harris, N. R. P., et al. (2015), Past changes in the vertical distribution of ozone – Part 3: Analysis and interpretation of trends, Atmos. Chem. Phys., 15(17), 9965-9982, doi:10.5194/acp-15-9965-2015.

Duflot, V., et al. (2015), Acetylene (C2H2) and hydrogen cyanide (HCN) from IASI satellite observations: global distributions, validation, and comparison with model, Atmos. Chem. Phys., 15(18), 10509-10527, doi:10.5194/acp-15-10509-2015.

Barthlott, S., et al. (2015), Using XCO2 retrievals for assessing the long-term consistency of NDACC/FTIR data sets, Atmos. Meas. Tech., 8(3), 1555-1573, doi:10.5194/amt-8-1555-2015.