MetaData File provided: July 1999.
Latest Revision : 08-August-2024.

Data License:

Data Set Description:

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Co-PI: John. ROBINSON
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Instrument: Infrared Fourier Transform Spectrometer (FTIR)

Site(s): Arrival Heights, Ross Island, Antarctica
77.83 S, 166.66 E, 220m

Measurement Quantities: Profile and total vertical column abundances above measurement site
(profile: volume mixing ratio .total column: number of molecules per sq. cm)

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Note:

Until the end of 2001, the Co-P.I. for this programme was Frank Murcray, who was at the University of Denver, USA.

Until the end of 2010, the P.I. for this programme was Stephen Wood,
formally of the National Institute for Water and Atmospheric Research Ltd (NIWA)

The current MIR-FTIR team would like to thank the former PI's for their past and continuing contribution to the current MIR research program.

Instrument Description and History:

MIR-FTIR measurements were made at Arrival Heights
with a Bomem DA2 FTS (NIWA005) (opd=50cm) and EOCOM FTS (opd = 20) from 1992 to 1996 and for some short campaigns
before that. HNO3 and HCl only.
This data has been reprocessed with the most current retrieval strategies, total column only.

A Bruker 120M (opd 257cm-1, 0.0035cm-1) was installed at the site in December 1996.
Full NDACC filter set and two detectors (MCT and InSb)
Solar absorption measurements are made in 6 bandpass region spanning 2 to 10 microns (700 to 4100 cm-1)

A Lauder designed tracker can track either sun or moon.

In 2006 a new laboratory was built, 50 metres away. instruments moved over in Dec 2006.

From 1996 to 2009 in the winter period lunar absorption measurements are made at 10 microns.

Operation is semi-automated and logistic support is provided by Antarctica New Zealand.

Since 2002 monthly HBr cell spectra measurements are made and analyzed with Frank Hase's LINEFIT code.

In November 2014 a Bruker-125HR has been installed at Arrival Heights using standard NDACC filters and detectors.
Spectra are taken at a 0.0035cm-1 resolution (257cm opd).
Both the 120M and 125HR operated in parallel over the period Nov 2014 to February 2016.
The inter-comparison was completed and the Bruker 120M is retired as of February 2016.
Analysis and results presented at the NDACC IRWG, 2017, Paris.
Results can be found at:
https://www.acom.ucar.edu/irwg/IRWG_2017_posters/Smale_AHT_comp_2017_poster_v1.pdf

The Bruker 120M was retired in February 2016.
The Bruker 125HR continues measurements.

In Dec 2017 a new solar tracker replaced the older one.

In the winer of 2019 lunar obs restarted and made when possible.

Effect of Covid-19: Measurements from Aug to Oct 2020 were effected by Covid, there were no measurements.
The instrument could not be fixed until Oct 2020.

Metrology laser failure on 24th Jan 2023, no measurements until it was fixed ~15th August 2023. From April to August is the polar night, so
only lost observations for Feb and Mar 2023.

Instrument IDs:
Bomem DA2: NIWA005 (1191-1995)
AHTS Bruker 120M: NIWA003 (1996-2016)
AHTS Bruker 125HR: NIWA004 (2014- present)

Algorithm Description:
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Vertical abundances for total and selected partial columns are retrieved by matching
synthetic spectra to the measured absorption spectra in selected micro-windows containing isolated and well characterized line(s) of the target gas.

The algorithm algorithm in use for the curve fitting is SFIT4 (version 0.9.4.4), developed by B.J.Connor,
C. P. Rinsland, J. Hannigan and M. Palm. It uses a forward
model that simulates the measured spectrum given a model atmosphere, instrument parameters and viewing direction. The SFIT4 codes use optimal estimation techniques and can vary mixing rations of fitted gases in individual layers to achieve the fit (profile fitting).

Even where the goal is the retrieval of total column, the profile fitting can give better
sensitivity, especially in the Antarctic context, where vertical profiles of target species
have larger seasonal perturbations. However, the algorithm does use a priori data and a decision
has to be made as to whether a priori profiles in the retrievals are kept constant for all days,
or if a priori profiles are chosen or adapted for the meteorological conditions on a given day.
For details of retrievals of particular molecules, contact the P.I.

Ancillary data:
-Line compilation : HITRAN 2000-2012 with published updates, TOON GFIT linelists 'ATM' also used.
(special files for ClONO2, CHClF2, ...)

-Physical models : PT profiles used are daily NMC.

Current retrieval strategy:
-SFIT4_v0944(f90) with FITBIN41 (f90) or WRAPDAT(IDL) batching codes
    Column and profile retrievals
        IRWG compliant micro-windows
        NCEP daily P,T profiles
        A priori species profiles: from WACCMv6 CCM model simulations
        48 layer atmosphere
        Hitran 2000-2012 and/or Geoff Toon's (JPL) ATM linelist (2012,2016) compilation (species dependent)
-Prepdat5 spectra pre-processing (f90)
        OPUS to BNR
        Contains hard-coded legacy timing adjustments, site specific coding.
-IDL post processing, visualization, QC/QA, HDF formatting
-Linefit14
-Monthly routine processing (bare minimum):
        HBr and N2O Cell tests, Pre-processing Spectra QA/QC, retrieval of O3, CO and CH4

Expected Precision/Accuracy of Instrument:
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Based on tests with NDACC N2O and HCl sealed cells,precision and accuracy are estimated at +/- 2% and +/- 4% respectively.
Uncertainty analysis is performed per retrieval and reported as systematic and random components.

NDACC IRWG N2O cell #18 measured in Arrival Heights 120M (NIWA003) and 125HR (NIWA004)

NDACC Submission to date:
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Profile: CO, N2O, HNO3, CH4, C2H6, HCl, HF, O3, HCN, OCS (from 1996 onwards)
Total column: ClONO2 (from 1996 onwards)
HDF4 format
Data template: GEOMS-TE-FTIR-002
Bruker 120M data till end of 2015. Bruker 125HR data is from 2015 onwards.

Data rules of use in NDACC HDF files:
These data have been provided with the understanding
that anyone accessing the data will contact the PI of the Lauder FTIR program, Dan Smale
(dan.smale@niwa.co.nz), to discuss the intended uses of the data. Measurement work at NIWA is funded
under a contract that requires identification of end-users of the data. Use of these data
without consultation with the programme PI may jeopardize the renewal of this contract and hence the

future of the FTIR measurement programme.'

Reference Articles:
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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, 2255-2277, doi:10.5194/acp-17-2255-2017, 2017.

Barthlott, S., et al. (2015) "Using XCO2 retrievals for assessing the long-term consistency of NDACC/FTIR data sets." Atmos. Meas. Tech. , amt-2014-260

Barthlott, S., et al. (2017) "Tropospheric water vapour isotopologue data (H216O, H218O, and HD16O) as obtained from NDACC/FTIR solar absorption spectra" http://www.earth-syst-sci-data.net/9/15/2017/

Blumenstock, Thomas, et al. "Characterization and potential for reducing optical resonances in Fourier transform infrared spectrometers of the Network for the Detection of Atmospheric Composition Change (NDACC)." Atmospheric Measurement Techniques 14.2 (2021): 1239-1252.

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, 1927-195

Cortesi, U., et al. (2007). "Geophysical validation of MIPAS-ENVISAT operational ozone data." Atmospheric Chemistry and Physics 7: 4807-4867.

De MaziÃ¨re, M., et al. (2007). "Validation of ACE-FTS v2.2 methane profiles from the upper troposphere to lower mesosphere." Atmospheric Chemistry and Physics 8: 2421-2435.

Dils, B., et al. (2006). "Comparisons between SCIAMACHY scientific products and ground-based FTIR DATA for total columns of CO, CH4, CO2 and N2O." Atmospheric Chemistry and Physics 6: 1953-1976.

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: 39.

Hannigan JW, et al., (2021) "Global atmospheric OCS trend analysis from 22 NDACC stations." Journal of Geophysical Research: Atmospheres. 2022 Feb 27;127(4):e2021JD035764.

Keys, J.G.; Johnston, P.V.; Blatherwick, R.D.; Murcray, F.J. (1993). Evidence of heterogeneous reactions involving nitrogen compounds in the Antarctic stratosphere. Nature 361: 49-51.

Keys, J.G.; Wood, S.W.; Jones, N.B.; Murcray, F.J. (1998). Spectral Measurements of HCl in the plume of the Antarctic volcano Mount Erebus. Geophysical Research Letters 25(13): 2421-2424.

Klekociuk, A. R., et al., (2019) "The Antarctic Ozone Hole during 2017", JSHES, DOI: 10.22499/3.6902.001

Klekociuk, A. R., et al. (2021) "The Antarctic ozone hole during 2018 and 2019." Journal of Southern Hemisphere Earth Systems Science 71.1 (2021): 66-91.

Klekociuk, A. R., et al, (2022) "The Antarctic ozone hole during 2020." Journal of Southern Hemisphere Earth Systems Science, 72(1), 19-37.

Kohlhepp, R., et al. (2012). "Observed and simulated time evolution of HCl, ClONO2, and HF total column abundances." Atmospheric Chemistry and Physics 12: 3527-3556.

Kreher, K.; Keys, J.G.; Johnston, P.V.; Platt, U.; Liu, X. (1996). Ground-based measurements of OClO and HCl in austral spring 1993 at Arrival Heights, Antarctica. Geophysical Research Letters 23(12): 1545-1548.

Kremser, S., et al. (2015). "Positive trends in Southern Hemisphere carbonyl sulfide", Geophys. Res. Lett., 42, 9473–9480, doi:10.1002/2015GL065879.

Kroger, K., et al. (2003). "Stratospheric ozone reaches new minima above McMurdo Station, Antarctica, between 1998 and 2001." Journal of Geophysical Research 108.

Liu, X.; Blatherwick, R.D.; Murcray, F.J.; Keys, J.G.; Solomon, S. (1992). Measurements and model calculations of HCl column amounts and related parameters over McMurdo during the austral spring in 1989. Journal of Geophysical Research 97(18): 20795-20804.

Mahieu, E., et al. (2008). "Validation of ACE-FTS v2.2 measurements of HCl, HF, CCl3F and CCl2F2 using space-, balloon- and ground-based instrument observations." Atmospheric Chemistry and Physics 8: 6199-6221.

Mercer, J. L., et al. (2007). "Comparison of measured and modelled ozone above McMurdo Station, Antarctica, 1989-2003, during austral winter/spring." Journal of Geophysical Research 112(D19307).

Murcray, F.J.; Goldman, A.; Blatherwick, R.; Matthews, W.A.; Jones, N.B. (1989). HNO3 and HCl amounts over McMurdo during the spring of 1987. Journal of Geophysical Research 94(D14): 16615-16619.

Murcray, F. J., A. Goldman, R. Blatherwick, W. A. Matthews, and N. B. Jones, (1989) HNO3 and HCl amounts over McMurdo during the spring of 1987, J. Geophys. Res., 94, 16615-16619, 1989.

Morgenstern, O., et al. (2012). "Long-range correlations in FTIR, satellite, and modeled CO in the Southern Hemisphere." Journal of Geophysical Research. doi:10.1029/2012JD017639

Olsen, K. S., et al. (2017) "Comparison of the GOSAT TANSO-FTS TIR CH4 volume mixing ratio vertical profiles with those measured by ACE-FTS, ESA MIPAS, IMK-IAA

MIPAS, and 16 NDACC stations" , Atmos. Meas. Tech., 10, 3697-3718, https://doi.org/10.5194/amt-10-3697-2017, 2017.

Rinsland, C. P., et al. (2000). "Correlation relationships of stratospheric molecular constituents from high spectral resolution, ground-based infrared solar absorption spectra." Journal of Geophysical Research - Atmospheres 105(D11): 14637-14652.

Rinsland, C. P., et al. (2005). "Long term trends in CH4 at northern mid-latitudes: comparison between ground-based infrared solar and surface sampling measurements." Journal of Quantitative Spectroscopy and Radiative Transfer 97(3): 457-466.

Rinsland, C. P., et al. (2005). "Long-term evolution in the tropospheric concentration of chlorofluorocarbon 12 (CCl2F2) derived from high-spectral resolution infrared solar absorption spectra: retrieval and comparison with in situ surface measurements." Journal of Quantitative Spectroscopy and Radiative Transfer 92: 201-209.

Risi, C., et al. (2012). "Process-evaluation of tropospheric humidity simulated by general circulation models using water vapor isotopologues: 1. Comparison between models and observations." Journal of Geophysical Research 117: D05303.

Ronsmans, G., et al (2016) "First characterization and validation of FORLI-HNO3 vertical profiles retrieved from IASI/Metop", Atmos. Meas. Tech., 9, 4783-4801, doi:10.5194/amt-9-4783-2016

Schneider, M., et al. (2012): "Ground-based remote sensing of tropospheric water vapour isotopologues within the project MUSICA", Atmos. Meas. Tech., 5, 3007-3027, doi:10.5194/amt-5-3007-2012, 2012 .

Sepulveda, E., et al (2014): "Tropospheric CH4 signals as observed by NDACC FTIR at globally distributed sites and comparison to GAW surface in situ measurements" Atmos. Meas. Tech., 7, 2337-2360, doi:10.5194/amt-7-2337-2014, 2014

Sha, M.K., et al, (2021) "Validation of methane and carbon monoxide from Sentinel-5 Precursor using TCCON and NDACC-IRWG stations." Atmos. Meas. Tech., 14(9): 6249-6304. 10.5194/amt-14-6249-2021

Solomon, S.; Keys, J.G. (1992). "Seasonal variations in Antarctic NOx chemistry". Journal of Geophysical Research 97(8): 7971-7978.

Smale, D., et al. (2021) "Evolution of observed ozone, trace gases, and meteorological variables over Arrival Heights, Antarctica (77.8° S, 166.7° E) during the 2019 Antarctic stratospheric sudden warming." Tellus B: Chemical and Physical Meteorology 73.1 (2021): 1-18.

Smale, D., et al. (2023) "Opportunistic observations of Mount Erebus volcanic plume HCl, HF and SO2 by high resolution solar occultation mid infra-red spectroscopy." Journal of Quantitative Spectroscopy and Radiative Transfer (2023): 108665

Strahan, S. E., et al. (2020) "Observed hemispheric asymmetry in stratospheric transport trends from 1994 to 2018." Geophysical Research Letters 47.17 (2020): e2020GL088567.

Strahan, S. E., et al., (2022). Unexpected Repartitioning of Stratospheric Inorganic Chlorine After the 2020 Australian Wildfires. Geophysical Research Letters, 49(14), e2022GL098290.

Vandenbussche S., et al., (2022) "Nitrous Oxide Profiling from Infrared Radiances (NOPIR): Algorithm Description, Application to 10 Years of IASI Observations and Quality Assessment. Remote Sensing." 2022 Apr 8;14(8):1810.

Vigouroux, C., et al. (2007). "Comparisons between ground-based FTIR and MIPAS N2O and HNO3 profiles before and after assimilation in BASCOE." Atmospheric Chemistry and Physics 7: 1-20.

Wang, D. Y., et al. (2007). "Validation of MIPAS HNO3 operational data." Atmospheric Chemistry and Physics 7: 4905-4934.

Wolff, M. A., et al. (2008). "Validation of HNO3, ClONO2, and N2O5 from the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS)." Atmospheric Chemistry and Physics 8: 3529-3562.

Wood, S. W., et al. (2004). "Ground-based nitric acid measurements at Arrival Heights, Antarctica, using solar and lunar Fourier transform infrared observations." Journal of Geophysical Research 109(D18307).

Wood, S. W., et al. (2002). "Validation of version 5.20 ILAS HNO3, CH4, N2O, O3 and NO2 using ground-based measurements at Arrival Heights and Kiruna." Journal of Geophysical Research 107(D24): 10.1029/2001JD000581.

Zeng, G., et al. (2012). "Trends and variations in CO, C2H6 and HCN in the Southern Hemisphere point to the declining anthropogenic emissions of CO and C2H6." Atmospheric Chemistry and Physics 12: 7543 - 7555.

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, 7217-7245, doi:10.5194/acp-15-7217-2015