MetaData File provided: September 2023.
Latest Revision: September 2023.

Data License:

Data Set Description:

PI: Martine De Mazière
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Instrument: Fourier Transform Infrared Spectrometer (FTIR)

Site(s): Maido, Reunion Island
NDACC Station Maido
21.08 S, 55.38 E, 2.16 km above sea level

Measurement Quantities: Vertical Total Column Abundances above Maïdo (0-120 km) in units of [molecules/cm^2]
Vertical profiles of partial column abundances above Maïdo (0-120 km) in units of [molecules/cm^2]

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Reference Articles:
Vigouroux, C. et al.: NDACC harmonized formaldehyde time-series from 21 FTIR stations covering a wide range of column abundances, Atmos. Meas. Tech., 11, 5049-5073, https://doi.org/10.5194/amt-11-5049-2018, 2018.

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Duflot, V., Dils, B., Baray, J. L., De Mazière, M., Attié, J. L., Vanhaelewyn, G., Senten, C., Vigouroux, C., Clain, G., and Delmas, R.: Analysis of the origin of the distribution of CO in the subtropical southern Indian Ocean in 2007, J. Geophys. Res., Vol. 115, No. D22, D22106, http://dx.doi.org/10.1029/2010JD013994, 2010.

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Senten, C., De Mazière, M., Dils, B., Hermans, C., Kruglanski, M., Neefs, E., Scolas, F., Vandaele, A.-C., Vanhaelewyn, G., Vigouroux, C., Carleer, M., Coheur, P.-F., Fally, S., Barret, B., Baray, J.-L., Delmas, R., Leveau, J., Metzger, J.-M., Mahieu, M., Boone, C., Walker, K. A., Bernath, P. F., and Strong K.: Technical Note: New ground-based FTIR measurements at Ile de La Réunion: observations, error analysis, and comparisons with independent data, ACP, 8, 3483-3508, 2008.

Neefs, E., De Mazière, M., Scolas, F., Hermans, C., and Hawat, T.: BARCOS, an automation and remote control system for atmospheric observations with a Bruker interferometer, Review of Scientific Instruments, 78, 3, 035109, doi:10.1063/1.2437144, 2007.

Instrument Description:
A Bruker IFS 125HR Fourier Transform Infra-red (FTIR) spectrometer has been installed at the Maido Observatory since March 2013, and performs continuous measurements since then.
It is equipped with a meteo station and the BARCOS system (Neefs et al., 2007) that allows to record spectra automatically and through remote control from Brussels.

The Bruker 125HR is equipped with two detectors: InSb and MCT, and with KBr beamsplitter.
The measurements cover the 750 - 5000cm-1 spectral range, using seven different filter bands, as recommended in the NDACC Infrared Working Group (IRWG).

A single spectrum is the average of at least one forward and one backward scan which can be taken in less than 3 minutes, but usually two or three forward & backward scans are averaged to increase the Signal to Noise Ratio.
The instrument can measure with a maximum of 257 cm Optical Path Difference (OPD).

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) 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 of partial columns.

The microwindows for NDACC target gases and interfering species follow the NDACC IRWG recommendations.

Spectra are recorded with different optical path differences, depending on the filter and the local measurement time.

Before archiving the data in the NDACC DHF, 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 threshold values depend on the target gas.

Ancillary Data:
Line compilation: The HITRAN 2008 line list with additional pseudo-line parameters is used in the forward calculation (except for HCHO). For interfering species the ATM line list (http://mark4sun.jpl.nasa.gov/toon/linelist/linelist.html) might be used instead (e.g. for H2O).

Physical models: A priori temperature and pressure profiles are derived from 6-hourly NCEP analyses to approx. 1.0 mbar altitude and WACCM monthly means above.
A priori profiles of trace gas volume mixing ratios are taken from the WACCM v6 model, where possible and/or appropriate.

The Instrumental Line Shape (ILS) is monitored with HBr cell (cell #30) spectra on a quasi-regular basis. The HBr cell spectra are analysed with Linefit v.9.0 [Hase, Applied Optics, 1999]. For some retrieved gases the ILS is taken into account in the retrieval process (either in the forward model or as a retrieval parameter).

For QA4ECV CO data product:

Line compilation: The ATM line list (http://mark4sun.jpl.nasa.gov/toon/linelist/linelist.html) is used also in the forward calculation of the target gas (CO).

Expected Precision/Accuracy of retrieved profiles/columns:
The uncertainty evaluations 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] in which the Kb values are calculated by SFIT4 and our best estimates of the uncertainties in temperature (S_temp) and solar zenith angle (S_sza) are used. Systematic forward model errors, i.e. errors due to uncertainties in line intensity (S_lint)and line widths (S_lwdth), are calculated based on uncertainties provided in HITRAN 2008. 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 total error (S_total) has been determined by adding all components in quadrature. For the most important contributions (temperature, measurement noise, interfering species, retrieval parameters, solar position, spectroscopy) this becomes:

S_total=sqrt((Sm^2+S_temp^2+S_int^2+S_retparam^2+S_sza^2)+(S_lint^2+S_lwdth^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 14(4):609-624, 1976.

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

[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 108, doi:10.1029/2002JD002299, 2003.

<u>Instrument History:</u>

Operational since March 2013. Upgraded in April 2023 to the M16 electronics system.