

MetaData File provided: December 2017.

Latest Revision: December 2017.

#### Data Set Description:

PI: Maria V. Makarova (SPbU)  
Co-I: Yana Virolainen (SPbU)  
Alexander Polyakov (SPbU)  
Instrument: Bruker IFS 125 HR Fourier Transform Infrared Spectrometer  
Site(s): St.Petersburg  
Peterhof, Russia,  
59.88N, 29.83E, 20m asl.

#### Measurement Quantities:

Total columns of more than 20 trace gases. Total columns (in molec/cm<sup>2</sup>) of CO, CH<sub>4</sub>, N<sub>2</sub>O, C<sub>2</sub>H<sub>6</sub>, HCN, O<sub>3</sub>, HCl, HF, HNO<sub>3</sub>, CLONO<sub>2</sub> are submitted into NDACC database.

#### Contact Information:

Name: Maria Makarova, Yana Virolainen, Alexander Polyakov  
Address: Dept. of Atmospheric Physics,  
Saint Petersburg State University (SPbU)  
1, Ulyanovskaya st., Peterhof, St. Petersburg,  
198504, Russia  
email: zaits@troll.phys.spbu.ru, yana.virolainen@spbu.ru, a.v.polyakov@spbu.ru  
phone: +7-812-4284347  
fax: +7-812-4287240

#### Selected Articles:

Gavrilov N.M., M.V. Makarova, A.V. Poberovskii, and Yu.M. Timofeyev, 2014: Comparisons of CH<sub>4</sub> ground-based FTIR measurements near Saint-Petersburg with GOSAT observations. *Atmos. Meas. Techn.*, 7, 1003-1010, doi: 10.5194/amt-7-1003-2014.

Timofeyev Yury, Yana Virolainen, Maria Makarova, Anatoly Poberovsky, Alexander Polyakov, Dmitry Ionov, Sergey Osipov, Hamud Imhasin, 2016: Ground-based spectroscopic measurements of atmospheric gas composition near Saint Petersburg (Russia). *J. Mol.Spectr.*, 323, May 2016, 2–14. DOI: 10.1016/j.jms.2015.12.007.

Virolainen, Y. A., Timofeyev, Y. M., Kostsov, V. S., Ionov, D. V., Kalinnikov, V. V., Makarova, M. V., Poberovsky, A. V., Zaitsev, N. A., Imhasin, H. H., Polyakov, A. V., Schneider, M., Hase, F., Barthlott, S., and Blumenstock, T., 2017: Quality assessment of integrated water vapour measurements at St. Petersburg site, Russia: FTIR vs. MW and GPS techniques. *Atmos. Meas. Tech.*, 10, 4521-4536, <https://doi.org/10.5194/amt-10-4521-2017>, 2017.

#### Instrument Description:

Bruker IFS 125 HR Fourier Transform Infrared Spectrometer started its operation at the St.Petersburg site in January, 2009. Solar tracking system for atmospheric observations was designed and performed at the Dept. of Atmospheric Physics, SPbU. The maximum optical path difference (OPD) for the Bruker

IFS 125 HR installed at the St.Petersburg site is 450 cm which corresponds to the spectral resolution of 0.002 cm<sup>-1</sup>.

Typical Bruker IFS 125 HR setup for the solar IR measurements:

- spectral resolution of 0.005 cm<sup>-1</sup> (OPD=180 cm);
- KBr beamsplitter (optionally - CaF);
- liquid nitrogen cooled MCT and InSb detectors;
- standard NDACC optical filter is used for measurements by MCT detector and two non-standard broadband filters are used for measurements by InSb detector.

Instrument alignment is controlled once a month using HBr or N<sub>2</sub>O gas cell spectra. Instrumental line shape parameters are derived from cell spectra by LINEFIT software (developed by F. Hase, IMK KIT).

#### Algorithm Description:

Two processing softwares are routinely used for spectra processing:

- SFIT4 V0.9.4.4 (for CO, CH<sub>4</sub>, N<sub>2</sub>O, C<sub>2</sub>H<sub>6</sub>, HCN, HCl, HF retrievals) implements both, Optimal Estimation and Tikhonov-Phillips approaches. Current version of SFIT includes procedure of uncertainty estimation, these uncertainties are included in the HDF archived data files (<https://www2.acom.ucar.edu/irwg>);

-PROFFIT 9.6 (for O<sub>3</sub>, HNO<sub>3</sub>, CLONO<sub>2</sub> retrievals) is used for the inversion of the spectra. PROFFIT is able to retrieve profiles and vertical column abundances of several species in several microwindows simultaneously. For the profile retrieval the Phillipps-Tikhonov approach is used. For some species the inversion is performed on a logarithmic scale to avoid negative vmr values.

Both retrieval codes use HITRAN 2008, NCEP T&P profiles, and gases (except H<sub>2</sub>O) a priori profiles from the WACCM V6. Pre-fitted water vapour profiles are used as a priori for gases retrievals.

#### Expected Precision/Accuracy of Instrument:

HDF-files contains corresponding error estimates (for each target gas, for every spectrum).

#### Instrument History:

- January 2009 - Bruker IFS 125 HR and self-made solar tracking system setup;
- August 2010 - instrument electronics failure (repaired in September 2010);
- May 2012 - HBr cell measurements were started;
- December 2017 - instrument maintenance by engineer from Bruker company.