

# The portable atmospheric research interferometric spectrometer for the infrared, PARIS-IR

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## Abstract

A new compact, portable Fourier transform spectrometer, called the Portable Atmospheric Research Interferometric Spectrometer for the Infrared (PARIS-IR), has been built for atmospheric remote sensing. The first comprehensive description of the configuration and performance of this instrument for ground-based and balloon-borne operation is provided. Sample atmospheric absorption spectra and representative results observed at the Waterloo Atmospheric Observatory (WAO) are given. The good agreement between PARIS-IR, Brewer spectrophotometer, and ozonesonde measurements of the column density of ozone at mid-latitudes demonstrate the performance and the reliability of the instrument.

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## 1. Introduction

Observations of the trace gas constituents in the Earth's atmosphere are important in the study of atmospheric chemistry and the development of models that can predict the possible evolution of this complicated system. Trace gases from volcanic eruptions, biomass burning and industrial sources are perturbing the environment. Conventional atmospheric measurements involve direct sampling, which is not always straightforward or risk-free and is inconvenient for long-term monitoring. An atmospheric absorption spectrum recorded using the Sun as a source contains spectral features that are characteristic of atmospheric composition. The intensity of the observed features provides quantitative information on the constituent concentrations.

In the infrared spectral region, Fourier transform spectrometers (FTSs) are the usual choice for atmospheric remote sensing because of their inherent advantages of high energy throughput and wide spectral coverage, relative to a grating spectrometer with a single detector element. In general, FTSs also have a 'multiplex'

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advantage, at least in the thermal infrared [1]. FTSs have been deployed on various satellites and planetary probes [e.g., 2–4], on balloon gondolas [e.g., 5,6], and on the ground [e.g., 7–10]. Remote sensing from a satellite can provide a global picture of changes in the trace gas distribution in the atmosphere. However, the use of spectrometers in space has, in turn, spurred the need for measurements from the ground because ground-truth measurements are required to verify the calibration and performance of satellite instruments. Portable instruments can provide calibration and validation data from multiple locations coincident with measurements from satellite instruments.

Field campaign measurements of industrial pollutant emissions [11–13] and volcanic gases [14] require equipment that is compact and portable. The weight, power requirements, and relative fragility of standard laboratory instruments make them difficult to use in field campaigns. Typically compact portable FTSs have low spectral resolution and cannot resolve individual rotational lines of trace gases in the upper atmosphere. Spectral line widths of minor species such as O<sub>3</sub> in the upper atmosphere are narrower than those of mainly tropospheric species such as CH<sub>4</sub> because the contribution of pressure broadening to the line width is much reduced. A typical portable spectrometer such as the ABB-Bomem MR100 series FTIR instrument (<http://www.abb.com/analytical>) operates in the 510–14,000 cm<sup>-1</sup> spectral region with a maximum spectral resolution of 1 cm<sup>-1</sup>. These instruments are typically used with an infrared glower to study species in the boundary layer, for example, for ‘fence-line’ [15] monitoring of chemical plant emissions. Such instruments, however, are not very useful for trace gas measurements in the stratosphere.

A new portable high-resolution Fourier transform spectrometer, named the Portable Atmospheric Research Interferometric Spectrometer for the Infrared (PARIS-IR), has been built by ABB-Bomem for the Waterloo Atmospheric Observatory (WAO). PARIS-IR has relatively high spectral resolution (0.02 cm<sup>-1</sup>) with a very compact design. A suntracker (also from ABB-Bomem) is used to provide radiance from the Sun to the spectrometer, and atmospheric absorption measurements can be made from sunrise to sunset. PARIS-IR is being used regularly to monitor atmospheric trace gases from the WAO, which is located on the roof of the Centre for Environmental and Information Technology, University of Waterloo (43°28′18″N, 80°32′32″W, 319 m above sea level). PARIS-IR has also participated in Canadian ground-based field campaigns to Eureka, Nunavut, in the high Arctic and in a balloon campaign in Vanscoy, Saskatchewan. From these solar absorption results, total column amounts are obtained for key atmospheric constituents such as ozone and other species involved in ozone chemistry (such as NO, NO<sub>2</sub>, HCl and chlorofluorocarbons) together with measurements of primarily tropospheric species such as CH<sub>4</sub>. PARIS-IR has a design similar to the ACE-FTS, which is the primary instrument on the Atmospheric Chemistry Experiment (ACE—also called SCISAT-1). The ACE-FTS is on a Canadian scientific satellite launched by NASA on 12 August 2003 for a nominal 2-year mission [16]. Because of their similar designs, the measurements recorded by PARIS-IR are providing correlative measurements for validating data from the ACE-FTS [17,18]. The purpose of this paper is to provide the first description of PARIS-IR and provide some examples of its performance.

## 2. PARIS-IR instrument

PARIS-IR and the sun tracker were constructed by ABB-Bomem, Inc., in Quebec City. PARIS-IR has the same resolution (0.02 cm<sup>-1</sup>) and spectral coverage region (750–4400 cm<sup>-1</sup>) as the ACE-FTS due to their similar design, and the use of components such as the beam splitter that were flight spares for the satellite instrument. PARIS-IR has a mass of about 66 kg, dimensions of 60 cm × 60 cm × 42 cm, and an average power consumption of 62 W. The instrument has a circular field of view (FOV) of 3.32 mrad on the Sun. It can sustain a mechanical shock of up to 10g ( $g = 9.8 \text{ m/s}^2$ ). These features make PARIS-IR an excellent instrument for field measurements.

The core of this compact, high-resolution spectrometer is a ‘double pendulum’ interferometer (DPI; Fig. 1). Two cube-corner reflectors mounted on a rotating structure (Fig. 1) driven by a magnetic voice coil around a pivot are used as moving elements to generate the optical path difference (OPD). The first DPI interferometer design was developed in the 1980s [19]. The advantages of DPI-type instruments are compact size, low power consumption and insensitivity to linear accelerations. The beam splitter and compensator are made from zinc selenide (ZnSe). The corner cubes are coated with protected gold and the only moving components are the cube-corner reflectors. A diode laser operating at 1.55 μm provides interference fringes to measure the OPD

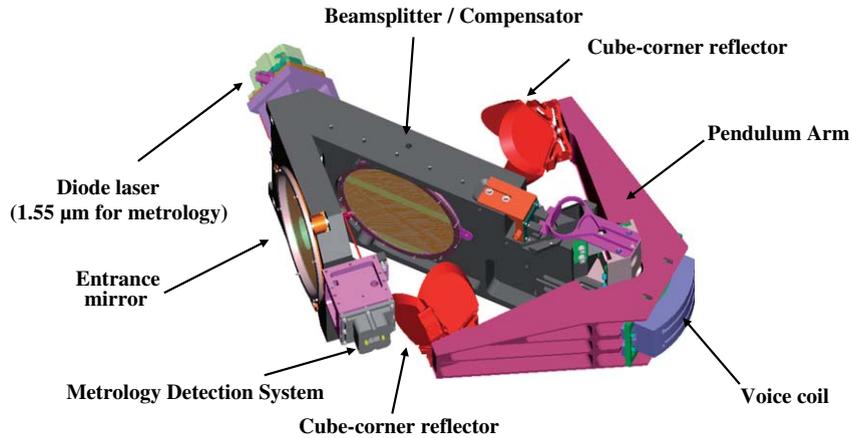


Fig. 1. DPI for the PARIS-IR instrument. Two cube-corner reflectors mounted on a rotating structure driven by a magnetic voice coil around a pivot are used as moving elements to generate the OPD.

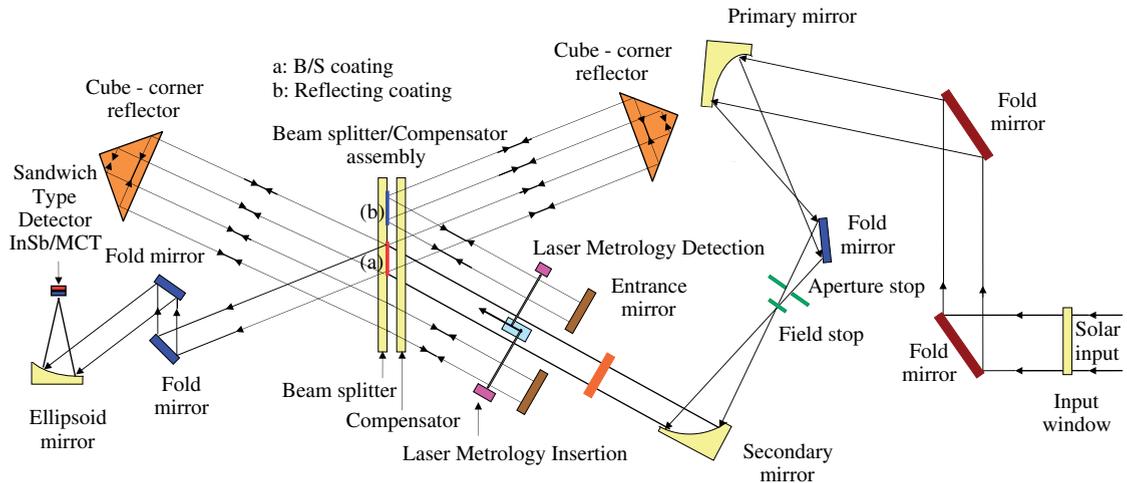


Fig. 2. Schematic diagram showing optical layout of the PARIS-IR instrument. The PARIS-IR optical design is fully compensated for tilt and shear of both moving and stationary optics inside the interferometer, mainly because the radiation is double-passed through the FTS using the ‘entrance mirror’.

and these are used to trigger the sampling of the interferogram. There are eight options for the maximum optical path difference (MOPD) setting, corresponding to 0.02, 0.1, 0.2, 1.0, 2.0, 5.0, 10.0, and 25 cm. These MOPD values correspond to spectral resolutions (defined as  $0.5/\text{MOPD}$ ) of approximately 25.0, 5.0, 2.5, 0.5, 0.25, 0.10, 0.05, and  $0.02\text{ cm}^{-1}$ , respectively. The spectral observation time will vary according to the MOPD setting and the scan speed of the interferometer. Four options for the scanning speed of the interferometer are available: 0.83, 1.25, 1.67 and  $2.5\text{ cm/s}$ .

The PARIS-IR optical design is fully compensated for tilt and shear of both moving and stationary optics inside the interferometer, mainly because of the radiation is double-passed through the FTS using the ‘entrance mirror’ (Fig. 1). The optical path layout is illustrated in Fig. 2. The pointing mirror in the sun tracker, controlled by the sun tracker servo-loop, locks on the radiometric center of the Sun and provides fine tracking while PARIS-IR is taking measurements. The solar beam is sent through the PARIS-IR input window by the sun tracker. The 44 mm diameter solar beam is directed to the optical bench by two flat mirrors ( $73\text{ mm} \times 73\text{ mm}$ ) coated with protected gold. The solar beam is then directed to the  $1.73 \times$  magnification telescope primary mirror. The primary mirror reflects the solar beam through the entrance aperture (5 mm

diameter) and field stop (0.5 mm diameter) to the collimator mirror. The collimated beam with a diameter of 25.4 mm is directed towards the interferometer. An infrared filter (30 mm diameter) is installed between the input optics and the interferometer to minimize the thermal load. The IR signal goes through a 25.4 mm diameter port in the entrance mirror. In order to mount the optics in a relatively small volume, the interferometer is double-passed and cube corner mirrors in both arms of the interferometer are scanned. The output of the interferometer is then directed by a series of flat mirrors and an ellipsoidal mirror into the detector. The stainless-steel detector Dewar has a capacity of 0.4 liters of liquid N<sub>2</sub> and a hold time of approximately 48 h. The two detectors (from Judson), a photovoltaic indium antimonide (InSb) and a photoconductive mercury cadmium telluride (MCT) detector, are mounted in a sandwich arrangement. Using these two detectors simultaneously, PARIS-IR covers the spectral region from 750 to 4400 cm<sup>-1</sup>. Double-sided interferograms are stored on the hard disk of the main control computer inside the PARIS-IR case. These data are transferred to an external data processing computer using a 10 Mb/s Ethernet communication port.

### 3. Measurements made from ground

As sunlight passes through the Earth's atmosphere, certain wavelengths are selectively absorbed by gaseous constituents. In the infrared region, the target species of PARIS-IR have characteristic, discrete absorptions whose positions and strengths are known from laboratory measurements of gaseous samples. We used the HITRAN 2004 [20] database of molecular line parameters to predict the transmission of radiation through the atmosphere. Our analysis uses a model atmosphere with a line-by-line calculation of simulated spectra, followed by comparison with the observed spectra using the SFIT2 computer program in our work. SFIT2 is widely used for the analysis of ground-based infrared solar spectra and was jointly developed at the NASA-Langley Research Center and at the National Institute of Water and Atmospheric Research at Lauder, New Zealand [21,22]. SFIT2 makes use of the optimal estimation formalism developed by Rodgers [23–25] to include a priori constituent profiles in the retrievals in a statistically sound manner. SFIT2 allows the simultaneous retrieval of a vertical profile and column density of the target molecule together with the total columns of interfering species.

Using ABB-Bomem's software package L1bDPS (version 1.2), the desired atmospheric spectra were generated from the double-sided interferograms recorded by PARIS-IR. The L1bDPS includes several necessary processes including wavenumber calibration, phase correction, detector non-linearity correction, channel spectrum correction, residual DC removal and Fourier transformation. The L1bDPS program is based on the level 0 (raw interferograms) to level 1 (calibrated spectra) software developed by ABB-Bomem for the ACE-FTS instrument [16].

The output frequency of PARIS-IR's diode laser, which is used to control the sampling of the interferogram, is affected by the ambient temperature. The spectra recorded by PARIS-IR thus require careful wavenumber calibration because of the drift of the diode laser frequency. The L1bDPS program can obtain the calibration factor needed for each interferogram based on unsaturated atmospheric lines of species such as N<sub>2</sub>O. The measured interferogram is not a real symmetric function because of experimental, instrumental, and computational limitations. A complete reconstruction of the spectrum thus requires a complex Fourier transformation to handle both amplitude and phase information. The needed phase correction, to obtain a real spectrum with only noise in the imaginary plane, is made by the L1bDPS program. In addition, the non-linear response of the photoconductive MCT detector must be corrected. The L1bDPS program obtains non-linearity characterization parameters by minimizing the out-of-band optical artifacts and uses them for non-linearity correction of the interferogram [26].

Fig. 3 displays typical ground-based infrared atmospheric solar absorption spectra generated from interferograms using the L1bDPS program. They have a 0.02 cm<sup>-1</sup> resolution and were observed at WAO on 3 November 2004 with a solar zenith angle of 65.77°. The left side in Fig. 3 shows the overview of a typical spectrum recorded using MCT (upper plot) and InSb (lower plot) detectors. The range of signal-to-noise ratios over the 750–4400 cm<sup>-1</sup> spectral region is from 150:1 to 300:1 (we typically co-add 20 scans recorded in 400 s). The right side of Fig. 3 shows several spectral segments (microwindows) used in the retrieval process. The retrieval process uses SFIT2 to extract the column densities of O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O and HCl target

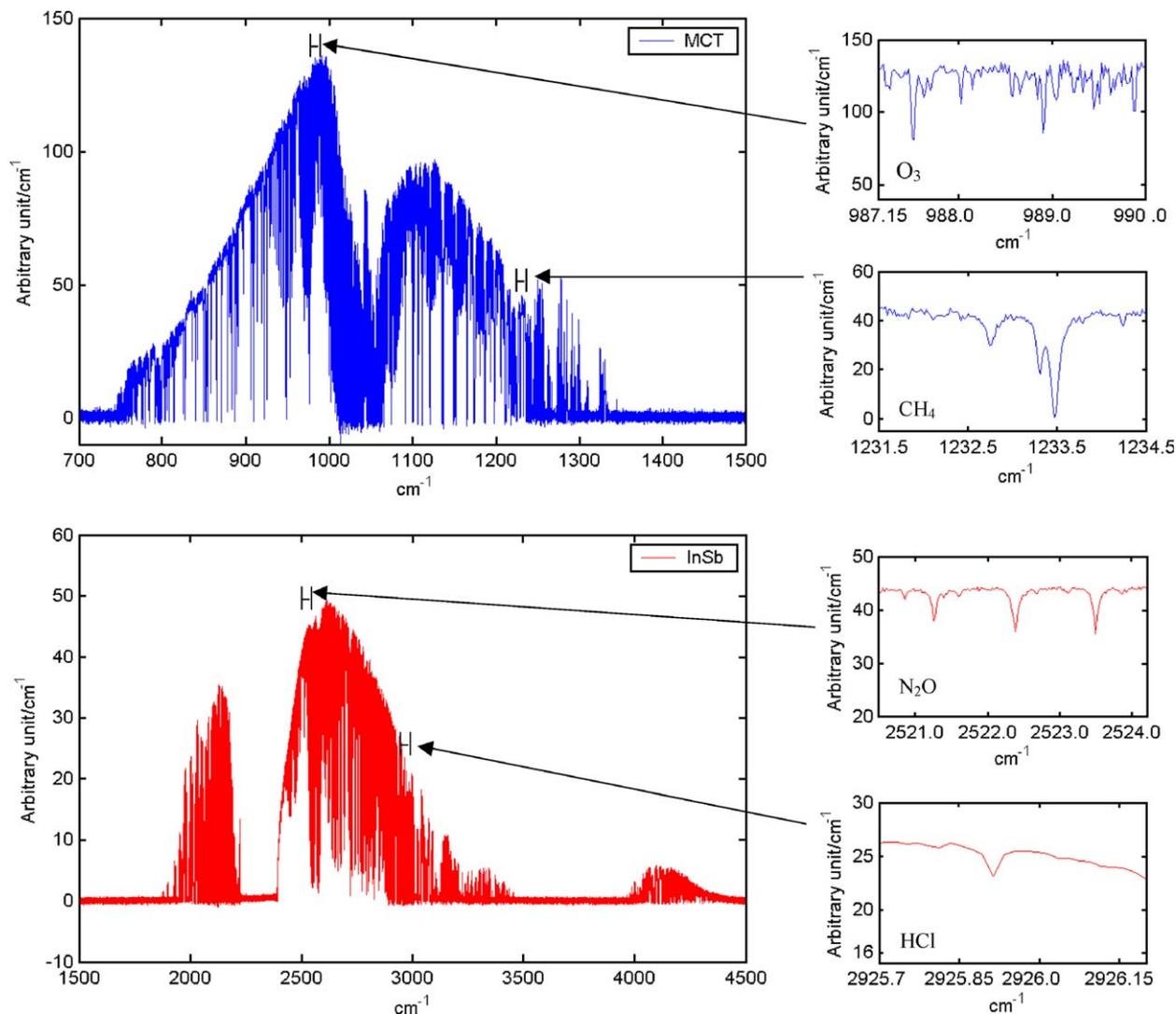


Fig. 3. Sample PARIS-IR solar absorption spectra (left upper: MCT band, left lower: InSb band) recorded with a solar zenith angle of  $65.77^\circ$  at the WAO on 3 November, 2004 (we typically co-add 20 scans recorded in 400 s).

molecules from the appropriate microwindows ( $\text{O}_3$ :  $987.15\text{--}990.0\text{ cm}^{-1}$ ;  $\text{CH}_4$ :  $1231.5\text{--}1234.5\text{ cm}^{-1}$ ;  $\text{N}_2\text{O}$ :  $2520.5\text{--}2524.2\text{ cm}^{-1}$ ;  $\text{HCl}$ :  $2925.65\text{--}2926.20\text{ cm}^{-1}$ ). In these microwindows, the absorption lines of the target species are well isolated, i.e., the absorption lines of the target molecules are minimally affected by the absorption of the interfering species such as  $\text{H}_2\text{O}$  and  $\text{CO}_2$ . These observed spectral lines shapes contain the possible contributions due to instrumental effects (such as slight optical misalignment) and observing conditions (e.g., clouds in the FOV). These effects are considered by including an Empirical Apodization Parameter Function (EAPF) in the spectral analysis [21,22]. Fig. 4 shows the instrument line shape function (ILS) of PARIS-IR obtained by Fourier transformation of the EAPF. The EAPF was derived from a  $\text{N}_2\text{O}$  gas cell spectrum in the  $2500\text{ cm}^{-1}$  region. The PARIS-IR line shape is symmetric and is nearly a sinc function. Careful characterization of the PARIS-IR line shape function is necessary in order to obtain reliable retrievals and more details about the EAPF are discussed in another paper on data analysis [27].

SFIT2 program requires a model atmosphere appropriate for the observations for the forward model used to simulate the spectra. Pressure and temperature profiles needed were constructed by combining the reanalysis data from the National Centers for Environmental Prediction weather model (NCEP) ([28],

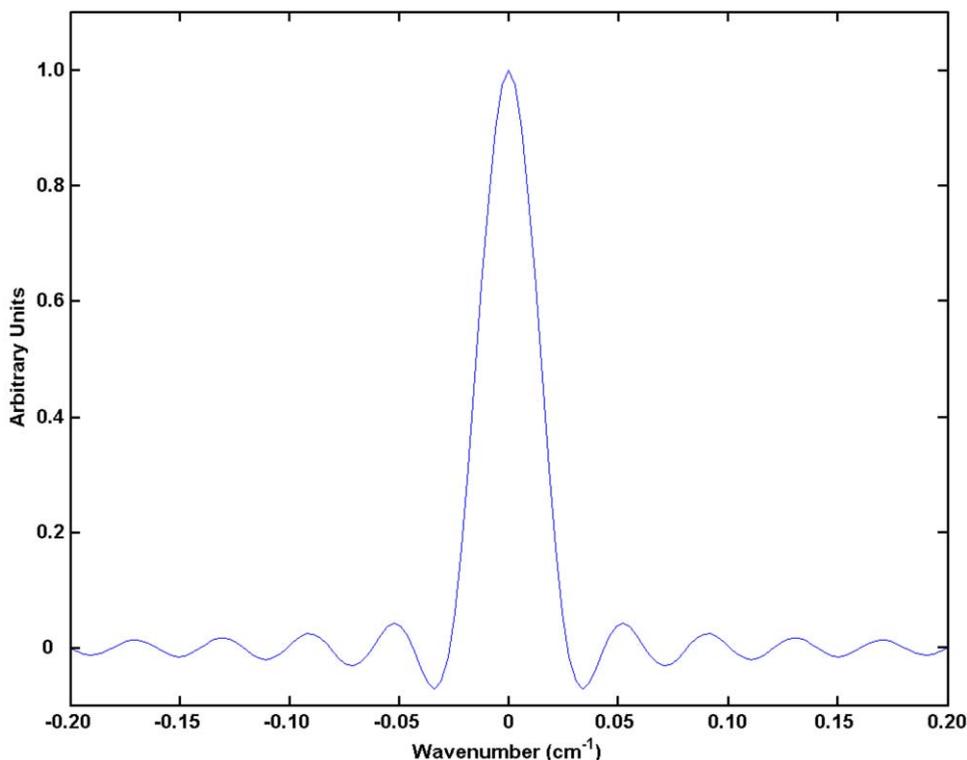


Fig. 4. ILS of the PARIS-IR instrument, which was derived from a  $\text{N}_2\text{O}$  gas cell spectrum around  $2500\text{ cm}^{-1}$ . The PARIS-IR line shape is symmetric and is nearly a sinc function.

<http://www.cdc.noaa.gov/cdc/reanalysis/>) and the Mass-Spectrometer-Incoherent-Scatter model (MSIS-2000) [29]. NCEP covers the surface to 50 km and the output of MSIS is used from 50 to 100 km. The model atmosphere also contains a priori volume mixing ratio (VMR) profiles of trace gases in the atmosphere. In this work, a priori VMRs were provided by the University of Toronto Atmospheric Observatory (TAO, about 95 km away from WAO). TAO was approved as a Complementary Measurement Station by the Network for the Detection of Stratospheric Change (NDSC) Steering Committee in March 2004 (<http://www.ndsc.ws/>). SFIT2 simulates spectra using information from the model atmosphere and line parameters from the HITRAN 2004 database [20]. The discrepancies are calculated from the comparison of simulated spectra and observed spectra using the optimal estimation method. VMR profiles of trace gases are adjusted to reduce the discrepancies between simulated spectra and observed spectra until the difference is within a specified convergence criterion.

Fig. 5 shows the fits and residuals for the observed and calculated spectra of  $\text{N}_2\text{O}$  and  $\text{O}_3$ . The root mean square of the residuals for the fits of  $\text{N}_2\text{O}$  and  $\text{O}_3$  spectra for the measurement day are less than 0.3% and 1%, respectively. The daily mean for  $\text{O}_3$  total columns observed using PARIS-IR at Waterloo on 3 November 2004 was 258 Dobson Units (1 Dobson Unit =  $2.686 \times 10^{16}$  molecules/ $\text{cm}^2$ ). On the same day, the average column density from the Brewer spectrophotometer operated by the Meteorological Service of Canada (MSC) at Toronto was 253 Dobson Units. The discrepancy is less than 2%. The statistical uncertainty in the retrieved PARIS-IR results is 2.6%. A detailed error budget discussion is given in the retrieval paper [27].

#### 4. PARIS-IR balloon configuration

High-altitude balloon measurements can provide concentration profiles of trace gases (up to the float altitude) by recording solar spectra during sunrise and sunset. PARIS-IR was designed to perform measurements from a balloon platform as well as from the ground. During August and September 2004,

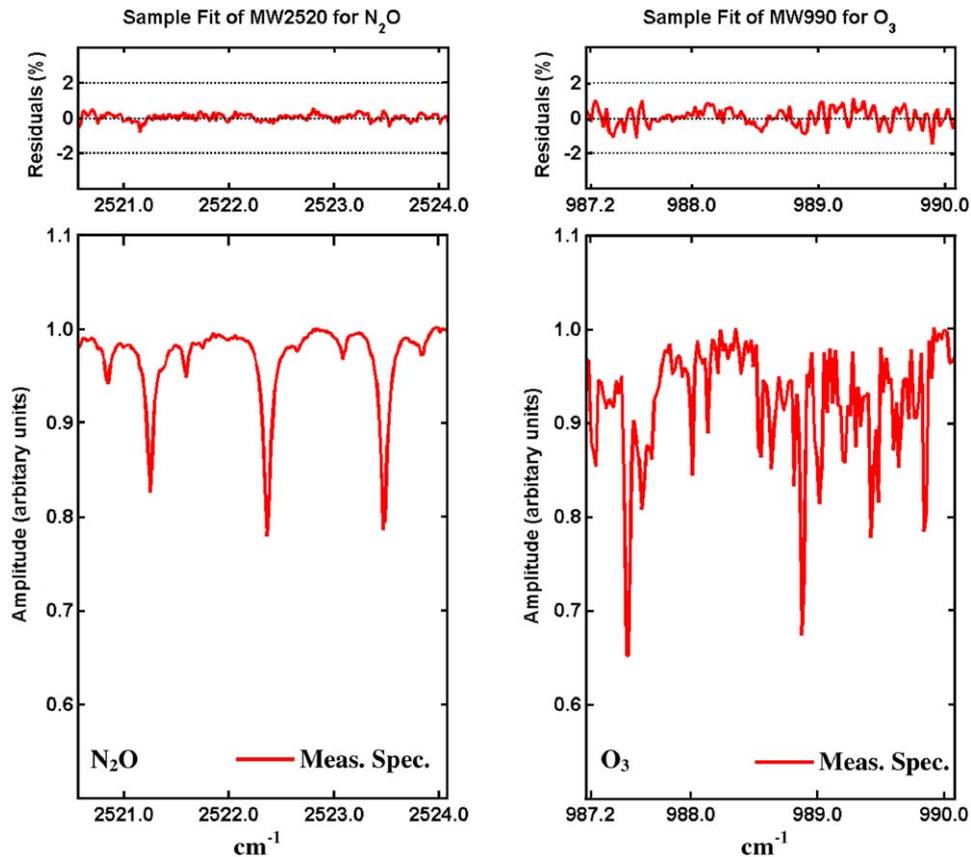


Fig. 5. Examples of fits for the mainly tropospheric species  $\text{N}_2\text{O}$  (left upper: fitting residuals, left lower: measured spectrum) and the mainly stratospheric species  $\text{O}_3$  (right upper: fitting residuals, right lower: measured spectrum). Solar absorption spectra used in these fits were recorded with a solar zenith angle of  $65.77^\circ$  at the WAO on 3 November, 2004 (we typically co-add 20 scans recorded in 400 s).

PARIS-IR was part of the payload of the Middle Atmosphere Nitrogen TRend Assessment (MANTRA 2004) balloon campaign [30]. The purpose of this mission was to investigate changes in the concentrations of ozone as well as nitrogen-containing and chlorine-containing compounds in the stratosphere [30]. No balloon-based data are available from PARIS-IR during MANTRA 2004 flight because of balloon failures, but some ground-based measurements were recorded.

Ground-based measurements were carried out on 13 August 2004 at the MSC Balloon Launch Facility in Vanscoy, Saskatchewan ( $52^\circ 12' \text{N}$ ,  $107^\circ 18' \text{W}$ ). The data were analyzed using the same procedure as discussed above. The total column of ozone observed by PARIS-IR for Vanscoy on 13 August 2004 was 307.4 Dobson Units. For the same day, total column amounts of ozone obtained from the Brewer spectrophotometer [31], SAOZ (Système d'Analyse par d'Observation Zenithale, a lightweight UV-visible diode array spectrometer) [32] and UV-visible grating spectrometer [33–35] at the same campaign station were 307.7, 305.8 and 288.0 Dobson Units, respectively. The partial column amount of ozone (from the surface to 33.82 km) measured by an ozonesonde [36] was 270.2 Dobson Units. The partial column of ozone from the surface to 33.5 km retrieved from PARIS-IR observations was 261.3 Dobson Units. The discrepancies between PARIS-IR, Brewer spectrophotometer, SAOZ, ozonesonde and the UV-visible grating spectrometer are less than 6.5%. The statistical uncertainty in the retrieved PARIS-IR results is 2.6%.

## 5. Summary

PARIS-IR has recorded ground-based solar absorption spectra from two mid-latitude stations: the WAO and the MSC Balloon Launch Facility in Vanscoy, Saskatchewan. The column density of ozone retrieved

from these spectra using SFIT2 shows good agreement with the results obtained from a number of other instruments. These results show PARIS-IR is performing well and observations are continuing at WAO for ACE-FTS validation.

The PARIS-IR instrument was adapted for balloon-based measurements and it participated in the MANTRA 2004 balloon campaign. Although no spectra were obtained during the flight, some useful engineering information was obtained on the thermal performance of the instrument.

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