



**HAL**  
open science

## **Odin/SMR limb observations of stratospheric trace gases: level 2 processing of C1O, N2O, HNO3, and O3**

Jakub Urban, N. Lautié, E. Le Flochmoën, C. Jiménez, P. Eriksson, J. de La Noë, E. Dupuy, M. Ekström, L. El Amraoui, U. Frisk, et al.

### ► To cite this version:

Jakub Urban, N. Lautié, E. Le Flochmoën, C. Jiménez, P. Eriksson, et al.. Odin/SMR limb observations of stratospheric trace gases: level 2 processing of C1O, N2O, HNO3, and O3. *Journal of Geophysical Research: Atmospheres*, 2005, 110 (D14), pp.D14307. 10.1029/2004JD005741 . hal-00256295

**HAL Id: hal-00256295**

**<https://hal.science/hal-00256295>**

Submitted on 25 Jun 2022

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Copyright

## Odin/SMR limb observations of stratospheric trace gases: Level 2 processing of ClO, N<sub>2</sub>O, HNO<sub>3</sub>, and O<sub>3</sub>

J. Urban,<sup>1,2</sup> N. Lauté,<sup>3</sup> E. Le Flochmoën,<sup>1,4</sup> C. Jiménez,<sup>3,5</sup> P. Eriksson,<sup>3</sup> J. de La Noë,<sup>1</sup> E. Dupuy,<sup>1</sup> M. Ekström,<sup>3</sup> L. El Amraoui,<sup>1,6</sup> U. Frisk,<sup>7</sup> D. Murtagh,<sup>3</sup> M. Olberg,<sup>8</sup> and P. Ricaud<sup>1,4</sup>

Received 23 December 2004; revised 13 April 2005; accepted 27 April 2005; published 29 July 2005.

[1] The Sub-Millimetre Radiometer (SMR) on board the Odin satellite, launched on 20 February 2001, observes key species with respect to stratospheric chemistry and dynamics such as O<sub>3</sub>, ClO, N<sub>2</sub>O, and HNO<sub>3</sub> using two bands centered at 501.8 and 544.6 GHz. We present the adopted methodology for level 2 processing and the achieved in-orbit measurement capabilities of the SMR radiometer for these species in terms of altitude range, altitude resolution, and measurement precision. The characteristics of the relevant level 2 data versions, namely version 1.2 of the operational processor as well as versions 222 and 223 of the reference code, are discussed and differences are evaluated. An analysis of systematic retrieval errors, resulting from spectroscopic and instrumental uncertainties, is also presented.

**Citation:** Urban, J., et al. (2005), Odin/SMR limb observations of stratospheric trace gases: Level 2 processing of ClO, N<sub>2</sub>O, HNO<sub>3</sub>, and O<sub>3</sub>, *J. Geophys. Res.*, 110, D14307, doi:10.1029/2004JD005741.

### 1. Introduction

[2] The Odin satellite was launched on 20 February 2001 into a circular quasi-polar low Earth orbit at ~600 km altitude. It carries two instruments, namely the Optical Spectrograph and Infrared Imaging System (OSIRIS) and the Sub-Millimetre Radiometer (SMR).

[3] The SMR instrument employs four tunable single-sideband Schottky-diode heterodyne receivers in the ~486–581 GHz spectral range as well as one mm-wave receiver at ~119 GHz. Observations of thermal emission of trace gases originating from the Earth's limb are performed in a time-sharing mode with astronomical observations using a 1.1-m telescope. Spectra are recorded by means of two high-resolution auto-correlators, one acousto-optical spectrometer, and a three-channel filter bank for the 119-GHz radiometer. Detailed technical information on the satellite and the SMR instrument is given by *Frisk et al.* [2003].

[4] In aeronomy mode, various target bands are dedicated to profile measurements of trace constituents relevant to stratospheric and mesospheric chemistry and dynamics such as O<sub>3</sub>, ClO, N<sub>2</sub>O, HNO<sub>3</sub>, H<sub>2</sub>O, CO, and NO, as well as isotopes of H<sub>2</sub>O and O<sub>3</sub> [e.g., *Murtagh et al.*, 2002; *Merino et al.*, 2002].

[5] Stratospheric mode measurements are performed typically twice per week using the two auto-correlator spectrometers centered at 501.8 and 544.6 GHz. We describe the adopted retrieval methodology and the achieved observation capabilities of the SMR radiometer for the study of the stratospheric target species O<sub>3</sub>, ClO, N<sub>2</sub>O, and HNO<sub>3</sub>. The ground-segment is first described in section 2. Section 3 gives an overview of theoretical and achieved in-orbit measurement capabilities for the stratospheric mode target species. Differences between the latest versions of the operational and reference level 2 data products are analyzed and discussed. Systematic errors of the level 2 data arising from instrumental and spectroscopic uncertainties are evaluated in section 4, and the characteristics of the Odin/SMR stratospheric mode level 2 data are summarized in section 5.

## 2. Odin/SMR Data Processing

### 2.1. Ground Segment

[6] The Odin satellite with its two instruments is operated by the Swedish Space Corporation. Calibrated spectra (level 1b) are produced from the SMR instruments raw data and the reconstructed attitude data of the satellite (level 0) at the Onsala Space Observatory in Sweden, both for the astronomy and aeronomy measurement modes. Detailed information on level 1 data processing is given by *Olberg et al.* [2003]. For the retrieval

<sup>1</sup>Observatoire Aquitain des Sciences de l'Univers, Floirac, France.

<sup>2</sup>Now at Department of Radio and Space Science, Chalmers University of Technology, Göteborg, Sweden.

<sup>3</sup>Department of Radio and Space Science, Chalmers University of Technology, Göteborg, Sweden.

<sup>4</sup>Now at Laboratoire d'Aérodynamique, Observatoire de Midi-Pyrénées, Toulouse, France.

<sup>5</sup>Now at Institute of Atmospheric and Environmental Science, School of GeoSciences, University of Edinburgh, Edinburgh, UK.

<sup>6</sup>Now at Météo France, Toulouse, France.

<sup>7</sup>Swedish Space Corporation, Solna, Sweden.

<sup>8</sup>Onsala Space Observatory, Chalmers University of Technology, Onsala, Sweden.

of vertical profiles from the spectral measurements of a limb scan (aeronomy level 2 processing), two similar data processors have been developed in Sweden and in France: within the SMR retrieval group, the Chalmers University of Technology (Gothenburg, Sweden) is in charge of the systematic production of the operational level 2 data (available at <http://www.rss.chalmers.se/geml>). The Observatoire Aquitain des Sciences de l'Univers (Bordeaux, France) provides a reference level 2 product with the aim of verification and validation of the operational data product. The overall objectives of the specifically designed reference code include the development and optimization of the retrieval methodology for the various measurement modes as well as the quality assessment of the operational code by comparison of results for scientifically interesting periods, but without aiming at the processing of the whole data set. The French level 2 data processor CTSO (for Chaîne de Traitement Scientifique Odin) has for this purpose been installed within the French atmospheric data bank ETHER (<http://ether.ipsl.jussieu.fr>), which also serves as a platform for distribution of the Odin/SMR level 2 data.

## 2.2. Forward and Retrieval Models

[7] Vertical profiles are retrieved from the spectral measurements of a limb scan by inverting the radiative transfer equation for a non-scattering atmosphere. Retrieval algorithms based on the Optimal Estimation Method (OEM) [Rodgers, 1976], a linear inversion method using statistical a priori knowledge of the retrieved parameters for regularization, were developed for the ground segment of Odin/SMR in Sweden and in France [Baron, 1999; Baron et al., 2001, 2002; Merino et al., 2001, 2002; Lautié et al., 2001; Lautié, 2003; Eriksson et al., 2002, 2005; Urban et al., 2002, 2004a].

[8] The modular 1-d forward and retrieval code for the millimeter and sub-millimeter wavelengths range MOLIERE-5 (Microwave Observation Line Estimation and REtrieval, version 5) is used for Odin/SMR level 1b → level 2 processing within CTSO/ETHER. The forward model part of MOLIERE-5 includes modules for spectroscopy (line-by-line calculation, water vapor, and dry air continua), radiative transfer (including refraction), and sensor characteristics (antenna, sideband, spectrometer). It also allows the computation of differential weighting functions (Jacobians) needed for the inversions. The forward model and an inversion module based on the Optimal Estimation Method are implemented within a framework allowing nonlinear retrievals to be performed according to a Newton Levenberg-Marquardt iteration scheme. For detailed information on the model, the reader is referred to Urban et al. [2004a].

[9] The Swedish level 2 processor Qsmr, aiming at fast operational data analysis, is based on the same basic principles and methods. The employed retrieval model Qpack [Eriksson et al., 2005] is built around the atmospheric radiative transfer model ARTS (Atmospheric Radiative Transfer Simulator), developed at the Chalmers University of Technology (Gothenburg, Sweden) and the University of Bremen (Germany) [Buehler et al., 2005].

[10] A systematic comparison of the forward models ARTS and MOLIERE-5 used within the Odin/SMR level 2 processors resulted in an excellent agreement of the

different modules for spectroscopy, radiative transfer and instrument modeling [Melsheimer et al., 2005].

## 3. Odin/SMR Observation Capabilities

### 3.1. Theoretical Capabilities

[11] In a first step, the nominal measurement capabilities of the SMR instrument with respect to the stratospheric mode target gases ClO, N<sub>2</sub>O, O<sub>3</sub>, and HNO<sub>3</sub> were investigated theoretically by means of nonlinear retrieval simulations assuming nominal instrument performance [Frisk et al., 2003]; that is, all instrumental parameters (antenna-, sideband-, spectrometer-response) were simulated according to their pre-flight characterization. A realistic receiver noise temperature of 3000 K (single-sideband) and an effective integration time of 0.875 s in the stratosphere below 50 km, corresponding to a spectrometer read-out every 1.5 km in terms of tangent-altitude, were assumed (1.75 s above 50 km). Note that Odin's scan velocity is kept constant at  $\sim 0.75 \text{ km s}^{-1}$ .

[12] Figure 1 shows the results of the MOLIERE-5 simulation runs, providing for each target species the nominal retrieval precision as well as altitude range and resolution. The theoretical retrieval capabilities are summarized in Table 1. In order to test and to demonstrate the robustness of the retrieval model, somewhat extreme cases were chosen: Vertical distributions characteristic for polar winter conditions were retrieved starting from a first guess corresponding to a midlatitude scenario.

[13] Results are in qualitative agreement with pre-flight studies performed by, for example, Baron et al. [2002] and Merino et al. [2002]. Small quantitative differences can be explained by the slightly different set-up for the pre-flight simulations, for example with respect to the assumptions made for the measurement error and a priori error covariance matrices. The simulation results of this work were obtained using the robust retrieval methodology developed for the CTSO-v223 and are here presented as a quantitative estimate for the best possible performance which could theoretically be expected from the SMR instrument for stratospheric mode measurements.

### 3.2. Level 2 Data Versions

[14] In order to account for the in-flight performance of the Odin/SMR instrument, the methodology and set-up adopted for level 2 processing has progressively been adapted and optimized. The discussed here most recent versions of the reference code CTSO are version 222 (in the following also called "CTSO-v222"), optimized for retrieval of ClO, N<sub>2</sub>O, and O<sub>3</sub> in the 501.8-GHz band, and version 223 (or "CTSO-v223"), which also gives satisfactory results for the 544.6-GHz band retrievals of O<sub>3</sub> and HNO<sub>3</sub>. The most recent version of the operational code, used for the systematic processing of the stratospheric mode measurements, is version 1.2 ("Chalmers-v1.2"). Particularities of the different versions of both reference and operational code are first summarized in this section. A detailed comparison is provided in section 3.4.

#### 3.2.1. CTSO-v222

[15] Version 222 of the reference code CTSO allows for simultaneous nonlinear retrievals of the volume mixing ratios (VMR) of ClO, N<sub>2</sub>O, and O<sub>3</sub> in the 501.8-GHz band.

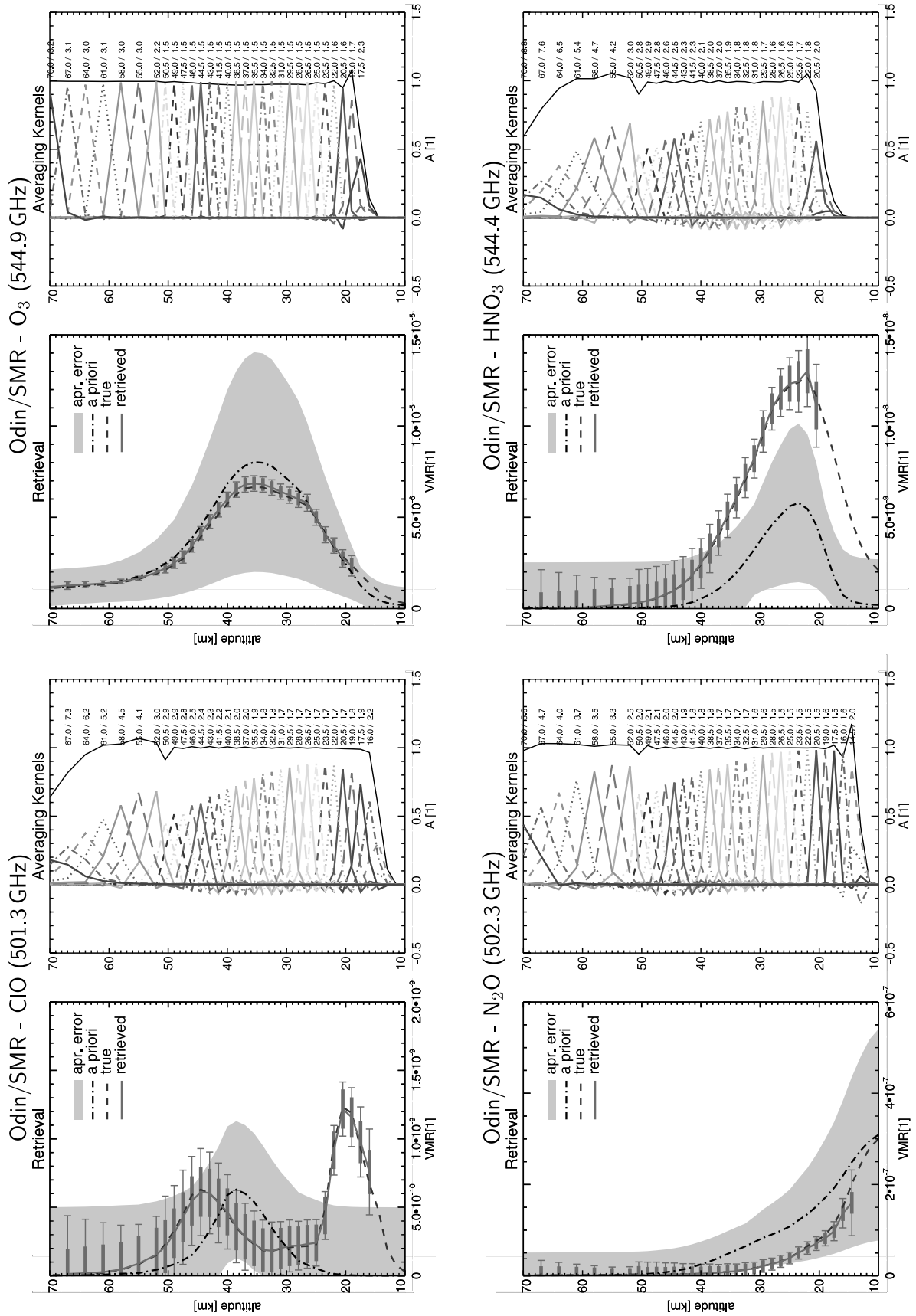


Figure 1

**Table 1.** Theoretical and Typically Achieved Capabilities of Odin/SMR for the Observation of Stratospheric ClO, N<sub>2</sub>O, O<sub>3</sub>, and HNO<sub>3</sub><sup>a</sup>

Species	Frequency, GHz	Precision (1- $\sigma$ )	Altitude Resolution	Altitude Range	Number of Iterations
<i>Theoretical Capabilities<sup>b</sup></i>					
O <sub>3</sub>	501.5	0.5–2 ppmv (25–30%)	~2 km	~19–50 km	2–3
ClO	501.3	0.15–0.2 ppbv	1.5–2 km	~16–67 km	2–3
N <sub>2</sub> O	502.3	15–35 ppbv (10–20% <30 km)	~1.5 km	~15–70 km	2–3
O <sub>3</sub>	544.9	0.2–0.4 ppmv (10–20%)	~1.5 km	~18–70 km	3–4
HNO <sub>3</sub>	544.4	≤1 ppbv (15–25% <30 km)	1.5–2 km	~21–67 km	3–4
<i>Achieved Capabilities CTSO-v222<sup>c,d</sup></i>					
O <sub>3</sub>	501.5	0.25–1.5 ppmv (20–25%)	~2.5 km	~17–45 km	2–3
ClO	501.3	0.15–0.25 ppbv	2–2.5 km	15–55 km	2–3
N <sub>2</sub> O	502.3	10–45 ppbv (5–15% <30 km)	~2 km	13–55 km	2–3
O <sub>3</sub>	544.9	0.2–0.5 ppmv (10–25%)	~2 km	14–70 km	3–4
HNO <sub>3</sub>	544.4	≤1 ppbv	2–3 km	20–50 km	3–4
<i>Achieved Capabilities CTSO-v223<sup>c,e</sup></i>					
O <sub>3</sub>	501.5	0.25–1.5 ppmv (20–25%)	3–3.5 km	~18–45 km	2–3
ClO	501.3	0.15–0.25 ppbv	2–2.5 km	15–55 km	2–3
N <sub>2</sub> O	502.3	15–45 ppbv (15–20% <30 km)	~1.5 km	14–55 km	2–3
O <sub>3</sub>	544.9	0.2–0.8 ppmv (10–40%)	~1.5 km	14–70 km	3–4
HNO <sub>3</sub>	544.4	≤1.5 ppbv	1.5–2 km	18–35 km	3–4
<i>Achieved Capabilities Chalmers-v1.2<sup>c,e,f</sup></i>					
O <sub>3</sub>	501.5	0.25–0.75 ppmv	3.5–4 km	21–45 km	4–5
ClO	501.3	0.05–0.15 ppbv	2–4 km	15–45 km	4–5
N <sub>2</sub> O	502.3	10–30 ppbv (5–15% <30 km)	2–4 km	15–35 km	4–5
O <sub>3</sub>	544.9	0.2–0.4 ppmv (10–20%)	2–3 km	17–60 km	5–6
HNO <sub>3</sub>	544.4	≤1 ppbv	2–2.5 km	18–35 km	5–6

<sup>a</sup>Indicated are target line frequencies, single-scan precisions and altitude resolutions (FWHM) in the lower stratosphere, approximate altitude ranges for a polar scenario, and the typical number of iterations required for reaching convergence.

<sup>b</sup>Retrieval grid given by nominal tangent-altitudes of stratospheric mode scan:  $\Delta z = 1.5$  km ( $z \leq 50$  km),  $\Delta z = 3$  km ( $z > 50$  km).

<sup>c</sup>Based on single-scan retrieval (latitude  $\sim 78.4^\circ$ S, 20/9/2002, orbit 217F).

<sup>d</sup>Retrieval grid  $\Delta z = 2$  km ( $z \leq 50$  km),  $\Delta z = 6$  km ( $z > 50$  km).

<sup>e</sup>Retrieval grid given by tangent-altitudes of scan:  $\Delta z \sim 1.5$  km ( $z \leq 50$  km),  $\Delta z \sim 6$  km ( $z > 50$  km).

<sup>f</sup>Smoothed in altitude (using non-diagonal a priori covariance matrix).

The usable bandwidth is 700 MHz, a 100-MHz-wide sub-band of the auto-correlator has been excluded owing to frequently occurring instabilities of the sub-band power level. The response function of the auto-correlator indicates a spectral resolution of  $\sim 2$  MHz and is taken into account in the forward calculations. A scan-bias is retrieved assuming an a priori uncertainty of 500 m, as estimated from the satellites attitude data. Moreover, a continuum profile is retrieved in order to account for water vapor and dry air continuum emissions which increase with decreasing tangent-altitudes. Profiles are retrieved on an altitude grid of 2 km resolution in the stratosphere and of 6 km resolution above 50 km and are defined as piecewise linear functions determined by the altitude levels of the retrieval grid. The assumed a priori error for the retrieved mixing ratios corresponds to 75% of the climatological a priori mixing ratios. Threshold values are used if the climatological

mixing ratio is too small: The minimum a priori error is limited to 1 ppmv for O<sub>3</sub>, 50 ppbv for N<sub>2</sub>O, 0.5 ppbv for ClO, and 0.1 ppbv for HNO<sub>3</sub>. A constant a priori error of 5 K is assumed for the temperature retrieval in the 544.6-GHz band. For the optically thin bands (ClO, O<sub>3</sub>, and N<sub>2</sub>O around 501.8 GHz), only channels with a total opacity smaller than 1.5 according to the climatological a priori profiles are used, a measure to linearize the inversion problem and to assure rapid convergence. In practice, only the lowest tangent-views are rejected using this criterion. In the case of bands containing optically thick lines (O<sub>3</sub> and HNO<sub>3</sub> band at 544.6 GHz), temperature information is retrieved simultaneously, in accordance with recommendations from dedicated studies [Baron *et al.*, 2001; Cailley, 2002]. Moreover, the measurement error is assumed to be 3 K higher than the theoretical noise calculated from the radiometer equation (4.5 K higher for the 544.6-GHz band),

**Figure 1.** Retrieval simulations for the Odin/SMR stratospheric mode target species using MOLIERE-5. (top left) ClO at 501.3 GHz; (bottom left) N<sub>2</sub>O at 502.5 GHz; (top right) O<sub>3</sub> at 544.9 GHz; (bottom right) HNO<sub>3</sub> at 544.4 GHz. Two plots are presented for each molecule. The plots on the left-hand side show the profiles used for simulating the measurement (dashed line) and the retrieved profile (solid line with error bars). Errors due to statistical measurement noise (thick error bars) and total errors, including also the error due to smoothing of the profile due to the limited altitude resolution, can be distinguished. The a priori (“first guess”) profile (dash-dotted line) and the assumed 1- $\sigma$  a priori uncertainty (shaded area) are presented as well. The plots on the right-hand side show the averaging kernel functions providing information on the altitude resolution associated with the retrieved parameters (FWHM values are indicated). The envelope is the sum of the averaging kernel functions for a given altitude, an indicator for the measurement response as a function of altitude. See color version of this figure in the HTML.



in order to account for baseline artifacts (e.g., offsets, ripples) present in the calibrated spectra (of level 1b, calibration version 4). The errors associated with the individual spectrometer channels are assumed to be uncorrelated, and the measurement error covariance matrix is consequently diagonal. A linear baseline is retrieved (offset and slope), applied to the whole scan, as well as a spectrometer frequency shift from the strong O<sub>3</sub> line in the 544.6-GHz band in order to account for a possible residual (non-corrected) Doppler shift. Spectroscopic line parameters for the line-by-line calculation are taken from the Verdandi database (<http://www.rss.chalmers.se/gem/Research/verdandi.html>) [Eriksson, 1999], which merges frequencies, line intensities, and lower state energies from the JPL catalog [Pickett *et al.*, 1998] with pressure broadening parameters from the HITRAN compilation [Rothman *et al.*, 2003], but also includes spectral parameters from other sources where appropriate. See Table 2 for an overview of the spectroscopic parameters used in the processing system.

[16] Level 2 data of the CTSO-v222 for the 501.8-GHz band, available since February 2003, have been used in the past for scientific studies concerning polar vortex chemistry and dynamics [e.g., Urban *et al.*, 2004c; Ricaud *et al.*, 2005a; Berthet *et al.*, 2005]. However, known spectroscopic uncertainties of the pressure broadening parameters for the 544.9-GHz O<sub>3</sub> line have prevented the use of version 222 data of this band.

### 3.2.2. CTSO-v223

[17] The CTSO-v223 retrieval scheme was developed in order to account for several identified instrumental and spectroscopic problems with the version 222 data analysis and is available since July 2003.

[18] First of all, CTSO-v223 profiles are retrieved on an altitude grid given by the actual tangent-altitudes of the Odin limb scans. This scheme allows to have access to the highest possible altitude resolution of the Odin/SMR measurements and provides at the same time a certain robustness since the integration time for a single Odin/SMR measurement changes between stratosphere and mesosphere (typically 0.875 s versus 3.5 s) and the altitude where the change occurs may vary by a few kilometers as do the lower and upper limits of the scan. Moreover, during a few orbits per day when the ground station at Esrange (Sweden) is not accessible for data down-link, the integration time in the stratosphere is prolonged ( $\sim 1.75$  s) in order to meet platform memory requirements.

[19] Second, the baseline retrieval was extended to the retrieval of an offset for each tangent altitude in order to account for frequently observed jumps of the spectral baseline of the order of a few Kelvin. This unphysical behavior, easily identifiable at high tangent-altitudes where the continuum level should be zero, is assumed to arise from gain variations during the calibration cycle or, more precisely, from uncertainties in the correction of the contributions of the antenna baffles to the measured power. The new scheme leads in particular to smoother retrievals for the 544.6-GHz band.

[20] Third, the instrument module of the version 223 forward model simulates the nominal behavior for image-band suppression and signal-band transmission, based on pre-flight laboratory measurements of the sideband ratio.

Thus the accurate modeling of the measurements is further improved.

[21] Finally, the a priori errors assumed for HNO<sub>3</sub> were slightly adapted in order to allow for a more stable profile retrieval from the HNO<sub>3</sub> band residing around 544.4 GHz on the wing of a strong ozone line centered at 544.9 GHz. The HNO<sub>3</sub> a priori error was slightly reduced to 50% of the climatological value, while the minimum value was slightly increased to 0.5 ppbv.

[22] Compared to version 222, CTSO-v223 single-profile data appear noisier, but provide a better altitude resolution. On the other hand, averaged data are somewhat smoother, since the CTSO-v223 retrieval scheme corrects for a number of systematic problems of the level 1b data, in particular the offsets at higher tangent altitudes.

[23] While, in general, all SMR data versions are based on the same set of spectroscopic parameters (see Table 2 for an overview), a known problem with the line broadening parameter of the 544.9-GHz ozone line was corrected for the CTSO-v223 algorithm. The values reported by Smith *et al.* [1997] of 3.4 MHz Torr<sup>-1</sup> and 0.69 for the temperature dependence coefficient were adopted, derived from parameters of the corresponding transition of the  $\nu_1$ -band in the infrared spectral region. For comparison, the "first guess" parameters used in version 222 were 4.25 MHz Torr<sup>-1</sup> and 0.53.

### 3.2.3. Chalmers-v1.2

[24] The retrieval scheme employed for version 1.2 of the operational code of the Chalmers University of Technology (Göteborg, Sweden) is in many aspects identical to the CTSO-v223 scheme. Differences are as follows: (1) Retrieved parameter is the logarithm of the volume mixing ratio divided by the a priori VMR; that is, negative mixing ratios (which might appear owing to measurement noise) are avoided, a measure which provides regularization for the single profile retrieval; (2) a relative a priori error of 50% is assumed, leading to stronger regularization than in the reference versions and as a consequence to a slightly reduced altitude range, as indicated by the measurement response data of the different data versions; (3) minimum threshold values for the a priori error are not used at all, which might cause a strong weighting of the a priori information at altitudes where the climatological a priori profile approaches zero; (4) smoothing of the profile in altitude is applied by assuming a correlation of retrieval parameters with altitude (off-diagonal elements of the a priori covariance matrix: linearly decreasing correlation function, half-width at 1/e of maximum:  $\sim 3$  km), leading to a reduced resolution in altitude while improving at the same time the retrieval precision; (5) the measurement covariance matrix is calculated directly from the theoretical noise of the measurement; (6) the minimum tangent-altitude of measurements of a scan which are used for the retrievals is determined empirically, e.g., 15 km at midlatitudes; (7) different parameters are used within the Levenberg-Marquardt iteration scheme, leading to slightly slower convergence compared to CTSO-v222 and -v223; (8) the continuum profile is retrieved on a reduced altitude grid; and (9) the spectrometer center frequency fit is omitted.

[25] In summary, the stronger regularization of the Chalmers-v1.2 data compared to the recent versions of the reference code CTSO leads to smoother and less noisy

**Table 2.** Spectroscopic Parameters Used Within the Odin/SMR Processing Chains for the Most Significant Lines Residing in the Stratospheric Mode Target Bands<sup>a</sup>

Species	Frequency, MHz	Intensity 300 K log <sub>10</sub> , nm <sup>2</sup> MHz	E <sub>low</sub> , cm <sup>-1</sup>	γ <sub>air</sub> <sup>0</sup> , 296 K, MHz Torr <sup>-1</sup>	γ <sub>self</sub> <sup>0</sup> , 296 K, MHz Torr <sup>-1</sup>	n <sub>air</sub> [1]	n <sub>self</sub> [1]	Level 2 Version
ClO	* 501264.3791	-2.1377	102.2295	3.23(13) <sup>b</sup>	3.35	0.69(6) <sup>b</sup>	0.50	v222, v223, v1.2
	* 501265.1728	-2.1701	102.2283					
	* 501265.8420	-2.2026	102.2279					
	* 501266.7152	-2.2351	102.2282					
	* 501267.8681	-2.1377	102.2300					
	* 501268.7569	-2.1701	102.2288					
	* 501269.4092	-2.2026	102.2284					
	* 501270.1533	-2.2351	102.2286					
O <sub>3</sub>	501112.0592	-5.2619	1094.0036	2.90	3.83	0.76	0.76	v222, v223, v1.2
	501220.2903	-6.3050	1375.4012	2.79	3.81	0.76	0.76	v222, v223, v1.2
	* 501476.3852	-5.4899	428.5805	2.77(5%) <sup>c</sup>	3.96	0.76(4) <sup>c</sup>	0.76	v222, v223, v1.2
O <sub>3</sub> -18-asym	501771.1392	-4.4777	1032.9718	2.79(3) <sup>d</sup>	3.72	0.78(6) <sup>d</sup>	0.76	v222, v223, v1.2
	501623.3065	-3.5967	212.2880	2.76	3.96	0.76	0.76	v222, v223, v1.2
N <sub>2</sub> O	* 502296.4230	-3.1600	159.1987	2.98(3%) <sup>e</sup>	2.95	0.71 <sup>e</sup>	0.77	v222, v223, v1.2
O <sub>3</sub>	* 544486.1463	-4.9548	965.4669	2.83	3.98	0.76	0.76	v222, v223, v1.2
	* 544857.4467	-3.4528	15.0520	4.25 <sup>f</sup>	4.27	0.53	0.76	v222, v1.2
O <sub>3</sub> -18-asym	544518.7134	-3.8554	292.2070	3.40(3) <sup>g</sup>	2.80	0.69(4) <sup>g</sup>	0.76	v222, v223, v1.2
HNO <sub>3</sub>	* 544252.9191	-2.8856	385.7943	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544252.9700	-2.8856	385.7943	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544283.3900	-2.9039	385.0016	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544283.4328	-2.9039	385.0016	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544309.0320	-2.9213	383.3659	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544309.0700	-2.9213	383.3659	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544330.5800	-2.9378	380.8881	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544330.5833	-2.9378	380.8881	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544349.0079	-2.9535	377.5686	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544349.0079	-2.9535	377.5686	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544365.3149	-2.9685	373.4082	3.95 <sup>h</sup>	4.34	0.89 <sup>h</sup>	0.75	v222, v223, v1.2
	* 544365.3200	-2.9685	373.4082	3.95 <sup>h</sup>	4.34	0.89 <sup>h</sup>	0.75	v222, v223, v1.2
	* 544380.6543	-2.9828	368.4071	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544380.6543	-2.9828	368.4071	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544396.4036	-2.9965	362.5655	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544396.4036	-2.9965	362.5655	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544414.3152	-3.0098	355.8836	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544414.3152	-3.0098	355.8836	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544436.7738	-3.0226	348.3610	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544436.7738	-3.0226	348.3610	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544467.2100	-3.0350	339.9971	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544467.2675	-3.0350	339.9971	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544511.2900	-3.0473	330.7908	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544511.2900	-3.0473	330.7908	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544578.1723	-3.0592	320.7400	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544578.1723	-3.0592	320.7400	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544685.0600	-3.0709	309.8412	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544685.0834	-3.0709	309.8412	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544866.6254	-3.0819	298.0881	4.34	4.34	0.75	0.75	v222, v223, v1.2
	* 544866.6600	-3.0819	298.0881	4.34	4.34	0.75	0.75	v222, v223, v1.2
544940.9095	-3.1664	244.9331	4.34	4.34	0.75	0.75	v222, v223, v1.2	

<sup>a</sup>Indicated are line center frequencies, integrated intensities, lower state energies, and air- and self-broadening parameters, as well as corresponding coefficients describing the temperature dependence. Pressure-shift is assumed to be negligible.

<sup>b</sup>From *Bauer et al.* [1998], based on measurement.

<sup>c</sup>From J. P. Colmont (Université de Lille, France, personal communication, 2002), based on calculation.

<sup>d</sup>From *Bauer et al.* [1998], based on measurement.

<sup>e</sup>From *Henry et al.* [1985], based on infrared measurements of the  $\nu_3$ -band.

<sup>f</sup>Our own first guess (assuring consistency of commissioning phase ozone, temperature, and scan-bias retrieval).

<sup>g</sup>From *Smith et al.* [1997], based on infrared measurements of the  $\nu_1$ -band.

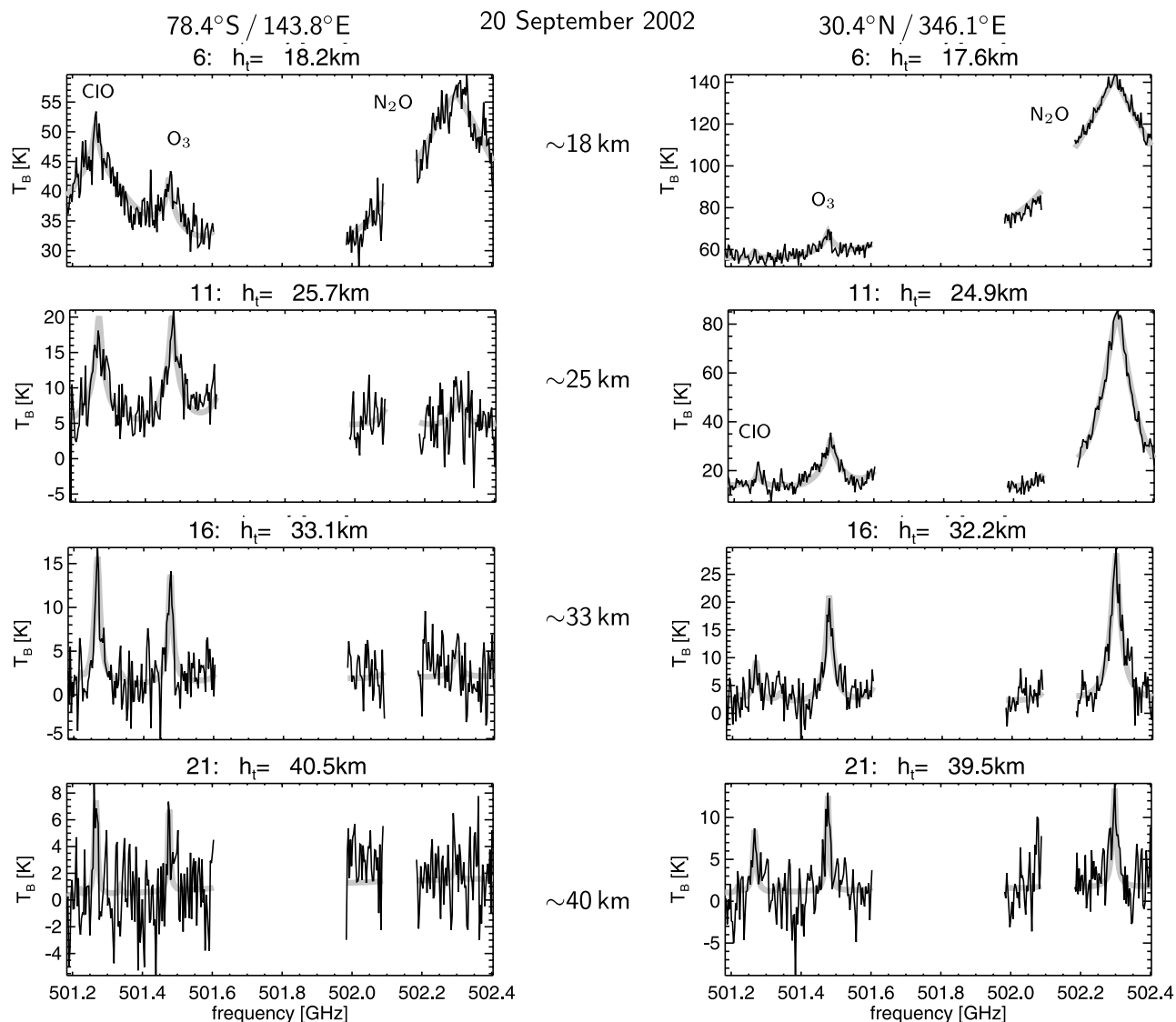
<sup>h</sup>From J. P. Colmont (Université de Lille, France, personal communication, 2002).

profiles with the drawback of a slightly reduced resolution and range in altitude. Note that Chalmers-v1.2 ozone retrievals are based on the same problematic spectroscopic line-broadening parameters for the 544.9-GHz line as version 222 (see Table 2).

### 3.3. Achieved Capabilities

[26] We investigate the typically achieved capabilities of the SMR instrument for the observation of stratospheric O<sub>3</sub>,

N<sub>2</sub>O, ClO, and HNO<sub>3</sub> using the reference analysis chain CTSO-v223. Figures 2 and 3 present for the 501.8-GHz band the results of a retrieval case study for typical limb-scans performed on 20 September 2002 at high latitudes (Antarctic polar vortex) and at midlatitudes. Spectral measurements and retrieved profiles of ClO, N<sub>2</sub>O, and O<sub>3</sub> are shown for both scenarios. Moreover, retrieval diagnostics such as retrieval errors and averaging kernel functions providing information on the achieved altitude resolution



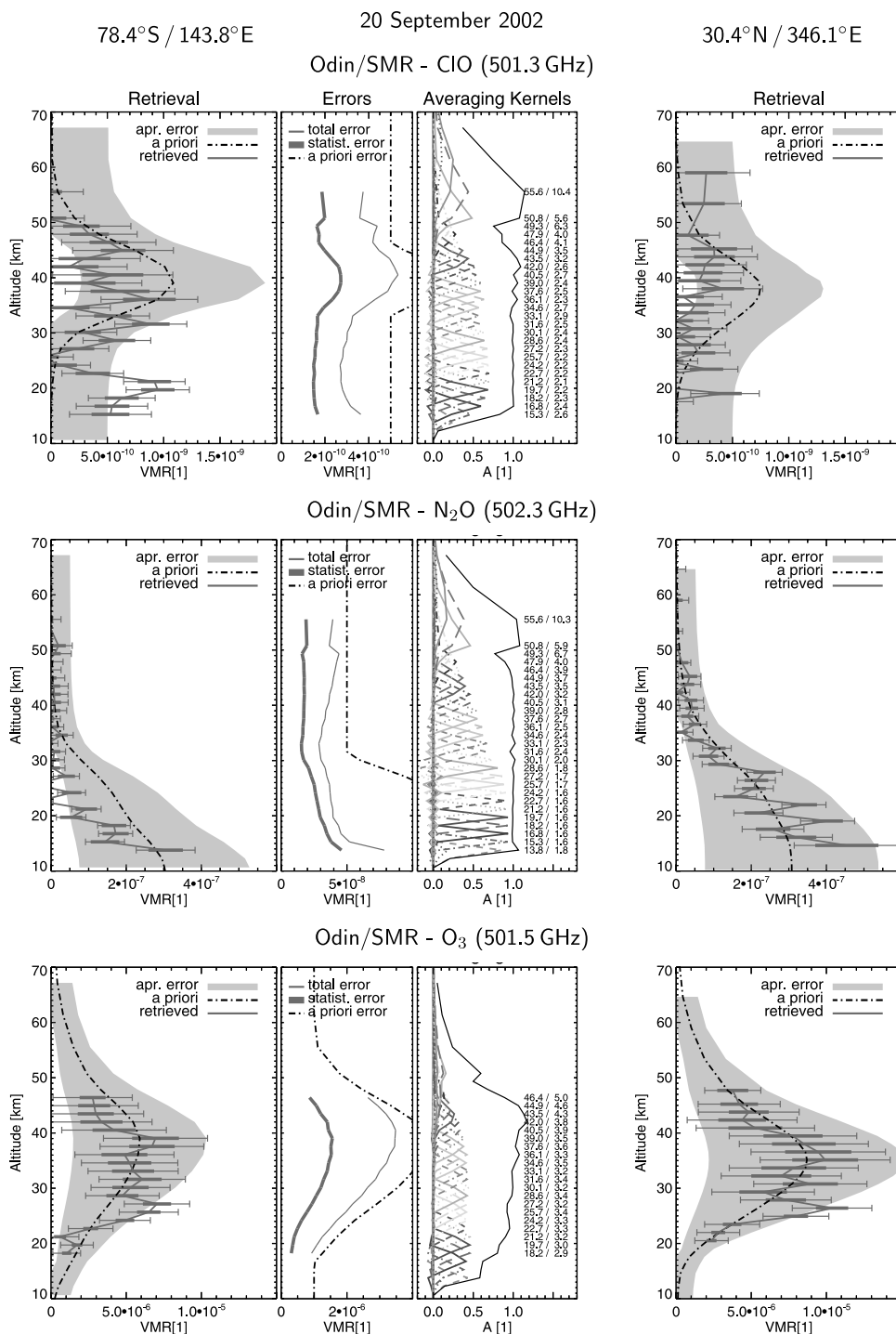
**Figure 2.** Example for spectral measurements of ClO, N<sub>2</sub>O, and O<sub>3</sub> taken by Odin/SMR with an auto-correlator spectrometer centered at 501.8 GHz on 20 September 2002. (left) High latitudes, southern winter hemisphere. (right) Midlatitudes, Northern Hemisphere. (top to bottom) Spectral measurements (thin black lines) and fits using MOLIERE-5.32 (thick shaded lines) for tangent altitudes of  $\sim$ 18, 25, 33, and 40 km.

and range are presented for the polar case. Information on ClO is here retrieved between 15 and 55 km, as indicated by values of the measurement response close to 1 in this range. In the lower stratosphere the altitude resolution is of the order of 2 km and the precision is approximately 0.15 ppbv. Slightly worse values are obtained in the upper stratosphere, for example, 0.25 ppbv and 2.7 km at 40 km. N<sub>2</sub>O and O<sub>3</sub> are measured and retrieved simultaneously with ClO in the 501.8-GHz band. Information on N<sub>2</sub>O is obtained in the stratosphere above about 14 km for the polar case. Approximate values for precision and altitude resolution for the lower stratosphere are 15–45 ppbv (15–20% below 30 km) and  $\sim$ 1.5 km. Profile information for ozone is obtained in the altitude range between about 18 and 45 km from the small line residing in this band. The altitude resolution is of about 3 km in the lower stratosphere, and the corresponding

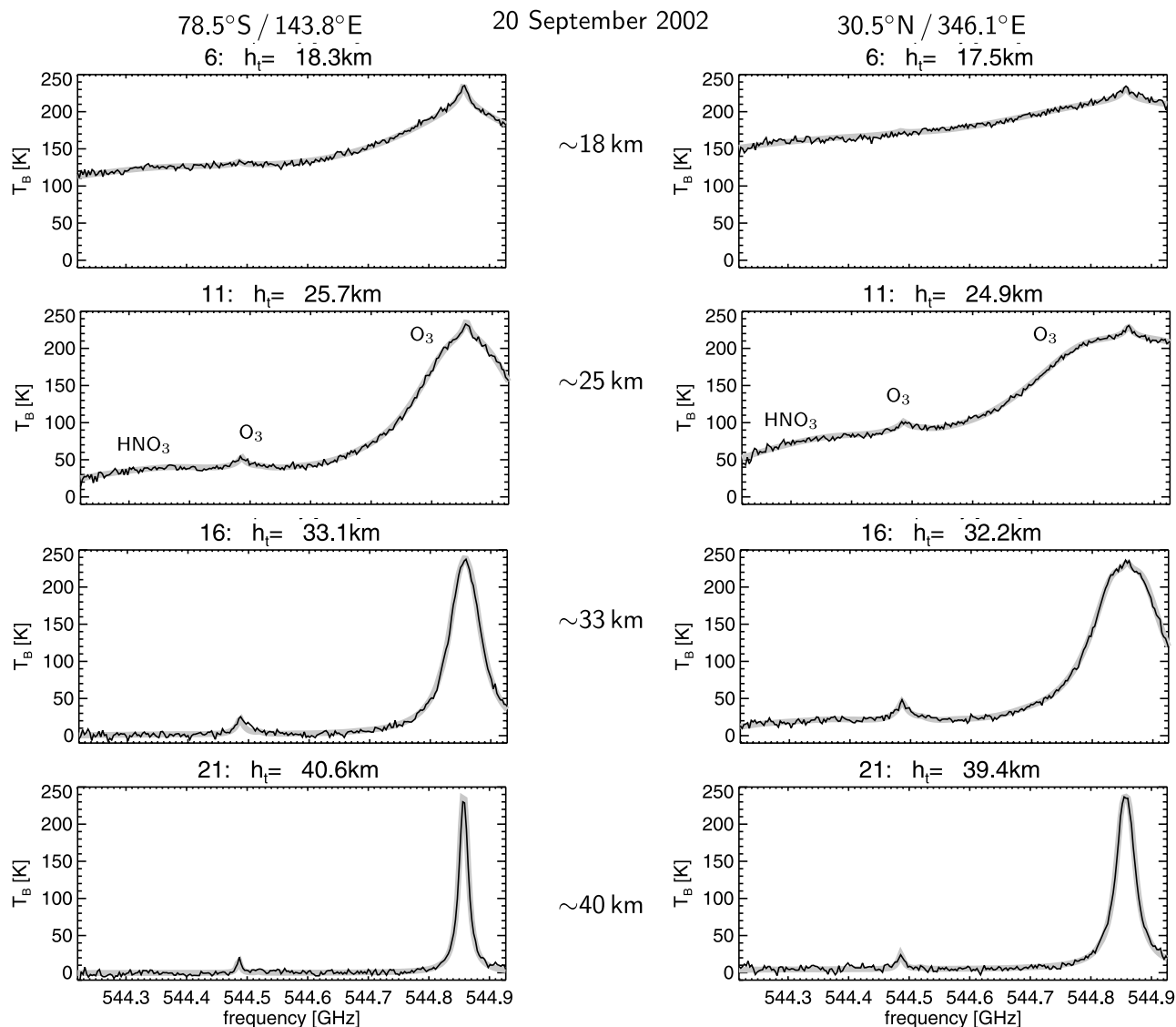
single-scan precision is of the order of 20–25% (e.g., 0.4 ppbv at 20 km).

[27] Figures 4 and 5 provide information on the achieved measurement capabilities for O<sub>3</sub> and HNO<sub>3</sub> which are simultaneously measured using the second auto-correlator spectrometer centered at 544.6 GHz. The strong ozone line at 544.9 GHz is the main ozone target line of Odin/SMR. Emissions from a smaller line at 544.5 GHz also contribute to the retrieval result for ozone in this band. For the polar case, ozone is retrieved from about 14 km up to the upper limit of the stratospheric scan of  $\sim$ 70 km. The altitude resolution of this ozone measurement is  $\sim$ 1.5 km throughout the stratosphere, limited mainly by the characteristics of the stratospheric mode scan with spectrometer read-out every 1.5 km in terms of tangent-altitudes below 50 km. The achieved single-profile precision is of about 10–15% in





**Figure 3.** Single-profile retrieval results for (top) ClO, (middle) N<sub>2</sub>O, and (bottom) O<sub>3</sub> as measured by Odin/SMR in the 501.8-GHz band on 20 September 2002 at (left) polar and (right) middle latitudes. Plots on the left- and right-hand side show retrieved profiles with error bars. Thick error bars indicate the error due to intrinsic receiver noise; thin error bars represent the total retrieval error including also the smoothing error due to the limited altitude resolution of the measurement. A priori profiles and errors are also plotted. Retrieval errors and diagnostics such as averaging kernel functions indicating altitude range (envelope) and resolution (FWHM) are shown for the polar case, only. Figure is based on CTSO-v223 data. See color version of this figure in the HTML.



**Figure 4.** Example for Odin/SMR measurements of  $\text{HNO}_3$  and  $\text{O}_3$  in the 544.6-GHz band taken on 20 September 2002 (thin black lines). (left) High latitudes, southern winter hemisphere. (right) Midlatitudes, Northern Hemisphere. The reproduction using the MOLIÈRE-5.32 forward model, calculated from the retrieved profiles, is also shown (thick shaded lines).

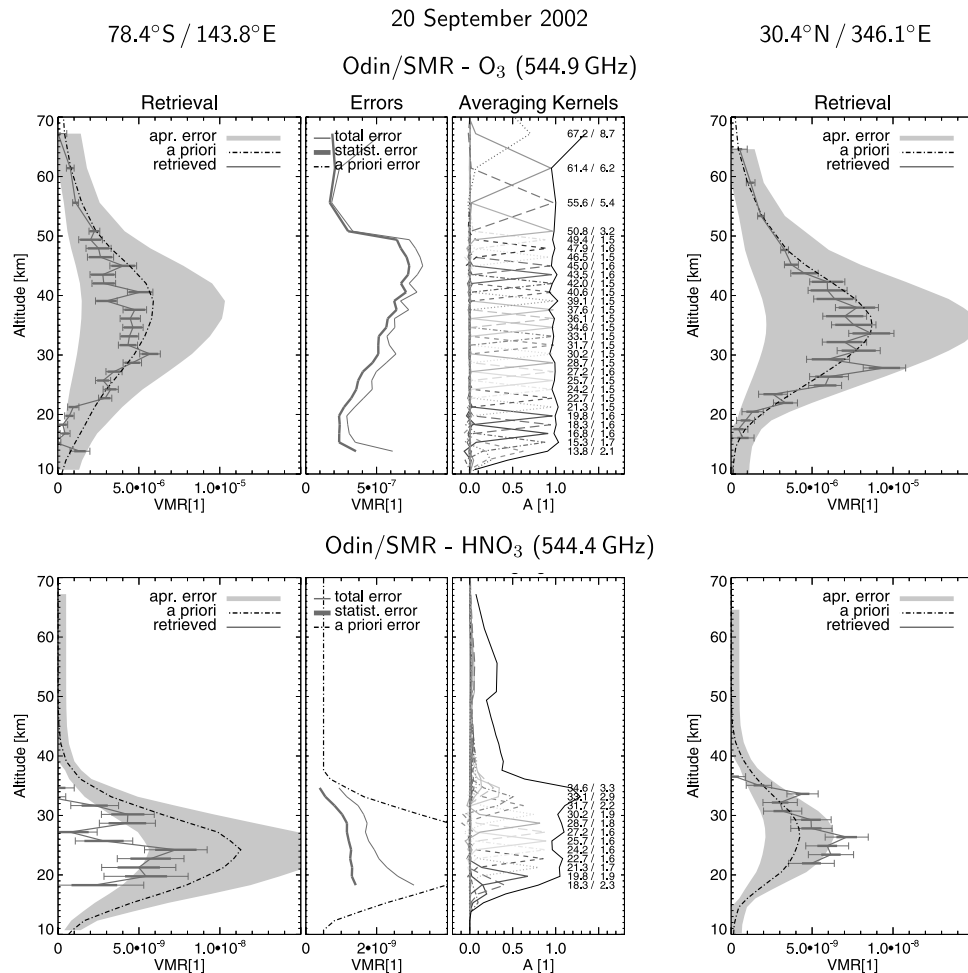
the lower stratosphere (e.g., 0.25 ppmv at 20 km). Note that the spectrometer read-out interval above 50 km is of the order of 5.5 km, a measure introduced to limit the overall data amount with respect to the spacecrafts memory and data down-link capabilities. This instrumental characteristic is directly reflected in the retrieval precision ( $\sim 0.2$  ppbv) and altitude resolution ( $\sim 6$  km) obtained for ozone above 50 km, as shown in Figure 4 for the polar case. Finally, information on  $\text{HNO}_3$  is retrieved between roughly 18 and 35 km with an altitude resolution in the order of 1.5–2 km and a corresponding single-profile precision of 1–1.5 ppbv.

[28] The achieved capabilities of Odin/SMR for the measurements of stratospheric mode target species are summarized in Table 1 for the relevant level 2 data versions. Compared to the theoretical capabilities, the achieved altitude resolutions and/or the related measurement precisions are slightly degraded for the target species having only relatively small emission lines such as  $\text{ClO}$ ,  $\text{HNO}_3$ , and  $\text{O}_3$

at 501.5 GHz. While upper limits of the retrieval altitude ranges are mainly determined by the signal-to-noise ratio of the measurements, the increasing absorption of the atmospheric water vapor continuum is the important limiting factor at the lowest altitudes. The respective lower limits at middle and low latitudes are typically 2 and 3–4 km higher than in the polar case discussed here due to the increasing tropopause height and water vapor absorption toward the tropics. Also note that the horizontal resolution of the limb measurements is in the order of 300 km, determined by the limb path in the tangent-layer. The satellite motion leads to an additional uncertainty of the profile position of similar magnitude.

### 3.4. Comparison

[29] A comparison of the most recent Odin/SMR level 2 data versions is presented in Figure 6. Shown are averages of profile retrievals of the stratospheric mode target species



**Figure 5.** Results of the CTSO-v223 retrieval case study for O<sub>3</sub> and HNO<sub>3</sub> measured by Odin/SMR in the 544.6-GHz band on 20 September 2002 at (left) polar and (right) middle latitudes. See caption of Figure 3 for explanation. See color version of this figure in the HTML.

ClO, N<sub>2</sub>O, and O<sub>3</sub> at 501.8 GHz as well as of O<sub>3</sub> and HNO<sub>3</sub> at 544.6 GHz for the limb measurements performed on four observation days: 19–20 September 2002, 25–26 September 2002, 20–21 March 2003, and 18–19 June 2003 (12:00 UT–12:00 UT).

[30] A large number of profiles was averaged for each species, and the error due to noise is consequently very small. The standard deviation, indicating the atmospheric variability, as well as the mean difference with respect to reference version 223 are also plotted. Only good quality Odin/SMR profiles (assigned flag QUALITY = 0) were considered, and the measurement response associated with each retrieved mixing ratio was required to be larger than  $\sim 0.9$ , a measure to assure that the information comes entirely from the measurement and the a priori contribution is negligible. Moreover, the logarithmic retrieval scheme of version 1.2 suggests that the logarithm of the mixing ratio should be averaged rather than the VMR, and this case was therefore investigated additionally.

[31] For the 501.8-GHz band target species, reference versions CTSO-v222 and CTSO-v223 give very similar results. For ClO and O<sub>3</sub>, version 1.2 of the operational code (Chalmers-v1.2) agrees well with the reference versions between about 25 and 45 km, while a considerable positive

bias is found toward the lower and upper limit of the altitude range covered by the measurements. In the case of ClO, this bias can slightly be reduced if the logarithm of the ClO mixing ratio is averaged. For N<sub>2</sub>O a small positive bias of  $\sim 10$  ppbv is found throughout the stratosphere for the mixing ratio average; larger differences are found below 20 km. Averaging of the logarithm of the mixing ratio yields here clearly smaller mixing ratios in the stratosphere which leads to a negative bias of 20–30 ppbv compared to the reference versions, while the large positive bias below 20 km remains unchanged.

[32] Concerning ozone measured in the 544.6-GHz band, a good agreement is found between all versions above  $\sim 50$  km, but considerable discrepancies are found below. Compared to the 501.8-GHz ozone retrievals of version 223, slightly smaller mixing ratios are found for the 544.6-GHz retrievals, for example,  $\sim 1$  ppmv below 30 km for version 223. Version 222 data give systematically very low mixing ratios around the ozone mixing ratio peak. This was identified to be caused by a wrong line broadening parameter used in this version for the ozone line at 544.9 GHz (see Table 2). Version 1.2 retrievals, based on the same spectroscopic parameters as version 222, yield nevertheless slightly larger mixing ratios than version 222.

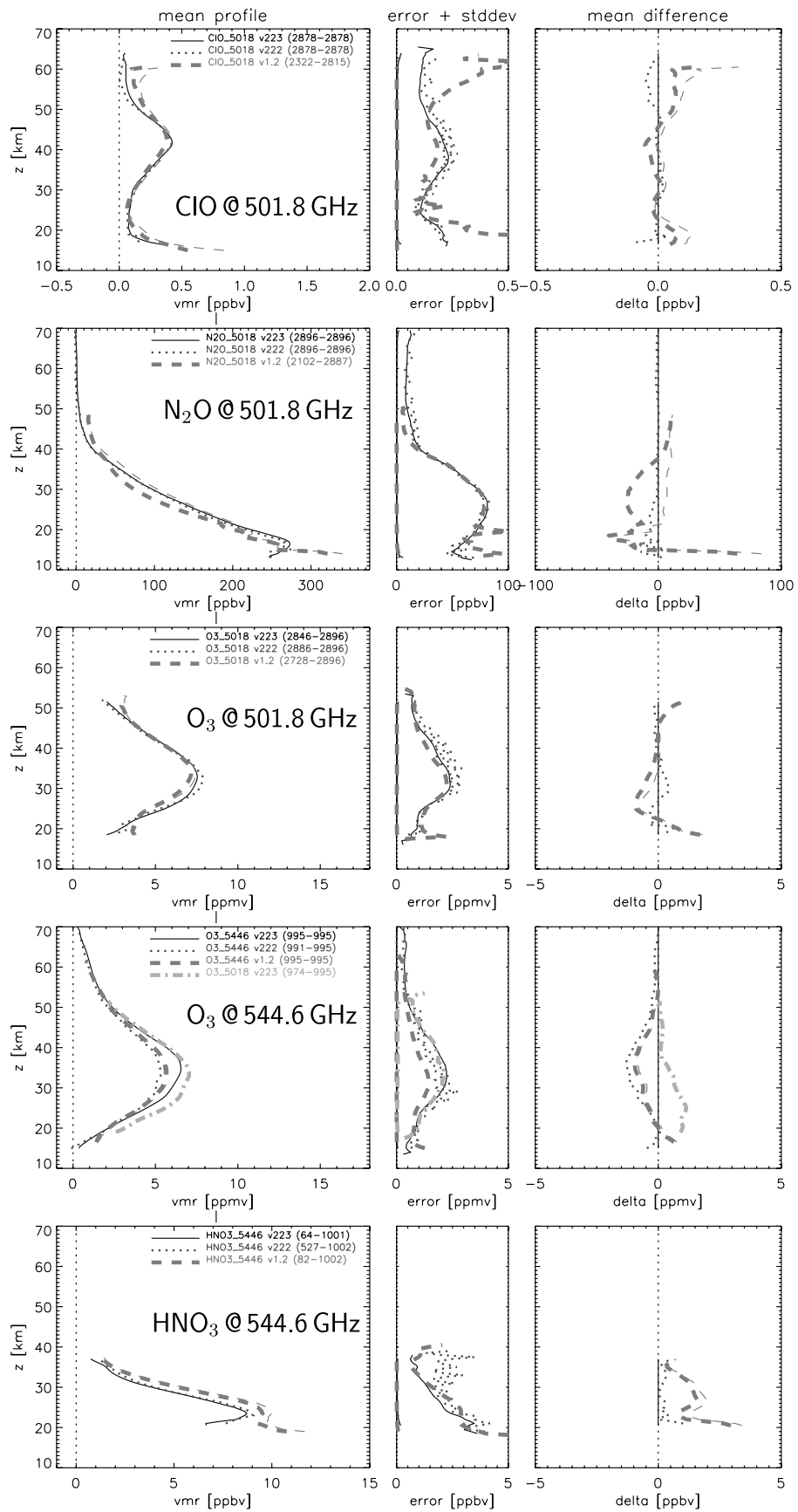


Figure 6

At altitudes below 20 km, the operational product is again characterized by a small positive bias compared to the reference versions. For  $\text{HNO}_3$ , all data versions agree reasonably in the altitude range from 25 km up to 40 km. Version 1.2 is slightly on the high side by 1–2 ppbv, while more considerable discrepancies persist below 25 km. Differences are slightly smaller if the logarithm is averaged.

[33] We assume that the systematic positive bias at the lowest and highest altitudes of the retrieval range is caused by a combination of different factors implying the logarithmic VMR retrieval employed by the Chalmers-v1.2 processing scheme. This technique provides reasonable regularization for a single-profile retrieval by avoiding negative mixing ratios, which otherwise might appear owing to measurement noise, but is susceptible to cause a systematic positive bias for averaged data at altitudes where the mixing ratios are smaller than 2–3 times the statistical 1- $\sigma$  uncertainty of a single profile measurement. The different regularization schemes and the altitude resolution might also play a role for the vertical distribution of the systematic deviations. Moreover, it was found by visual inspection that the larger differences at the top and the bottom of the averaged profiles are partly caused by some obviously unreasonable profiles in version 1.2, which are not correctly flagged. This is also indicated by the larger standard deviation of version 1.2, for example, for  $\text{N}_2\text{O}$  below 20 km and for  $\text{ClO}$  below 25 km and above 45 km. The incorrectly flagged profiles cannot be easily eliminated by automatic filtering, since only limited diagnostic information is available in the level 2 files. Improvement of the quality parameter of the operational product will therefore be important for future data releases, while for now the data user is advised to account for the limited altitude range and to use version 1.2 data with caution, depending on species and application. Averaging of the logarithm of the version 1.2 mixing ratios may yield in some cases better results, and more sophisticated filtering, such as median filtering, might also be a solution for certain applications. Please note that an assessment of the quality for each stratospheric mode target species by comparison with independent validation measurements is subject to further work and will be published elsewhere.

## 4. Systematic Errors

### 4.1. Instrumental Errors

[34] Uncertainties of the radiometric calibration as well as in the parameters used by the instrument module of the forward model might cause systematic biases in the retrieved mixing ratios. The most important instrumental sources of error for the Odin/SMR limb observations are discussed below.

#### 4.1.1. Calibration Error

[35] The calibration procedure is described in detail by *Olberg et al.* [2003] and shall only briefly be recalled here for the convenience of the reader. The calibrated brightness temperature  $T_{A,i}$  of a spectrometer channel  $i$  is given by

$$T_{A,i} = \frac{1}{\eta^A} \left( \frac{c_i^A - c_i^S}{g_i} - T_{sp} \right) \quad (1)$$

with

$$g_i = \frac{c_i^L - c_i^S}{\eta^L \epsilon T_L - \eta^S T_S + (\eta^S - \eta^L) T_{amb}} \quad (2)$$

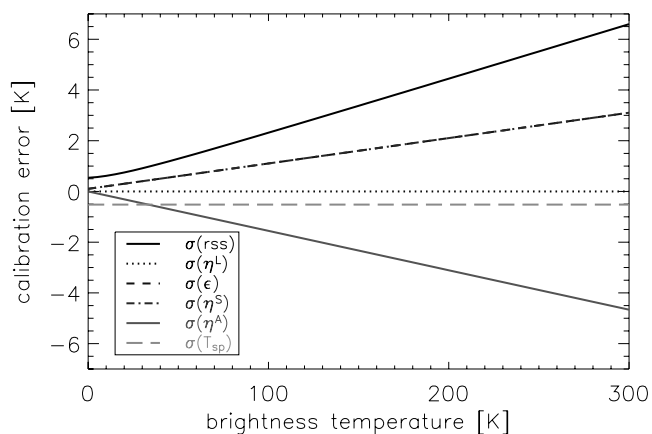
and

$$T_{sp} = -\eta^S T_S + (\eta^S - \eta^A) T_{amb}. \quad (3)$$

[36] The measured quantities  $c_i^A$ ,  $c_i^S$ , and  $c_i^L$  designate, respectively, the digital values of the thermal radiation detected in the direction of the atmosphere using the main telescope (A), in the direction of the cold sky (S), and in the direction of the internal hot load (L). The reference data (S, L) are measured in appropriate cycles and are properly interpolated onto the times of the atmospheric observations (A) in order to account for orbital gain variations. The receiver gain is denoted  $g_i$ , and the transmission coefficients  $\eta^A$ ,  $\eta^S$ , and  $\eta^L$  express the fact that part of the beam is terminated within the instrument at the unknown ambient temperature  $T_{amb}$ .  $T_S$  is the known background brightness temperature of the sky, and the brightness temperature  $T_L$  corresponds to the temperature of the internal calibration load which is measured to  $\sim 0.1$  K. The emissivity of the load material is denoted  $\epsilon$ . The quantities  $\epsilon$ ,  $\eta^L$ , and  $\eta^S$  are expected to be very close to 1 with a maximum uncertainty of 1%. The spill-over contribution  $T_{sp}$  is typically of the order of 10 K and is for each scan directly determined from the uppermost limb-views with an estimated precision of  $\sim 0.5$  K. The assumption of  $T_{amb} \approx 300$  K with an uncertainty of 100 K then allows estimation of the coefficient  $\eta^A$  and its uncertainty. Typical values are of the order of  $0.97 \pm 0.015$ . The root-sum-square calibration error, resulting from an error propagation analysis, is shown in Figure 7 along with the individual contributions. This systematic error is roughly of the order of 2% of the calibrated brightness temperature  $T_{A,i}$  with a minimum value of 0.5 K. These values should be interpreted as a conservative estimate for the Odin/SMR calibration uncertainty, since consistency considerations based on the comparison of measured and modeled continuum (window channel) brightness temperatures for the lowest opaque tangent-

**Figure 6.** Comparison of level 2 reference versions CTSO-v222 and CTSO-v223 with operational level 2 data of version 1.2. (left) Global averages of stratospheric mode data measured on four observation days (19–20 September 2002, 25–26 September 2002, 20–21 March 2003, and 18–19 June 2003), (middle) the statistical error ( $\sim 0$ ) and the standard deviation of the averaged measurements, and (right) the bias with respect to reference version CTSO-v223. The number of averaged mixing ratios per altitude level is indicated in the legend (values in parentheses: minimum and maximum number of averaged mixing ratios). For version 1.2, the thick dashed line indicates the result for the case that the logarithm of the mixing ratio was averaged, while the thin dashed line indicates the usual result if mixing ratios were averaged directly.



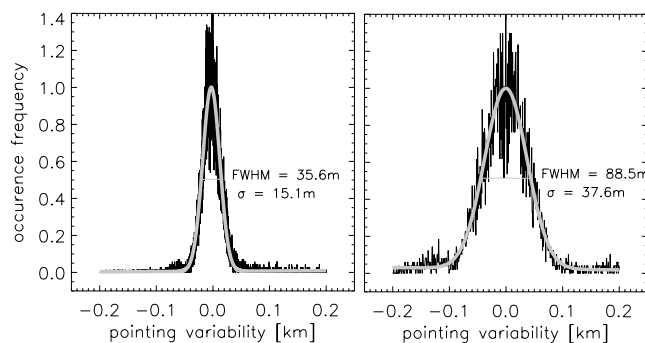


**Figure 7.** Estimation of the Odin/SMR calibration error as a function of brightness temperature. Individual error contributions are indicated (see legend and text for explanations). See color version of this figure in the HTML.

views, calculated using ECMWF temperatures and climatological data, indicate slightly smaller differences.

#### 4.1.2. Pointing Uncertainty

[37] The tangent-altitudes of the individual limb-views of a scan are obtained from the satellite's altitude data. In order to account for uncertainties in the absolute values of the geometrical tangent-altitudes and in the atmospheric pressure profile used in the retrieval, the standard processing algorithms retrieve an offset on the mean pointing angle of a limb-scan from the information contained in the pressure-broadened spectral lines. Typically, the tangent-altitude offset is determined with a precision of the order of  $\sim 100$  m. The corresponding uncertainties of the retrieved mixing ratios is already included in the retrieval error covariance matrix calculated by the Optimal Estimation Method. In addition, we consider here uncertainties in the determination of the individual tangent-altitudes. A statistical investigation of the differences between consecutive limb-views (see



**Figure 8.** Variability in the determination of Odin/SMR tangent-altitudes derived from a large number of stratospheric mode limb-scans. (left) Spectrometer read-out corresponding to 1.5 km in terms of tangent-altitude (stratosphere). (right) The 5.5-km read-out interval (mesosphere). Fitted Gauss-functions are also shown. Corresponding values of the full-width-at-half-maximum (FWHM) of the Gauss-functions and the 1- $\sigma$  standard deviations are indicated.

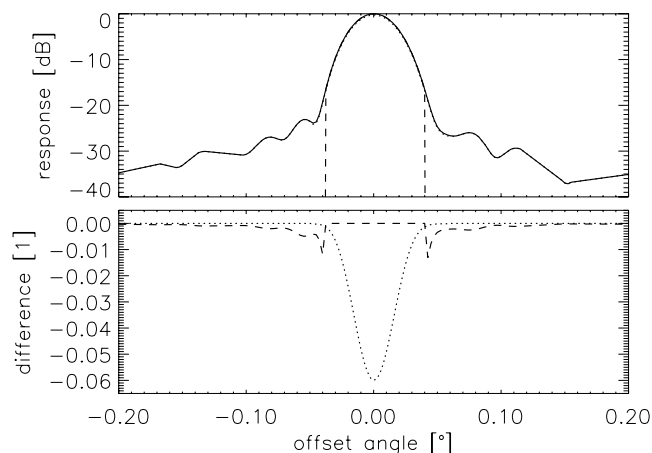
Figure 8) yielded random 1- $\sigma$  deviations from the nominal values of  $\sim 15$  m for the spectrometer read-out every 1.5 km (stratosphere) and of  $\sim 38$  m for the 5.5-km read-out interval (mesosphere), as well as of  $\sim 27$  m for the 3-km read-out interval (reduced stratospheric scan, not shown). These values for the variability of the tangent-altitude step between consecutive spectrometer read-outs should be interpreted as upper limits for the statistical uncertainty in the knowledge of the individual tangent-altitudes, after removal of an overall bias for the whole scan by the retrieval.

#### 4.1.3. Antenna Knowledge

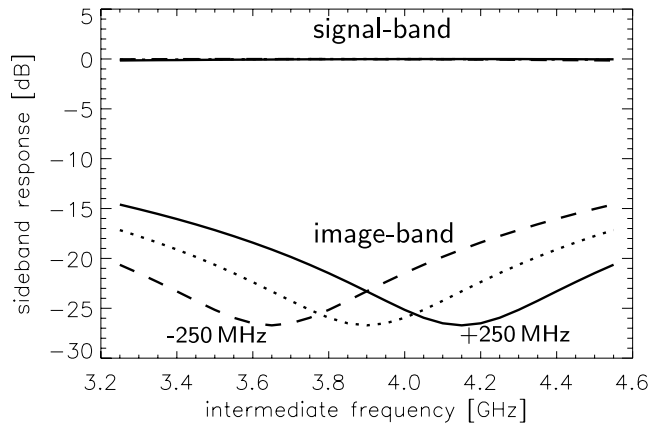
[38] The antenna response function used in the forward models is based on pre-launch measurements and modeling. A verification of the major antenna and pointing characteristics was also done several times in orbit by mapping of Jupiter [Frisk et al., 2003]. A main beam efficiency of  $87 \pm 6\%$  was found, assuring that in-orbit values are very close to theoretical expectations ( $\sim 89\%$ ). Following the results of these investigations, we adopt an uncertainty of 6% for the main beam efficiency. Moreover, a worst-case knowledge error for the antenna sidelobe contribution was simulated by cutting the antenna pattern at  $-17$  dB, the theoretical value for the interception of the main beam by the baffle. The total antenna knowledge error is the root-sum-square value of these two contributions (see Figure 9).

#### 4.1.4. Sideband Response Knowledge

[39] Sideband response characteristics of the Odin/SMR Martin-Puplett-type sideband filters have been measured in the laboratory before the launch. While no obvious systematic contamination of the stratospheric mode target bands by strong lines from the image bands could be detected in orbit, such effects have nevertheless been seen in other measurement modes [Lautié, 2003; Urban et al., 2004b]. We accordingly assume an uncertainty in the path length difference of the Martin-Puplett interferometer corresponding to a spectral shift of the suppression curve of about



**Figure 9.** (top) Odin/SMR antenna response function at 540 GHz, integrated over the azimuth angle (in logarithmic units (dB)). Also shown are the extreme scenarios of (1) a response function with main beam efficiency reduced by 6% (dotted line), as well as with sidelobes cut at the  $-17$ -dB level by the baffles (dashed line). The bottom plot shows the differences to the nominal case (in linear units (1)), for clarity.



**Figure 10.** Sideband response function for the 501.8-GHz band. Shown is the nominal case (dotted line), derived from pre-flight laboratory measurements, as well as estimated worst-case scenarios (solid and dashed lines).

$\pm 250$  MHz leading to a value of  $\sim 15$  dB instead of  $\sim 18$  dB for the image band suppression at the band edges (at the intermediate frequencies of 3.3 and 4.5 GHz, see Figure 10). The root-mean square value of the two resulting retrieval errors is used for the error analysis.

#### 4.1.5. Spectrometer Resolution

[40] In aeronomy mode, the auto-correlator spectrometers are operated since November 2001 with a processed bandwidth of  $\sim 700$  MHz and a spectral resolution of  $\sim 2$  MHz (due to Hanning smoothing) for each of the  $\sim 700$  channels. See *Olberg et al.* [2003] for detailed information on the spectrometer data processing. Main uncertainties of the resulting auto-correlator channel response function are (1) a temperature drift of the sampling clocks of 0.5%, causing an error smaller than 10 kHz for the spectral resolution, as well as (2) a more significant representation error of  $\leq 5\%$ , which leads to an uncertainty of up to 100 kHz in the spectral resolution modeled by the forward model during level 2 data processing. We consider the root-sum-square value of these contributions.

[41] For the error analysis, we first calculated spectral errors for all of the aforementioned individual instrumental uncertainties using the MOLIERE-5 forward model. The modeled errors in the spectra of a limb-scan  $\Delta y$  were then linearly mapped to errors in the retrieved mixing ratios  $\Delta x$  using the contribution functions  $D$  of the retrieval,

$$\Delta x = D \Delta y. \quad (4)$$

In case of the statistical pointing error, spectra were first calculated for 200 random scans characterized by the standard deviation of the difference between consecutive Odin tangent-altitudes. A root-mean square retrieval error was then determined from the individually determined retrieval errors. See, for example, *Urban* [2003] and *Verdes et al.* [2002] for a more detailed discussion of this method and *Urban et al.* [2004a] for a definition of the contribution functions in MOLIERE-5.

[42] The resulting uncertainties of the retrieved mixing ratios are presented in Figures 11 and 12 (left panels). The most critical instrumental error for all target species is the

calibration error. Since this error is roughly proportional to the brightness temperature (see Figure 7), the error decreases for the optically thin band around 501.8 GHz with altitude. For the target species of the 544.6-GHz band, in particular ozone, largest errors are found in the altitude range of the ozone mixing ratio maximum, which reflects the fact that the strong ozone line at 544.9 GHz is saturated even in the middle and upper stratosphere. Also important is the uncertainty of the sideband ratio, which contributes to the instrumental error budget of the target species. The other instrumental parameters are much less important, in particular for the 501.8-GHz band. The antenna and pointing errors give still a small contribution to the total instrumental error, in particular for the 544.6-GHz band targets species, while the uncertainty of the spectrometer resolution is completely negligible.

## 4.2. Model Errors

### 4.2.1. Spectroscopic Parameters

[43] Now we focus on spectroscopic parameters of the forward model. Any uncertainty in a model parameter  $b$  of the forward model  $F(x, b)$  which is not retrieved but assumed to be known is translated into a retrieval error. Here  $x$  stands here for the vector of retrieved parameters. The foreign air broadening parameters  $\gamma_{air}^0$  of target and interfering lines (given at reference pressure and temperature  $P_0$  and  $T_0$ ) as well as the coefficients  $n$  describing the temperature dependence according to

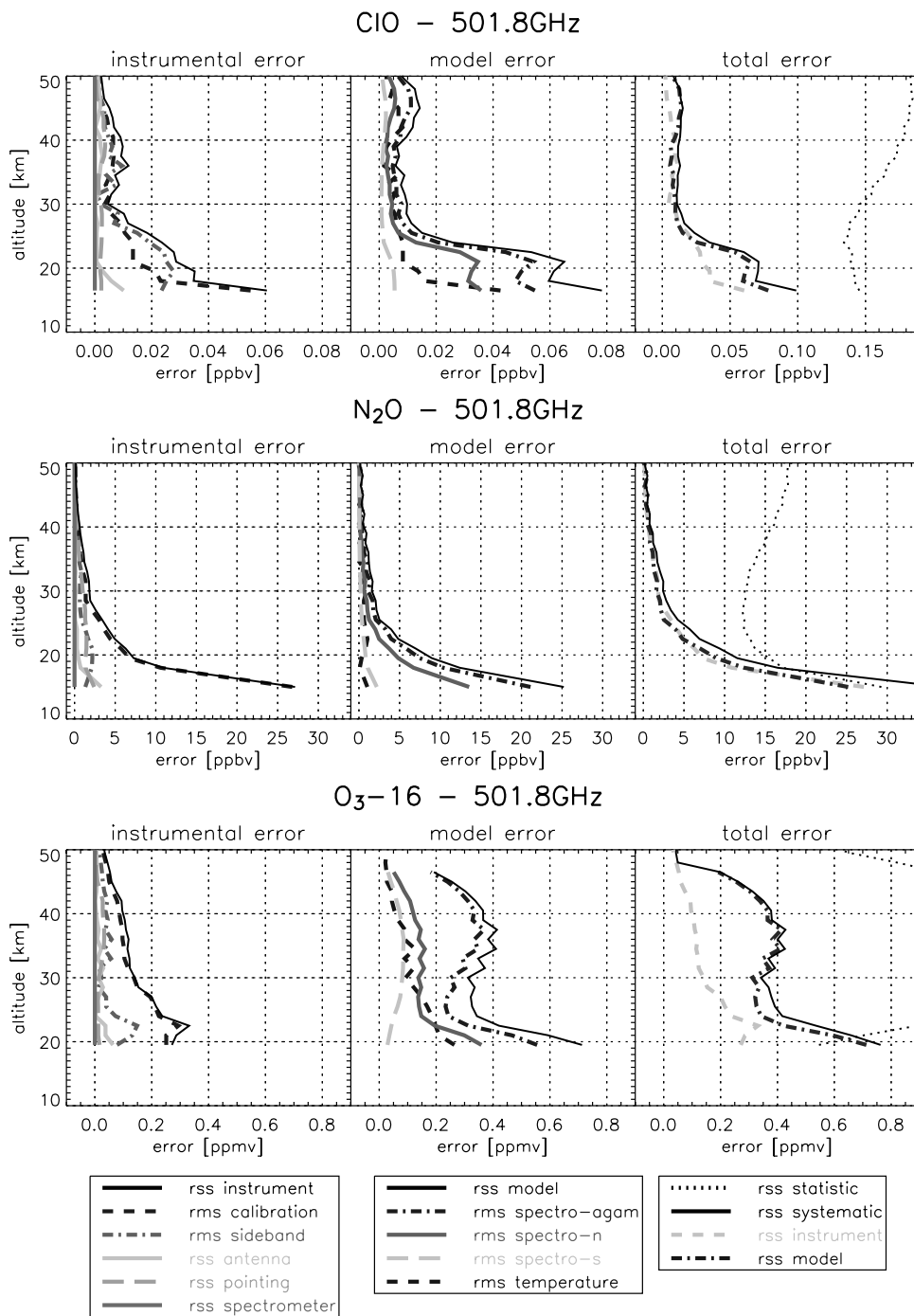
$$\gamma_{air} = \gamma_{air}^0 \cdot (P/P_0)(T/T_0)^{-n} \quad (5)$$

are known to be the most critical spectroscopic model parameters [*Bauer et al.*, 1998; *Bühler*, 1999]. The spectroscopic retrieval errors with respect to these parameters have therefore been determined for the major Odin/SMR stratospheric mode target species. Two cases were investigated separately: First, errors of 5% were assumed for the line-broadening parameters of target and interfering lines and, second, a 10% uncertainty was assumed for the exponent appearing in the semi-empirical law of the temperature dependence of the broadening parameter. Typically, these uncertainties may only be obtained when the parameters are measured in the laboratory, which is the case for the major stratospheric mode target lines (see Table 2). In addition, we also investigated retrieval errors due to a 1% uncertainty in the catalog value for the line intensity.

[44] The spectroscopic retrieval error was estimated following a linear approach described by *Rodgers* [1990]. The errors of the spectroscopic parameters in the forward model are specified in the model parameter covariance matrix  $S_b$ . The resulting error covariance matrix for the retrieved parameters can then be calculated using

$$S_s = (D \cdot K_b) \cdot S_b \cdot (D \cdot K_b)^T, \quad (6)$$

where  $K_b = \partial F(x, b)/\partial b$  represents the weighting function matrix with respect to the model parameters  $b$  and  $D$  is the contribution function matrix of the retrieval. See, for example, *Urban* [2003] for a more detailed description concerning this application.

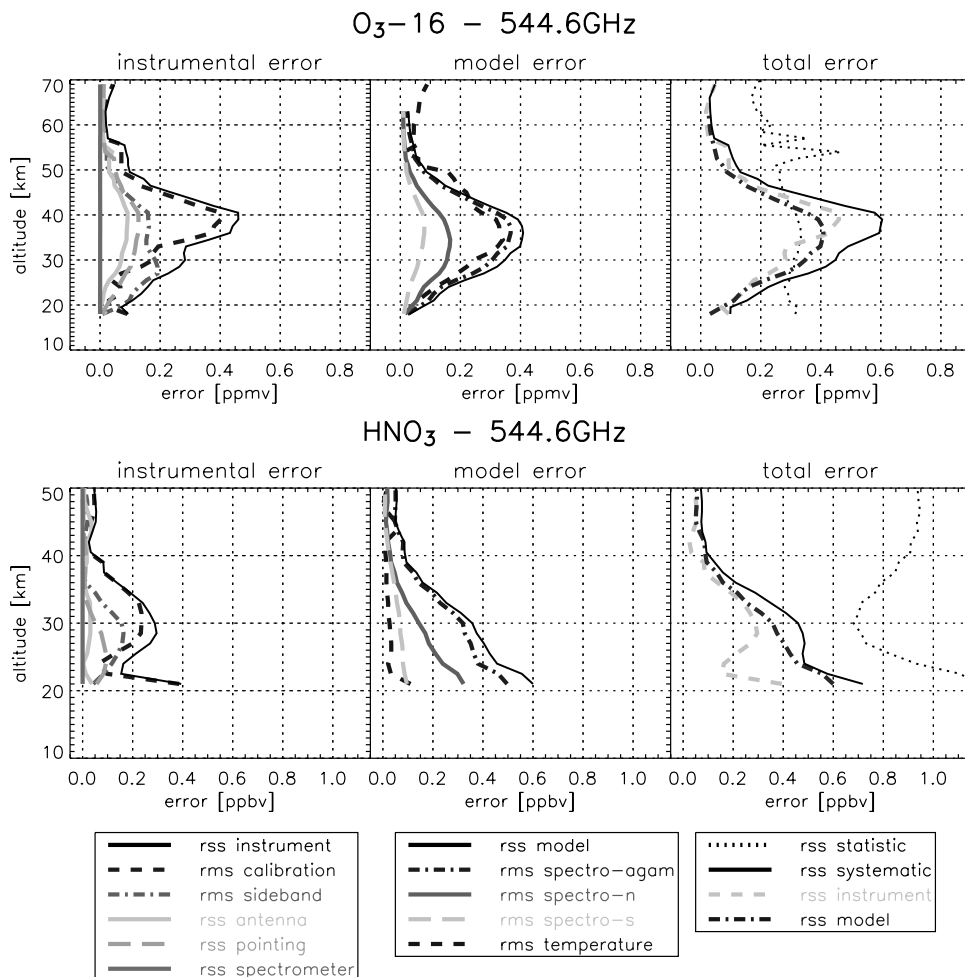


**Figure 11.** (left) Instrumental, (middle) spectroscopic, and (right) total systematic errors for the Odin/SMR stratospheric mode target species of the 501.8-GHz band (spectro-agam, retrieval error due to uncertainties of collisional line broadening parameters in air; spectro-n, temperature dependency uncertainty of collisional broadening; spectro-s, uncertainty of spectral line intensities). See color version of this figure in the HTML.

[45] The resulting retrieval errors due to uncertainties in the line broadening parameters are shown in Figures 13 and 14 for the 501.8-GHz and 544.6-GHz bands, respectively. The sensitivity of the retrieval to 5% errors in the line broadening parameters is roughly twice as large as the sensitivity to 10% uncertainties of the exponent in the temperature dependence law. The assumed 1% uncertainties

in the line intensities lead to a factor of 5–10 smaller retrieval errors. Spectroscopic retrieval errors with respect to the exponents of the temperature dependence law and the intensities are not explicitly shown, but are taken into account for the error budget.

[46] Important foreign broadening parameters for the error budget correspond naturally to the major target lines



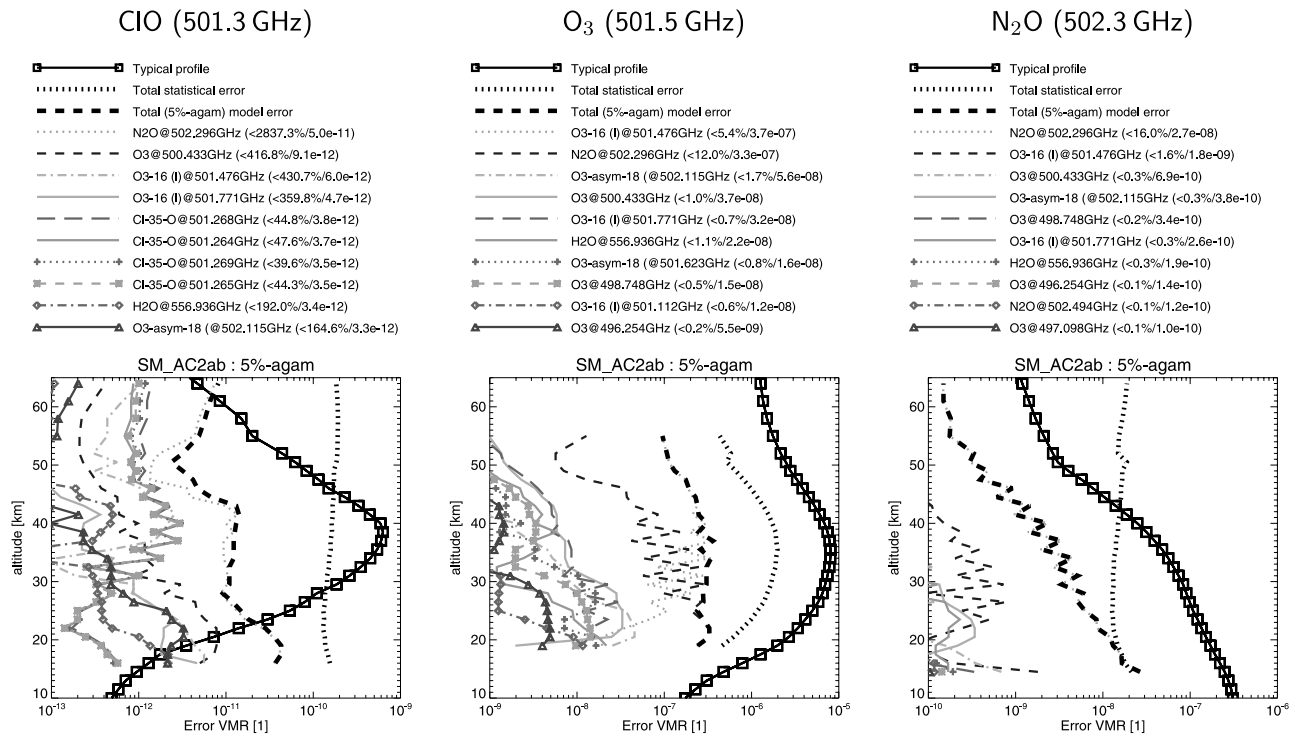
**Figure 12.** (left) Instrumental, (middle) spectroscopic, and (right) total systematic errors for the Odin/SMR stratospheric mode target species of the 544.6-GHz band. See color version of this figure in the HTML.

themselves: ClO at 501.3 GHz, O<sub>3</sub> at 501.5 GHz, and N<sub>2</sub>O at 502.3 GHz in the 501.8-GHz band, as well as O<sub>3</sub> at 544.9 GHz and the HNO<sub>3</sub>-band around 544.4 GHz in the 544.6-GHz band. The spectroscopic error of N<sub>2</sub>O at 502.3 GHz turns out to be critical for the simultaneous retrieval of ClO and O<sub>3</sub> in the 501.8-GHz band, since it gives a non-negligible contribution to the error budget of these species at ~25 km and below. The resulting spectroscopic retrieval errors for the 501.8-GHz band can be considered as a worst case scenario, since the major parameters were indeed measured or calculated to 5% or better. Concerning the 544.6-GHz band, the HNO<sub>3</sub> retrieval is at low altitudes significantly affected by the spectroscopic errors of the strong ozone line at 544.9 GHz, but also at higher altitudes by spectroscopic uncertainties of the close 544.5-GHz ozone line. One also should note the importance of the spectroscopic line broadening parameters of the somewhat smaller 544.5-GHz ozone line for the ozone retrieval. Its contribution is very critical in particular since spectroscopic parameters of this line have not yet been measured at all in the laboratory and the uncertainty of its pressure broadening parameter might therefore be considerably larger than 5%. Other lines than the above mentioned have only a very small

impact on the retrieval, and the contribution of their spectroscopic uncertainties is negligible.

[47] New measurements of spectroscopic line broadening parameters for the 544.9-GHz ozone line, the principal Odin/SMR ozone target line, were reported by *Amano and Yamada* [2004]. The measurements indicate a value of 3.15 MHz Torr<sup>-1</sup> and were just recently revised to 3.11 MHz Torr<sup>-1</sup> [*Yamada and Amano*, 2005]. For comparison, the parameter derived from measurements in the infrared spectral region of 3.4 MHz Torr<sup>-1</sup> reported by *Smith et al.* [1997] is larger by ~9%. However, retrieval tests revealed that the parameters proposed by *Smith et al.* [1997] give slightly better agreement with retrieval results from the 501.8-GHz band, and this value was therefore adopted at the time when the CTSO-v223 level 2 processing chain was implemented. The ambiguity between results reported from the direct line-broadening measurements and values extrapolated from the  $\nu_1$ -band has still to be resolved by experimental confirmation. Future Odin/SMR level 2 data versions will certainly rely on the measured line-broadening parameters and temperature dependence of the 544.9-GHz ozone line. It should be noted that experimental verification for other target lines, for example, for O<sub>3</sub>





**Figure 13.** Spectroscopic retrieval errors resulting from 5% errors in the collisional air broadening parameters (agam) for the Odin/SMR stratospheric mode target species ClO, O<sub>3</sub>, and N<sub>2</sub>O measured in the 501.8-GHz band. Retrieval errors resulting from individual lines as well as the total spectroscopic errors are plotted (see legend). The total statistical retrieval error and a typical profile are indicated for comparison. See color version of this figure in the HTML.

at 501.5 GHz, O<sub>3</sub> at 544.5 GHz, and N<sub>2</sub>O at 502.3 GHz, would also be highly beneficial for the Odin/SMR stratospheric mode level 2 data quality.

#### 4.2.2. Temperature Knowledge

[48] Uncertainty of the temperature profile used by the retrieval model is also susceptible to cause systematic retrieval errors. The Odin/SMR level 2 analysis uses temperature data from the European Centre of Medium-range Weather Forecast (ECMWF) in the stratosphere as well as data from a model climatology in the mesosphere [Hedin, 1991]. Moreover, temperature information is simultaneously retrieved if contained in the spectral measurements, a measure which reduces the sensitivity of the retrieval result to uncertainties in the temperature data. As a worst case, we investigated therefore the effect of a constant temperature error of  $\pm 2$  K on the retrieval result using the linear mapping technique. Results are shown in Figures 11 and 12 (middle panel) along with the spectroscopic model errors. While the model error is in general dominated by the spectroscopic errors, the temperature error gives a significant contribution in particular for the ozone retrieval from the strong, saturated ozone line in the 544.6-GHz band. Temperature is therefore retrieved in this band. The uncertainty estimated here due to a systematic temperature error is consequently not added to the error budget of this band's target species since a possible temperature bias would be retrieved in the altitude range where the spectral measurement is sensitive to temperature. Moreover, the statistical error of the temperature retrieval is included in the species

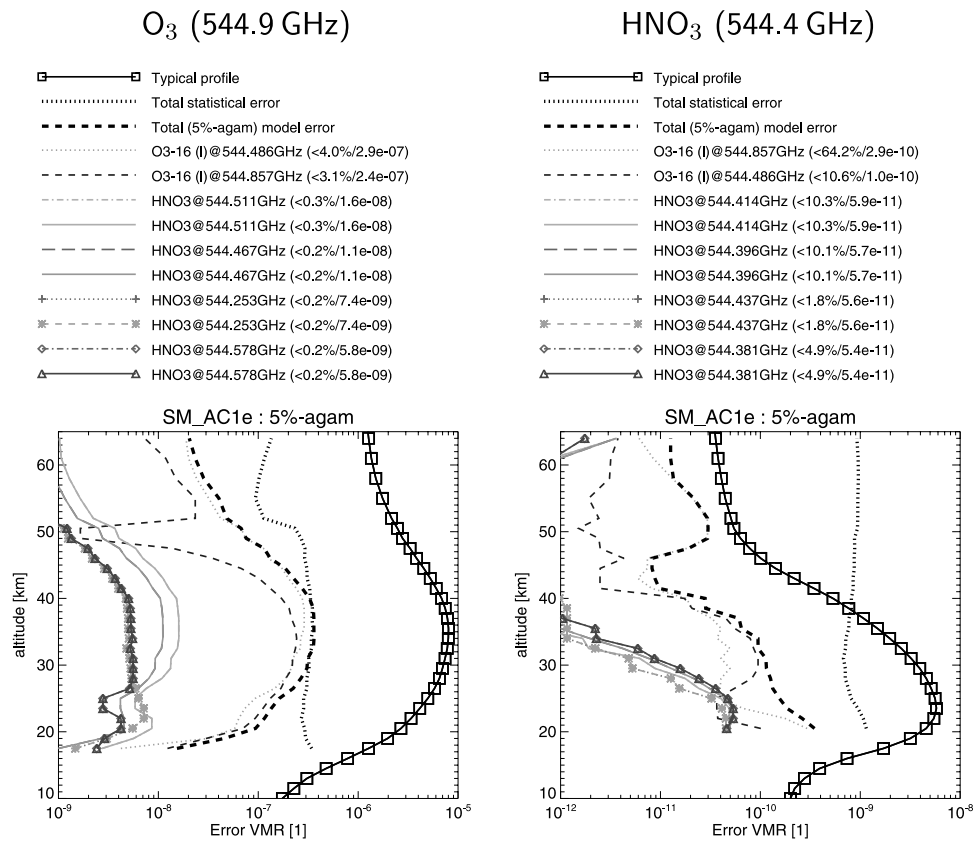
retrieval error covariance matrices and vice versa, since all parameters are retrieved simultaneously.

#### 4.3. Error Budget

[49] The estimated total systematic retrieval errors resulting from the aforementioned individual instrumental and spectroscopic contributions are shown in Figures 11 and 12 (right panel) for all stratospheric mode target species and are also summarized in Table 3. The statistical errors due to intrinsic receiver noise for a single-profile retrieval are plotted in the figures for comparison.

[50] The total systematic error for ClO measured in the 501.8-GHz band is smaller than 0.02 ppbv above 30 km ( $< 5\%$ ) and increases below to values of 0.07 ppbv at 20 km and 0.1 ppbv at 16.5 km. Spectroscopic and instrumental errors are roughly of equal importance. The total systematic error of N<sub>2</sub>O increases from values smaller than 3 ppbv above 30 km with decreasing altitude to values of 12 ppbv at 20 km. Below 20 km the increasing calibration uncertainties and the additional contributions of the spectroscopic error lead to a total systematic error of  $\sim 35$  ppbv around 15 km. In terms of relative units with respect to our midlatitude reference profile, shown in Figure 1, the systematic error is lower than 5% between 20 and 40 km and of the order of 5–15% below. The ozone retrieval in the 501.8-GHz band is dominated by the spectroscopic model error. The total systematic error is lower than 0.4 ppmv above 25 km and increases to  $\sim 0.75$  ppmv at 20 km. In terms of relative units, the error is of the order of 5% above 30 km and increases below up to 35% at 20 km.





**Figure 14.** Spectroscopic retrieval errors resulting from 5% errors in the line broadening parameters (agam) for the Odin/SMR stratospheric mode targets O<sub>3</sub> and HNO<sub>3</sub> measured in the 544.6-GHz band. See caption of Figure 13 for description. See color version of this figure in the HTML.

[51] For ozone measured in the 544.6-GHz band the total systematic error is determined by calibration and spectroscopic uncertainties. A maximum total systematic error of  $\sim 0.6$  ppmv is found at the altitude of the ozone mixing ratio maximum, while the error decreases considerably above and below. Values lower than 0.2 ppmv are obtained above 50 km and below 25 km. The relative error with respect to our midlatitude reference profile varies between 3 and 8% over the altitude range of the measurement. For HNO<sub>3</sub>, measured in the same band, a total systematic error of  $\sim 0.5$  ppbv at 25–30 km is found. The error increases below 25 km owing to the influence of the spectroscopic uncertainties up to a value of  $\sim 0.7$  ppbv at the lower limit of

the exploitable altitude range around 21 km. In other words, the total systematic uncertainty for HNO<sub>3</sub> is better than 15% between 20 and 35 km.

## 5. Summary

[52] In this work we first described the theoretical capabilities of the Sub-Millimetre Radiometer (SMR) on board the Odin satellite for the measurements of main stratospheric mode target species ClO, N<sub>2</sub>O, O<sub>3</sub>, and HNO<sub>3</sub>. The optimized robust retrieval methodologies for treating calibrated spectra (of level 1b, calibration version 4) were then presented, and differences between the operational (Chal-

**Table 3.** Estimated Systematic Errors of Odin/SMR Measurements of Stratospheric ClO, N<sub>2</sub>O, O<sub>3</sub>, and HNO<sub>3</sub><sup>a</sup>

Species	Frequency, GHz	Altitude Range, km	Systematic Errors		
			Instrumental	Model	Total
O <sub>3</sub>	501.5	25–50	$\leq 0.2$ ppmv	$\leq 0.4$ ppmv	$\leq 0.4$ ppmv
		<25	0.2–0.3 ppmv	0.35–0.7 ppmv	0.4–0.75 ppmv
ClO	501.3	25–50	$\leq 0.02$ ppbv	$\leq 0.01$ ppbv	$\leq 0.02$ ppbv
		<25	0.02–0.06 ppbv	0.01–0.08 ppbv	0.02–0.10 ppbv
N <sub>2</sub> O	502.3	20–50	$\leq 7$ ppbv	$\leq 8$ ppbv	$\leq 12$ ppbv
		<20	7–27 ppbv	8–25 ppbv	12–35 ppbv
O <sub>3</sub>	544.9	25–50	0.15–0.5 ppmv	0.2–0.4 ppmv	0.3–0.6 ppmv
		<25, >50	$\leq 0.15$ ppmv	$\leq 0.2$ ppmv	$\leq 0.25$ ppmv
HNO <sub>3</sub>	544.4	25–50	$\leq 0.3$ ppbv	$\leq 0.4$ ppbv	$\leq 0.5$ ppbv
		<25	$\leq 0.4$ ppbv	0.4–0.6 ppbv	0.5–0.7 ppbv
		<25	$\leq 0.4$ ppbv	0.4–0.6 ppbv	0.5–0.7 ppbv

<sup>a</sup>Indicated are instrumental, spectroscopic, and total systematic errors.

mers-v1.2) and reference (CTSO-v222,-v223) level 2 products were evaluated. An analysis of systematic instrumental and model uncertainties was also presented. Results are summarized in Tables 1 and 3 for the stratospheric mode target species and the different level 2 data versions.

[53] The most recent and elaborated data version is the reference product CTSO-v223. For a measurement inside the polar vortex, ClO is retrieved from a line at 501.3 GHz between 15 and 55 km with a vertical resolution of 2–2.5 km and a single-scan precision of 0.15–0.25 ppbv. The estimated systematic error including instrumental and spectroscopic uncertainties is smaller than 0.02 ppbv above 25 km and increases below up to 0.1 ppbv at ~16 km. Information on N<sub>2</sub>O is obtained from a line in the same band (at 502.3 GHz) in the stratosphere above 14 km with an altitude resolution of 1.5 km and a precision of 15–45 ppbv (15–20% below 30 km). The systematic error is smaller than 2–3 ppbv above 30 km. It increases to values of 12 ppbv at 20 km and 35 ppbv at 15 km. A small ozone line in this band allows retrieval of profile information between 18 and 45 km with an altitude resolution of 3–3.5 km, a precision of 0.25–1.5 ppmv (20–25%), and a systematic uncertainty of 0.75 ppmv around 20 km and of below 0.4 ppmv above 25 km. The main Odin/SMR ozone line at 544.9 GHz gives profile information from 14–70 km with 1.5 km resolution and a statistical error of 0.2–0.8 ppmv (10–15% between 18 and 45 km). The systematic error was found to be about 0.6 ppmv around the ozone mixing ratio maximum and lower than 0.2 ppmv above 50 and below 25 km. HNO<sub>3</sub> is retrieved between 18 and 35 km with a resolution of 1.5–2 km and a single-scan precision of better than 1.5 ppbv. For HNO<sub>3</sub>, the systematic uncertainty is 0.5–0.7 ppbv between 20 and 25 km and better than 0.5 ppbv above. The lower altitude limit of the Odin/SMR species retrieval is in general approximately 2 and 4 km higher at middle and low latitudes, respectively, owing to increased water vapor absorption.

[54] The operational code (Chalmers-v1.2), smoothed in altitude, gives in general a slightly improved measurement precision compared to the reference code (CTSO-v223) at the cost of a slightly degraded resolution in altitude. Compared to the reference codes CTSO-v222 and CTSO-v223, which agree relatively well throughout the stratosphere for ClO, N<sub>2</sub>O, HNO<sub>3</sub>, and O<sub>3</sub> in the 501.8 GHz band, Chalmers-v1.2 data appear to show systematically slightly higher mixing ratios, in particular at the upper and lower limits of the species retrieval altitude ranges.

[55] Ozone retrievals in the 544.6-GHz band yield considerably smaller mixing ratios compared to the 501.8-GHz ozone retrievals. Largest discrepancies were found for CTSO-v222 and Chalmers-v1.2 around the ozone mixing ratio peak. This was identified to be caused by a wrong line broadening parameter for the ozone line at 544.9 GHz used in these two older versions (see Table 2).

## 6. Conclusions

[56] A users choice of a version would very much depend on the species and application. Chalmers-v1.2 data, the operational level 2 product, has the advantage to be systematically processed and covers therefore the whole Odin measurement period starting in November 2001, based on

about 10 stratospheric mode measurement days per month. The reference level 2 processor (CTSO-v222, CTSO-v223) aims first of all at the verification and validation of the operational data product, and data are therefore not systematically produced. However, version 222 data of the 501.8-GHz target species ClO, N<sub>2</sub>O, and O<sub>3</sub> are already available for various periods of particular scientific interest (Arctic winter 2002–2003, Antarctic vortex split 2002). Version 223, the most recent and advanced version, provides in particular the best altitude resolution as well as good results for the 544.6-GHz band measurements of O<sub>3</sub> and HNO<sub>3</sub>. Data could be produced on request for scientifically interesting periods.

[57] In general, only good quality Odin/SMR profiles (assigned flag QUALITY = 0) shall be used for scientific studies, and the measurement response associated to each retrieved mixing ratio shall be larger than ~0.9, a measure to assure that the information comes entirely from the measurement and the contribution of the climatological a priori profile used by the “Optimal Estimation” retrieval is negligible. Both values, quality flag and measurement response, are provided in the Odin/SMR level 2 HDF data files. Data are available at <http://www.rss.chalmers.se/gem/> and <http://ether.ipsl.jussieu.fr>.

[58] A quality assessment of the Odin/SMR stratospheric mode level 2 products by comparison with independent measurements is the subject of individual studies focusing on nitrous oxide [Urban *et al.*, 2005], chlorine monoxide, ozone, and nitric acid. Future work on a unified level 2 data version includes a further refinement with respect to the quality of both level 1b data and operational level 2 product, for example, by optimization of the retrieval methodology and of the relevant instrumental and spectroscopic input parameters identified here.

[59] **Acknowledgments.** Odin is a Swedish-led satellite project funded jointly by the Swedish National Space Board (SNSB), the Canadian Space Agency (CSA), the National Technology Agency of Finland (Tekes), and the Centre National d’Etudes Spatiales (CNES) in France. The Swedish Space Corporation has been the industrial prime contractor. This research was supported in France by contracts from CNES and from the Programme National de Chimie Atmosphérique (PNCA) and in Sweden by SNSB. The authors wish to acknowledge P. Baron and F. Merino for their early work on the implemented retrieval algorithms as well as C. Boone, F. Girod, Y. Planchais, and A. Jones for their contribution to level 2 data processing. We are most grateful to the work of the Swedish team assuring the successful operation of the satellite.

## References

- Amano, T., and M. Yamada (2004), Pressure broadening measurements at Ibaraki: BrO and O<sub>3</sub>, in *Proceedings of the International Workshop on Critical Evaluation of mm-/Submm-Wave Spectroscopic Data for Atmospheric Observations*, edited by T. Amano, Y. Kasai, and T. Manabe, Commun. Res. Lab., Tokyo, Ibaraki Univ., Mito, Japan.
- Baron, P. (1999), Développement et validation du code MOLIERE: Chaîne de traitement des mesures micro-ondes du satellite Odin, Ph.D. thesis, Univ. Bordeaux 1, Talence, France.
- Baron, P., F. Merino, and D. Murtagh (2001), Simultaneous retrievals of temperature and volume mixing ratio constituents from non-oxygen Odin submillimeter bands, *Appl. Opt.*, **40**(33), 6102–6110.
- Baron, P., P. Ricaud, J. de La Noë, J. E. P. Eriksson, F. Merino, M. Ridal, and D. P. Murtagh (2002), Studies for the Odin Sub-Millimetre Radiometer: II. Retrieval methodology, *Can. J. Phys.*, **80**(4), 341–356.
- Bauer, A., M. Birk, S. Bühler, J. Colmont, A. von Engeln, K. Künzi, A. Perrin, D. Priem, G. Wagner, and G. Wlodarczak (1998), Study on a spectroscopic data base for millimeter and submillimeter wavelengths, *Tech. Rep. ESTEC/Contract 11581/95/NL/CN*, Eur. Space Res. and Technol. Cent., Noordwijk, Netherlands.

- Berthet, G., P. Ricaud, F. Lefèvre, E. Le Flochmoën, J. Urban, B. Barret, N. Lautié, E. Dupuy, J. de La Noë, and D. Murtagh (2005), Nighttime chlorine monoxide observations by the Odin satellite and implications for the ClO/Cl<sub>2</sub>O<sub>2</sub> equilibrium, *Geophys. Res. Lett.*, *32*, L11812, doi:10.1029/2005GL022649.
- Buehler, S., P. Eriksson, T. Kuhn, A. von Engeln, and C. Verdes (2005), ARTS, the Atmospheric Radiative Transfer Simulator, *J. Quant. Spectrosc. Radiat. Transfer*, *91*, 63–65, doi:10.1016/j.jqsrt.2004.05.051.
- Bühler, S. (1999), Microwave limb sounding of the stratosphere and upper troposphere, Ph.D. thesis, Univ. of Bremen, Bremen, Germany.
- Cailley, G. (2002), Étude de la restitution de la température à partir des mesures de l'instrument SMR à bord du satellite Odin, Master's thesis, Univ. Bordeaux 1 et Toulouse III, DEA Astrophys., Planétol., Sci. et Techn. Spatiales, Talence, France.
- Eriksson, P. (1999), Microwave radiometric observations of the middle atmosphere: Simulations and inversions, Ph.D. thesis, School of Electr. and Comput. Eng., Chalmers Univ. of Technol., Göteborg, Sweden.
- Eriksson, P., F. Merino, D. Murtagh, P. Baron, P. Ricaud, and J. de La Noë (2002), Studies for the Odin Sub-Millimetre Radiometer: I. Radiative transfer and instrument simulation, *Can. J. Phys.*, *80*(4), 321–340.
- Eriksson, P., C. Jiménez, and S. Buehler (2005), Qpack: A tool for instrument simulation and retrieval work, *J. Quant. Spectrosc. Radiat. Transfer*, *91*, 47–61, doi:10.1016/j.jqsrt.2004.05.050.
- Frisk, U., et al. (2003), The Odin satellite: I. Radiometer design and test, *Astron. Astrophys.*, *402*(3), L27–34.
- Hedin, A. (1991), Extension of the MSIS thermosphere model into the middle and lower atmosphere, *J. Geophys. Res.*, *96*(A2), 1159–1172.
- Henry, A., M. Margottin-Maclou, and N. Lacombe (1985), N<sub>2</sub> and O<sub>2</sub> broadening parameters in the ν<sub>3</sub> band of <sup>14</sup>N<sub>2</sub><sup>16</sup>O, *J. Mol. Spectrosc.*, *111*, 291–300.
- Lautié, N. (2003), Traitement des mesures satellitaires sub-millimétriques effectuées par Odin/SMR; étude non-linéaire de la vapeur d'eau. Étude stratosphérique de HCN au moyen de mesures micro-ondes, Ph.D. thesis, Univ. Pierre et Marie Curie, Paris.
- Lautié, N., et al. (2001), Retrieval of trace gas profiles from Odin/SMR limb measurements: Non-linear retrieval scheme for H<sub>2</sub>O at 556.9 GHz, in *International Symposium On Submillimeter Wave Earth Observation From Space - III, 8–9 Oct. 2001, Delmenhorst, Germany*, edited by S. Bühler, pp. 93–105, Logos Verlag, Berlin.
- Melsheimer, C., et al. (2005), Intercomparison of general purpose clear-sky atmospheric radiative transfer models for the millimeter/sub-millimeter spectral range, *Radio Sci.*, *40*, RS1007, doi:10.1029/2004RS003110.
- Merino, F., et al. (2001), The Odin Operational Code (an optimized forward and retrieval code), *Rep. AP-39*, Arrhenius Lab., Meteorol. Inst. of Stockholm Univ., Stockholm.
- Merino, F., D. P. Murtagh, M. Ridal, J. E. P. Eriksson, P. Baron, P. Ricaud, and J. de La Noë (2002), Studies for the Odin Sub-Millimetre Radiometer: III. Performance simulations, *Can. J. Phys.*, *80*(4), 357–373.
- Murtagh, D., et al. (2002), An overview of the Odin atmospheric mission, *Can. J. Phys.*, *80*(4), 309–319.
- Olberg, M., et al. (2003), The Odin satellite: II. Radiometer data processing and calibration, *Astron. Astrophys.*, *402*(3), L35–38.
- Pickett, H., R. Poynter, E. Cohen, M. Delitsky, J. Pearson, and H. Müller (1998), Submillimeter, millimeter, and microwave spectral line catalog, *J. Quant. Spectrosc. Radiat. Transfer*, *60*(5), 883–890.
- Ricaud, P., et al. (2005), Polar vortex evolution during the 2002 Antarctic major warming as observed by the Odin satellite, *J. Geophys. Res.*, *110*, D05302, doi:10.1029/2004JD005018.
- Rodgers, C. D. (1976), Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation, *Rev. Geophys.*, *14*(4), 609–624.
- Rodgers, C. D. (1990), Characterization and error analysis of profiles retrieved from remote sounding measurements, *J. Geophys. Res.*, *95*(D5), 5587–5595.
- Rothman, L., et al. (2003), The HITRAN Molecular Spectroscopic Database: Edition of 2000 including updates through 2001, *J. Quant. Spectrosc. Radiat. Transfer*, *82*, 5–44.
- Smith, M., V. Devi, D. Benner, and C. Rinsland (1997), Temperature dependence of air-broadening and shift coefficients of O<sub>3</sub> lines in the ν<sub>1</sub> band, *J. Mol. Spectrosc.*, *182*, 239–259.
- Urban, J. (2003), Optimal sub-millimeter bands for passive limb observations of stratospheric HBr, BrO, HOCl, and HO<sub>2</sub> from space, *J. Quant. Spectrosc. Radiat. Transfer*, *76*, 145–178.
- Urban, J., et al. (2002), Trace gas retrieval from Odin/SMR limb observations: Stratospheric mode, in *Proceedings of the 6th European Symposium on Stratospheric Ozone, 2–6 Sept. 2002, Göteborg, Sweden*, edited by N. Harris, G. Amanatidis, and J. Levine, pp. 474–477, Eur. Union, Cambridge, UK.
- Urban, J., P. Baron, N. Lautié, K. Dassas, N. Schneider, P. Ricaud, and J. de La Noë (2004a), MOLIERE (v5): A versatile forward- and inversion model for the millimeter and sub-millimeter wavelength range, *J. Quant. Spectrosc. Radiat. Transfer*, *83*(3–4), 529–554.
- Urban, J., et al. (2004b), Odin/SMR observations of stratospheric water vapour and its isotopes: Requirements on spectroscopy, in *Proceedings of the International Workshop on Critical Evaluation of mm/Submillimeter Spectroscopic Data for Atmospheric Observations*, edited by T. Amano et al., Commun. Res. Lab., Ibaraki Univ., Tokyo.
- Urban, J., et al. (2004c), The Northern Hemisphere stratospheric vortex during the 2002–03 winter: Subsidence, chlorine activation and ozone loss observed by the Odin sub-millimetre radiometer, *Geophys. Res. Lett.*, *31*, L07103, doi:10.1029/2003GL019089.
- Urban, J., et al. (2005), Odin/SMR limb observations of stratospheric trace gases: Validation of N<sub>2</sub>O, *J. Geophys. Res.*, *110*, D09301, doi:10.1029/2004JD005394.
- Verdes, C., S. Bühler, A. von Engeln, T. Kuhn, K. Künzi, P. Eriksson, and B. Sinnhuber (2002), Pointing and temperature retrieval from millimeter-submillimeter limb soundings, *J. Geophys. Res.*, *107*(D16), 4299, doi:10.1029/2001JD000777.
- Yamada, M. M., and T. Amano (2005), Pressure broadening measurement of submillimeter wave lines of O<sub>3</sub>, *J. Quant. Spectrosc. Radiat. Transfer*, *95*, 221–230.

J. de La Noë and E. Dupuy, Observatoire Aquitain des Sciences de l'Univers, Université Bordeaux 1, L3AB, F-33270 Floirac, France.

M. Ekström, P. Eriksson, N. Lautié, D. Murtagh, and J. Urban, Department of Radio and Space Science, Chalmers University of Technology, Hörsalsvägen 11, SE-412 96 Göteborg, Sweden. (jo.urban@rss.chalmers.se)

L. El Amraoui, Météo-France, CNRM, 42 avenue Gaspard Coriolis, F-31057 Toulouse, France.

U. Frisk, Swedish Space Corporation, Box 4207, SE-171 04 Solna, Sweden.

C. Jiménez, Institute of Atmospheric and Environmental Science, School of GeoSciences, University of Edinburgh JCMB, Mayfield Road, Edinburgh EH9 3JZ, UK.

E. Le Flochmoën and P. Ricaud, Laboratoire d'Aérodynamique, Observatoire de Midi-Pyrénées, F-31400 Toulouse, France.

M. Olberg, Onsala Space Observatory, Chalmers University of Technology, SE-439 92 Onsala, Sweden.