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First near-global retrievals of OH rotational temperatures from satellite-based Meinel band emission measurements

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[1] For the first time near-global retrievals of mesopause OH rotational temperatures from satellite-borne Meinel band emission measurements are presented. The measurements of the OH (3-1) Meinel band near 1.5 micron were performed with the SCIAMACHY instrument on the European Space Agency's environmental satellite Envisat. The derived OH (3-1) rotational temperatures are shown to be in reasonable agreement with the CIRA (1986) atmosphere temperatures for the seasons and latitudes considered. The derived temperatures are in good agreement with ground-based measurements of the OH rotational temperature performed with a CEDAR Mesospheric Temperature Mapper (MTM) at Maui, Hawaii (21°N/204°E), with the GRound based Infrared P-branch Spectrometer I (GRIPS-I) at Hohenpeißenberg (47°N/11°E) and with GRIPS-II at Wuppertal (51°N/7°E). The SCIAMACHY limb nighttime observations provide a unique data set of near-global OH rotational temperature to study seasonal and geographical variations, dynamical processes and possibly long-term temperature trends, if an extended data set becomes available in the future.

INDEX TERMS: 0310 Atmospheric Composition and Structure: Airglow and aurora; 0350 Atmospheric Composition and Structure: Pressure, density, and temperature; 0394 Atmospheric Composition and Structure: Instruments and techniques; 1610 Global Change: Atmosphere (0315, 0325); 1640 Global Change: Remote sensing. **Citation:** von Savigny, C., et al. (2004), First near-global retrievals of OH rotational temperatures from satellite-based Meinel band emission measurements, *Geophys. Res. Lett.*, *31*, L15111, doi:10.1029/2004GL020410.

1. Introduction

[2] Hydroxyl molecules in the mesopause region are known to be formed and vibrationally-rotationally excited through the reaction

$$O_3 + H \longrightarrow OH(v' \leq 9) + O_2 + 3.3\ eV \tag{1}$$

leading to an emission layer centered at about 87 km [e.g., *Baker and Stair*, 1988] with a width of 8–10 km. Measurements of the relative intensities of at least two rotational lines of a vibrational OH Meinel band can be used to remotely sense the rotational OH temperature at the altitude of the OH emission. This approach has been used for several decades for ground-based retrievals of mesopause temperatures [e.g., *Bittner et al.*, 2002, and references therein]. The retrievability of OH rotational temperatures from space-based spectroscopic measurements was demonstrated by *Mende et al.* [1988], who retrieved the OH temperature from a single spectrum of the OH (8-3) Meinel band obtained with a Fabry-Perot imager flown on the space shuttle mission STS 41-G.

[3] The advantage of ground-based observations is that the local time variation of the rotational temperature can be measured. However, as the shape and peak altitude of the OH emission layer are variable, a correct interpretation of ground-based measurements of OH rotational temperatures, as well as their long-term trends, requires simultaneous measurements of the vertical OH emission rate profile. Satellite-based observations are not affected by clouds and allow for global coverage, usually within a few days. But with satellites in sun-synchronous orbits the local time variation of atmospheric phenomena cannot be investigated. Furthermore, satellite instruments often integrate over relatively large spatial scales. Therefore, the synergy of satellite and ground-based observations can yield important complementary information: *She and Lowe* [1998] combined ground-based measurements of the OH (3-1) rotational temperature with satellite observations of the

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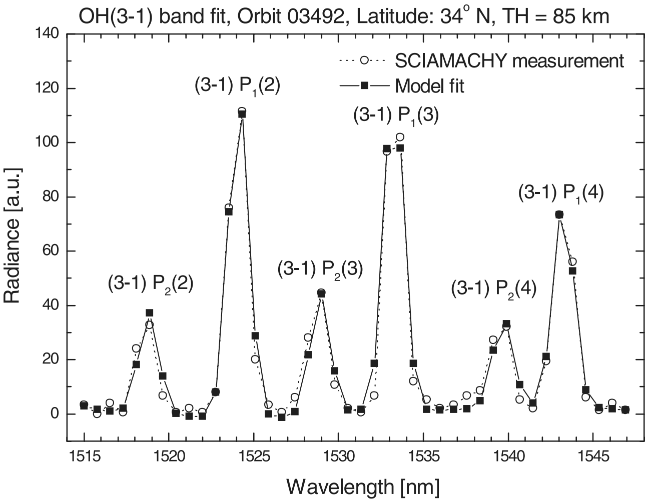

Figure 1. Example of a SCIAMACHY OH (3-1) nighttime limb emission spectrum at 85 km tangent height. Also shown is the model spectral fit.

OH (8-3) $P_1(3)$ vertical volume emission rate made with WINDII on UARS to facilitate a more accurate interpretation of the derived OH rotational temperatures.

[4] With SCIAMACHY [*Bovensmann et al.*, 1999], the Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY rotational OH temperatures can for the first time be retrieved from space-borne observations of the OH Meinel band emissions with near-global coverage. This paper presents initial nighttime OH rotational temperature retrieval results from SCIAMACHY.

2. SCIAMACHY on Envisat

[5] SCIAMACHY [*Bovensmann et al.*, 1999] is an 8-channel grating spectrometer on ESA's Envisat launched on March 1st 2002 into a polar, sun-synchronous orbit with an inclination of 98.7° and a descending node at 10:00 local solar time (LST). Beside nadir and occultation observations SCIAMACHY also makes spectroscopic observations of scattered solar radiation and atmospheric airglow emissions in limb geometry, over the wavelength range 220 nm to 2380 nm with a wavelength dependent spectral resolution between 0.2 and 1.5 nm. Limb measurements are also performed every second orbit on the Earth's nightside in a special mesosphere/upper atmosphere observation mode covering tangent heights from 75 km to 150 km in steps of about 3.3 km. The SCIAMACHY vertical geometric field of view (FOV) in limb-viewing mode is 2.8 km. The horizontal resolution of the measurements is about 960 km perpendicular to the satellite track and approximately 550 km along track. For the retrieval of OH rotational temperatures the limb emission spectra at a tangent height of 85 km are used (1.5 seconds integration time). The limb observations on the night side cover about 70° in terms of latitude during each orbit - with a gap of about 15 ° - and the minimum and maximum latitude covered each day exhibits a slow seasonal variation, leading to absolute limits of the latitudes that can be measured of 30°S and 70°N.

[6] The OH (3-1) Meinel band used in this study is measured in SCIAMACHY channel 6 (1000 nm–1750 nm). Uncalibrated data (so-called Level 0 data) is used here, since only relative intensities are needed for rotational temperature retrievals. The dark current and electronic offset corrections were made by subtracting the spectrum measured at the highest tangent height (150 km) from the used limb spectra. The SCIAMACHY channel 6 radiance response for unpolarized radiation was used for the radiance response.

3. Methodology

3.1. Rotational Temperature Retrieval From SCIAMACHY

[7] For lower rotational states the population of those rotational levels in the vibrational state $\nu' = 3$ is in local thermodynamical equilibrium (LTE) with the ambient air. This is because the collisional frequency at 86 km altitude is about 3×10^4 s^{-1}, while the lifetime of OH at $\nu' = 3$ is about 0.014 s [*Kovacs*, 1969]. Thus, excited OH($\nu' = 3$) undergoes several hundred collisions before it radiates, and the rotational temperature is close to the neutral kinetic temperature T_{kin}. The relative population of the different rotational states J is given by Boltzmann's distribution:

$$N_J \propto (2J+1) \times e^{-E_J/k_B T_{kin}} \qquad (2)$$

where N_J is the number of molecules with rotational quantum number J, $(2J+1)$ is the degeneracy factor, E_J the energy of the rotational state J, and k_B Boltzmann's constant. Equation (2) allows the determination of T_{kin} from measurements of the relative intensities of at least two rotational OH lines.

[8] The synthetic OH (3-1) Meinel band spectra needed for the determination of temperatures from the SCIAMACHY observations were calculated using the energy levels derived from the *Coxon* [1980], the *Coxon and Foster* [1982] term values, and the *Kovacs* [1969] line strength factors. The simulated spectra are first convolved on a high spectral resolution wavelength grid (0.01 nm) with the SCIAMACHY channel 6 instrument function (Gaussian with FWHM = 1.36 nm) and the convolved spectrum is binned into the SCIAMACHY wavelength pixels. The retrieval is performed with an iterative approach. First a linear least squares fit – including a third-order polynomial – is performed to (a) determine the scaling factor between the observed and simulated spectra, and (b) subtract a possible offset. In a second step a non-linear fit is performed using Levenberg-Marquard's scheme employing the synthetic OH spectral model described above as a forward model with the rotational temperature and a wavelength shift as model parameters. The wavelength range used extends from 1515 nm to 1547 nm, and includes 6 OH (3-1) rotational lines: $P_2(2)$, $P_1(2)$, $P_2(3)$, $P_1(3)$, $P_2(4)$, and $P_1(4)$. A sample OH (3-1) emission spectrum at a tangent height of 85 km together with the model fit is shown in Figure 1. The temperature retrieval error for an individual measurement varies between 5 and 8 K.

[9] A sensitivity study was performed to estimate the impact of different sets of transition probabilities on the retrieved SCIAMACHY OH temperatures. Apart from the *Kovacs* [1969] line strengths, the *Mies* [1974] (used for GRIPS-I and GRIPS-II) and the *Goldman et al.* [1998]

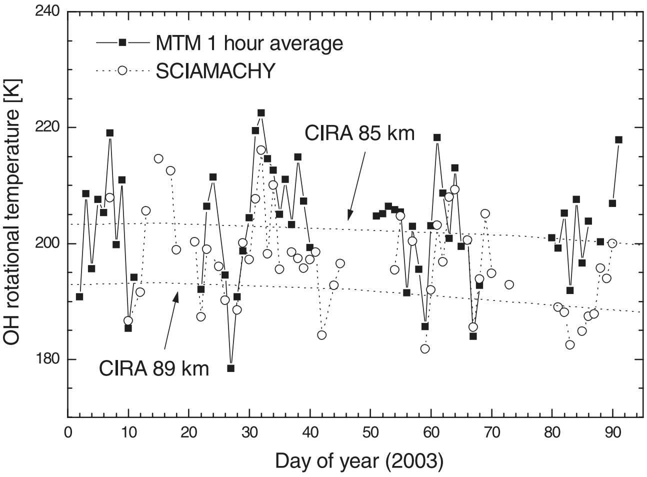

Figure 2. Comparison of SCIAMACHY OH (3-1) rotational temperatures with collocated (±10° latitude/±20° longitude) 1-hour averages of ground-based MTM OH (6-2) rotational temperatures in early 2003 at Hawaii (21°N/203°E).

(used for MTM) Einstein coefficients were employed and Envisat orbit 09936 on January 24, 2004 was chosen as a sample data set. The OH temperatures obtained with the *Kovacs* [1969] line strengths were on average 1.1 K higher than the temperatures obtained with the *Mies* [1974] transition probabilities, and 3.2 K higher than the ones retrieved with the *Goldman et al.* [1998] transition probabilities.

3.2. Ground-Based Measurements of OH Rotational Temperatures

[10] The SCIAMACHY OH rotational temperatures are compared to ground-based measurements from three stations: the CEDAR MTM (Mesospheric Temperature Mapper) instrument at Maui, Hawaii (21°N/204°E) [e.g., *Pendleton et al.*, 2000], the GRIPS-I instrument at Hohenpeißenberg (47°N/11°E) and GRIPS-II at Wuppertal (51°N/7°E) [*Bittner et al.*, 2002]. GRIPS-I and GRIPS II derive OH (3-1) rotational temperatures from a semi-logarithmic relationship between the intensities of the $P_1(2)$, $P_1(3)$ and $P_1(4)$ rotational lines of the OH (3-1) vibrational branch (1.524–1.543 μm). GRIPS-I has a FOV of 16 km × 22 km at mesopause altitudes. The FOV of GRIPS-II is with 29 km × 41 km slightly larger. Temperature measurements are taken every 4–5 minutes with GRIPS-I and in 1.5 minute intervals with GRIPS-II. The statistical and systematic errors of the nightly mean OH temperatures are less than 2.0 K each. For further details see *Bittner et al.* [2002] and references therein.

[11] The FOV of the MTM instrument corresponds to 180 km diameter at the OH emission altitude. However, for this comparative study data from a 4.5 km by 4.5 km square region centered on the zenith were used. The MTM samples both the OH (6-2) band and the O_2 (0,1) atmospheric band every 5.5 minutes. Comparison of the MTM OH (6-2) band rotational temperatures with ground-based lidar measurements indicates an uncertainty of ±5 K for nightly mean values as referenced to the 87 km level lidar measurements. However, the precision of the individual measurements is estimated to better than 2 K in 3 minutes (or 0.5 K in 1 hour) [*Pendleton et al.*, 2000].

4. Results and Discussion

[12] Due to tidal variations of the mesopause temperatures, the SCIAMACHY OH temperatures can only be directly compared with ground-based observations if the LST of the observations is also considered. The SCIAMACHY limb emission observations used in this study were all performed between 9 and 10 pm LST. For the initial comparisons presented here the ground-based temperature measurements were averaged over 1 hour around the LST of the SCIAMACHY overpass. All available SCIAMACHY measurements on a given day with tangent points within ±10° latitude/±20° longitude of the ground-based site (up to 8 individual measurements) were averaged. The gaps in the data sets are due to (a) overcast conditions making ground-based observations impossible, (b) ground-based measurements being limited to low-moon periods, (c) SCIAMACHY decontamination periods when detectors are not cooled, and (d) no SCIAMACHY measurements available satisfying the above coincidence criteria.

[13] Figure 2 shows the comparison of the SCIAMACHY and the MTM OH temperatures for days 1–92 of the year 2003. The temperatures measured with the two instruments are in good quantitative agreement except for the last 15 days which are under further investigation. The mean temperature difference between the collocated MTM and SCIAMACHY observations (i.e., T_{MTM} - $T_{SCIAMACHY}$) is 7.1 K (standard deviation: 11.4 K) for 36 nights with collocated observations during the period considered. If only days 1 to 70 are considered the mean difference is 5.1 K (standard deviation: 11.5 K). More importantly, the SCIAMACHY OH temperatures show the same day-to-day variability as observed in the ground-based MTM temperatures, especially during the extended periods: days 20 to 35 and days 50 to 70. Also shown in Figure 2 are the CIRA (1986) temperatures at 85 km and 89 km. These exhibit

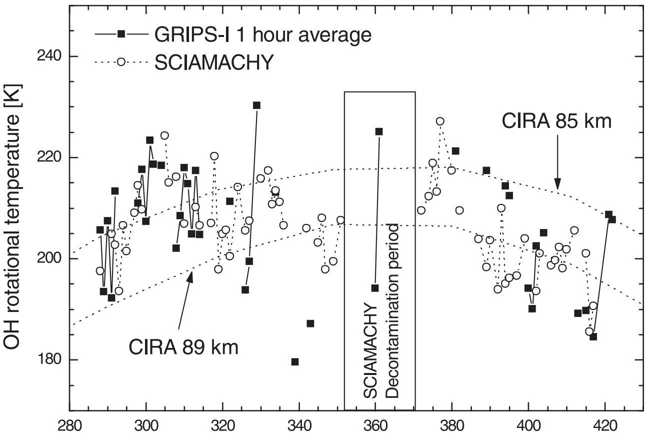

Figure 3. Comparison of SCIAMACHY OH (3-1) rotational temperatures with collocated GRIPS-I 1-hour averages of ground-based OH (3-1) rotational temperature measurements at Hohenpeißenberg (47°N/11°E) for the period October 15, 2003 through February 26, 2004.

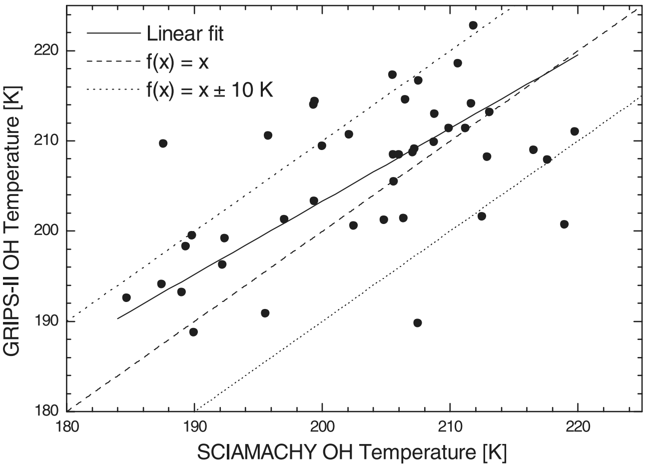

Figure 4. Scatter plot of collocated SCIAMACHY and GRIPS-II (Wuppertal: 51°N/7°E) OH (3-1) rotational temperature measurements. The solid line is the linear least squares fit of the data points, and the dashed line corresponds to $f(x) = x$.

similar trends to those evident in SCIAMACHY and the MTM OH temperatures.

[14] The GRIPS-I OH temperatures, routinely derived at Hohenpeißenberg since October 2003, are in Figure 3 compared with SCIAMACHY OH temperatures between October 15, 2003 (day 288) and February 26, 2004 (day 422). Again, the SCIAMACHY OH temperatures are in good quantitative agreement with the ground-based temperatures. The only period with significant differences between the two data sets occurs around day 340, when the GRIPS-I OH temperatures are systematically lower by about 20 K. The mean difference between the GRIPS-I and the SCIAMACHY temperatures (i.e., T_{GRIPS} - $T_{SCIAMACHY}$) is 2.6 K (standard deviation: 11.1 K) for 19 nights with collocated observations during the period considered. The comparison with GRIPS II data at Wuppertal yields similar results. Data from January to March 2003 and winter 2003/2004 yields 43 coincidences. The mean difference between GRIPS II and SCIAMACHY is 2.7 K (standard deviation: 8.5 K). Figure 4 shows a comparison of the collocated SCIAMACHY and GRIPS-II OH temperature retrievals. The correlation coefficient between the SCIAMACHY and the GRIPS-II temperatures in Figure 4 is 0.55. This relatively small value is most likely mainly due to atmospheric variability and the partly significant distances between the sampled atmospheric volumes. The small difference between the comparisons with the two GRIPS instruments provides independent evidence for the excellent agreement between GRIPS-I and GRIPS-II.

[15] The comparison of the SCIAMACHY OH temperatures with the ground-based stations showed periods with good agreement in terms of both absolute temperatures and the day-to-day variability, but also periods with systematic differences. In order to assess the comparability of the SCIAMACHY and the ground-based OH temperatures the differences between the measurements must be discussed. One aspect that may cause discrepancies in the retrieved temperatures are the large differences in the horizontal coverage of the measurements. SCIAMACHY samples an area of 960 km (across track) by about 550 km (along track), whereas the instantaneous FOV of the ground-based instruments is significantly smaller (on the order of 20 km × 20 km). Furthermore, the retrieved OH temperatures present averages over a certain altitude range, weighted by the vertical variation of the OH volume emission rate. For SCIAMACHY limb emission measurements the altitude range, where the OH emission signal mainly comes from, does not only depend on the vertical OH emission rate profile, but also on the tangent height used (here about 85 km). Initial results (not presented here) on the inversion of the integrated limb emission rates to vertical emission rate profiles indicate that the mean emission altitudes for ground-based and space-borne limb observations differ usually only by a few hundred meters if the SCIAMACHY limb emission spectrum at 85 km altitude is employed. However, if the OH emission rate profile is shifted vertically, or its vertical shape is distorted (as, e.g., in the case of double-peak structures [*Melo et al.*, 2000]), then the mean emission altitudes of the ground-based and the space-borne observations can differ by a few km, leading to differences in the observed OH temperatures.

[16] Considering these differences in observation geometries, FOV and retrieval techniques the good agreement between the different temperature data sets is remarkable and indicates that the SCIAMACHY nighttime OH (3-1) limb emission measurements can be used to retrieve rotational temperatures on a near-global scale and on a daily basis.

5. Conclusions

[17] We presented retrievals of OH rotational temperatures from satellite-based spectroscopic measurements of the nighttime OH (3-1) Meinel band emission. The retrieved OH temperatures are in good agreement with ground-based measurements of the OH (3-1) rotational temperature at Hohenpeißenberg and Wuppertal, and with OH (6-2) rotational temperatures measured at Hawaii. The mean difference between the GRIPS-I (II) and the SCIAMACHY rotational temperature measurements at Hohenpeißenberg (Wuppertal) is 2.6 K (2.7 K) for 19 (43) nights with collocated observations during early 2003 and winter 2003/2004. In terms of the Hawaii overpasses, 36 nights of collocated SCIAMACHY and ground-based measurements in early 2003 yielded a mean difference of 7.1 K. The retrieval of vertical OH emission rate profiles, allowing for both a better interpretation of the measurements and a more accurate comparison with ground-based temperature measurements, is work in progress.

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