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Revised temperature dependent ozone absorption cross section spectra (Bogumil et al.) measured with the sciamachy satellite spectrometer

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Abstract

Ozone absorption cross section spectra and other trace gases had been measured using the Scanning Imaging Absorption spectroMeter for Atmospheric ChartographHY (SCIAMACHY) satellite instrument at relevant atmospheric conditions. The measured cross sections were relative cross sections and were converted to absolute values using published data. Using the SCIAMACHY's FM cross sections as published by Bogumil et al. (2003) in the SCIAMACHY retrievals of total ozone leads to an over-estimation in the total ozone by 5 % compared to collocated GOME data. This work presents the procedures followed to correct the ozone cross section data as published in Bogumil et al. (2003) starting from original raw data (optical density spectra) from the original measurements. The revised data agrees well within 3 % with other published ozone cross-sections and preserves the correct temperature dependence in the Hartley, Huggins, Chappuis and Wolf bands. SCIAMACHY's total ozone columns retrieved using the revised cross section data are shown to be within 1 % compared to the ozone amounts retrieved routinely from SCIAMACHY.

1 Introduction

The Scanning Imaging Abortion spectroMeter for Atmospheric ChartographHY (SCIAMACHY) spectrometer (Burrows et al., 1995; Bovensmann et al., 1999) is a moderate resolution (0.2–1.5 nm) passive remote sensing instrument launched in 2002 onboard 20 ESA's ENVISAT (ENVIronmental SATellite). It is an eight channel grating spectrometer that collects at the top of the atmosphere the upwelling backscattered and cloud or surface reflected solar fluxes in the ultra-violet (UV), visible and near-infrared (NIR) spectral regions (230–2380 nm). SCIAMACHY has two scanning mirrors that perform alternative nadir and limb observation modes as well as lunar and solar occultations 25 (Bovensmann et al., 1999). Total column amounts and vertical distributions of atmospheric trace gases relevant to ozone chemistry and global warming are inferred from

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SCIAMACHY's data. In addition to other geophysical parameters including mesopause temperature, cloud coverage and top height, aerosols, Mg II index (solar activity) and polar stratospheric clouds are retrieved (Gottwald and Bovensmann, 2011).

Ozone (O_3), an important trace gas, shields the damaging UV radiation in the stratosphere (protects life). In the troposphere, it acts as a pollutant due to its high oxidation potential that may cause respiratory problems and destroys plant tissues. It plays a significant role in the radiative budget, absorbing UV-visible solar radiation in the stratosphere and infrared radiations emitted by Earth in the troposphere. Long-term datasets of total ozone columns and vertical profile are essential to confirm whether the ozone depleting substances and ozone depletion are reduced according to Montreal Protocol and ozone recovery is achieved (WMO, 2010). Global and long term measurements of atmospheric minor constituents are key factors in understanding physical and chemical processes in our atmosphere in a changing climate.

SCIAMACHY provides ten years (2003–2012) of ozone data (operations ceased on 8 April 2012 after losing communication with ENVISAT). This data together with that retrieved from GOME (1995–2005) onboard ERS-2 since 1995 (Burrows et al., 1999b) and GOME-2 (2007–present) launched in 2006 onboard of EUMETSAT's MetOp-A (Callies et al., 2000; Munro et al., 2006.) and two additional GOME-2 spectrometers as part of the MetOp programme MetOp B and C, will enable a homogeneous dataset in nadir observations since all instruments have very similar observation principles and differ slightly in spectral resolution. The consistency among the total column trace gas data from multiple space-borne instruments requires cautious investigation of the relevant parameters that present a significant source of error in the data processing, among them is the absorption cross section. Laboratory measurements of temperature dependent absorption cross section spectra for ozone and most trace gases were conducted in 1998–2000 using SCIAMACHY's spectrometer over a wide range of temperatures (203–293 K) (Bogumil et al., 2003). The measurements were carried out before setting the satellite in orbit. The so-called satellite FM (flight model) measurements were also performed for GOME (Burrows et al., 1998, 1999a) and GOME-2 (Gür, 2006; Gür

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et al., 2006; Chehade et al., 2012). The satellite FM data were relative cross section measurements and were scaled to absolute values using published literature data.

Accurate reference spectra (cross section) are key parameters in the retrieval of atmospheric trace gases. They are also required to homogenise the datasets acquired from different satellite platforms. GOME, SCIAMACHY and GOME-2 spectrometers provide global total ozone columns spanning over more than a decade since 1995. An instrumental drift of less than 1 % per decade is needed to identify changes in the long-term trends as a response to the Montreal protocol. The use of SCIAMACHY ozone FM cross-sections in the SCIAMACHY total ozone retrieval in the 325–335 nm spectral range (Huggins band) resulted in systematic differences of about 3–5 % when compared to collocated GOME data (Eskes et al., 2005). The GOME total ozone data retrieved using the GOME FM cross-sections agree very well with ground observations (Weber et al., 2005; Balis et al., 2007). This indicates that the approaches used to determine the absolute absorption cross sections were not consistent for the two instruments.

This work presents the re-analysis (correction) of SCIAMACHY FM ozone cross section in the spectral range 230–1070 nm between 203 and 293 K as published by Bogumil et al. (2003). Section 2 briefly describes the measurement campaigns and the procedures of reanalysing the data. Section 3 shows the validation of the revised cross sections by comparing them with published data in the different ozone bands with a focus on the Huggins band. Section 4 presents total ozone column retrievals from SCIAMACHY observations using the revised SCIAMACHY FM ozone cross section data compared to the reference retrieval.

2 Re-analysis of SCIAMACHY FM (Bogumil et al.) ozone cross-section

The absorption cross section spectra of O₃, NO₂, SO₂, OCIO, H₂CO, CO, CO₂, CH₄, HO₂, N₂O and H₂CO were measured in the 230–2380 nm spectral range at several temperatures between 203 and 293 K using the Calibration Apparatus for Trace Gas

Absorption Spectroscopy (CATGAS) connected to the SCIAMACHY FM spectrometer during the instrument calibration phase prior to its launch (Bogumil et al., 2003). The measured cross section spectra were also used to characterise the instrumental line shape (ILS) and to improve the straylight properties and wavelength calibration of
5 SCIAMACHY. Bogumil et al. (2003) presents a detailed description of the spectrometer, experimental setup (CATGAS apparatus), measurement procedure and method used to obtain the absolute cross sections.

Measurements of the cross sections are based on absorption spectroscopy, in which the intensity $I(\lambda)$ of the light at wavelength λ transmitted through an absorbing medium 10 of number density (n , molecule cm $^{-3}$) inside a gas cell, is a function of temperature T , pressure P , the length of the cell (l , cm), the absorption cross-section of the absorbing medium (σ , cm 2 molecule $^{-1}$) and the initial light intensity $I_0(\lambda)$ according to the Beer–Lambert law

$$I = I_0 e^{-\sigma \cdot n \cdot l}. \quad (1)$$

15 The concentrations and optical path lengths of the absorbing gas ($n \cdot l$) in Eq. (1) were not measured as ozone was contained in an oxygen mixture under continuous flow conditions. The optical density (OD), the ratio of light intensities with and without the gas absorber ($OD = \ln(I_0/I)$) was, therefore, scaled to absolute cross section by referencing them to published literature data.

20 The absorption measurements were done for each gas and temperature according the following procedure: a reference spectrum of light source with the gas carrier N₂ in the cell was recorded. The cell was evacuated and then filled with the absorber medium. An absorption spectrum was measured after the equilibrium conditions were achieved in the cell, and then the cell was pumped out. To monitor the stability of light (light drifts), another reference light spectrum was measured. Before each procedure, 25 a dark spectrum was recorded with the optical path to the spectrometer blocked by a shutter.

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2.1 Manual concatenation

The ozone absorption cross section varies over eight orders of magnitudes over the relevant SCIAMACHY spectral region up to 1070 nm. In order to cover this large dynamical range a set of absorption measurements, with varying ozone concentrations and optical path lengths was carried out that cover the entire UV, visible and NIR spectral region. All measurements were corrected for dark current and the reference intensity $I_0(\lambda)$ was calculated by linearly interpolating in time from the reference spectra (without absorber) before and after the absorption measurement. The optical densities were then calculated for all measurements at five temperatures between 203 and 193 K. A single continuous absorption cross section in arbitrary optical density units covering the entire SCIAMACHY's ozone wavelength range was obtained by gluing the useful parts of each absorption measurement by matching overlapping regions. An example of the new concatenation is shown in Figs. 1 and 2.

2.2 Absorption cross sections

The concatenated absorption cross section spectra for each temperature were scaled to absolute absorption cross section using Bass and Paur cross section data (Bass and Paur, 1985; Paur and Bass, 1985) since they were measured with high spectral resolution and cover the same temperatures at which SCIAMACHY FM data were measured. The Bass Paur data were convolved with the wavelength dependent SCIAMACHY slit function varying from about 0.2 to 0.4 nm. The instrument slit function varies in channel 2 and was determined by matching a high resolution solar spectrum, measured with the Fourier transform spectrometer at the McMath solar telescope at Kitt Peak, Arizona (Kurucz, 1995), to the SCIAMACHY measured solar spectrum in a non-linear least squares fit. The OD spectra are scaled directly in the 312–335 nm range to the convolved Bass Paur data for each temperature.

Figure 3 shows SCIAMACHY's temperature dependent cross section spectra in absolute units displaying the Hartley, Huggins, Chappuis and Wulf bands. The revised

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The improvements are due to the procedures followed to correct the ozone cross sections. The major improvements in this study were that different raw measurements were used to derive OD spectra, the overlap regions were optimized for concatenation, and, finally, the literature data were properly convolved to SCIAMACHY spectral resolution before scaling the unitless concatenated cross-section spectra. The improvements
5 can be clearly seen in Fig. 5.

3 Comparisons with literature data

To investigate the quality of the revised cross section data, they are compared with published literature data: BMD (Brion et al., 1993, 1998; Malicet et al., 1995; Daumont et al., 1992), Bass and Paur (Bass and Paur, 1985; Paur and Bass, 1985), Burrows (Burrows et al., 1999a) and Burkholder and Talukdar (Burkholder and Talukdar, 1994)
10 data as well as SCIAMACHY FM version 3.0 data (Bogumil et al., 2003). The comparisons are performed over broad wavelength intervals highlighting the Huggins and Chappuis bands where ozone is most commonly retrieved from nadir and limb viewing instruments and cross sections changes rapidly with temperature and wavelength. The
15 comparisons follow the procedures performed in the ESA study by Orphal (2002) and also summarised in Orphal (2003).

3.1 Integrated cross-sections at different temperatures

The integrated absorption cross-section is a good tool to compare the data in different regions since it is insensitive to the spectral resolution and wavelength calibration. The
20 comparisons are done over integrated regions according to those given by the 2002 ESA study (Orphal, 2002) and listed in Tables 1, 2, and 3:

- Hartley–Huggins band between 245 and 340 nm.
- Huggins band between 325 and 340 nm.

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- Chappuis band between 410 and 690 nm.

The comparisons exhibit an excellent agreement with the high spectral resolution literature data in the Huggins band, the revised data fit to within 1 % (Table 2). The data of Burrows (GOME FM) shows higher values. In the Hartley band, consistency between the data is very good (Table 1). The SCIAMACHY revised integrated cross-section data in the Chappuis band agrees very well with the mean values, they are larger than the values of Burkholder and Talukdar and smaller than Burrows data (Table 3). In this band, integrated cross sections shows a weak temperature dependence (increase with increasing temperature) which is consistent with Burkholder and Talukdar but not with Burrows.

3.2 Temperature parameterizations and smoothness comparisons

The Bass Paur temperature parameterization of the cross-section data approximates the cross-section at any temperatures as follows

$$\sigma(\lambda, T) = a_0(\lambda) \left[1 + a_1(\lambda) \cdot T + a_2(\lambda) \cdot T^2 \right]. \quad (2)$$

It is used in the radiation transfer model as part of the total ozone retrieval (see Section 4). Figure 7 shows the fitted quadratic temperature coefficients ($a_1(\lambda)$ and $a_2(\lambda)$) of the revised data together with that of other data. The comparison between the temperature coefficients of the different data is a good tool to examine the difference between them.

The first quadratic temperature coefficients ($a_1(\lambda)$) of the different data (in the upper panel) agree very well especially in the DOAS retrieval window (shaded area), larger differences are observed for Bogumil et al. (2003) version 3.0 data. The second temperature coefficients ($a_2(\lambda)$) do not match as well.

The smoothness of the temperature behavior of the absorption cross-sections is another mean to study the quality of the data. Figure 8 shows the temperature

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dependence (Eq. 2) in comparison with the measured absorption cross-section at an absorption maximum (328 nm) and minimum (330 nm) in the DOAS window.

The differences between the measured cross-section and the temperature parameterization are within 2 %. Figure 7 shows that the deviations from the quadratic temperature dependence of the revised data is similar to Bogumil et al. (2003) data.

3.3 Direct comparisons in the DOAS window (325–335 nm)

A more quantitative and direct comparison between the revised FM data and the high spectral resolution data (Brion and Bass and Paur) cannot be performed in the Huggins, due to differences in spectral resolution and wavelength calibration of the data. A non-linear least square fit is applied to match high resolution cross-sections, like Bass–Paur and BMD, to SCIAMACHY data. From this DOAS type fit a (differential) scaling factor and wavelength shift can be determined that can be directly translated into expected changes in retrieved total ozone. The fitting program is well explained in Weber et al. (2011) and Chehade et al. (2012) and retrieves six parameters:

- A scaling factor to adjust the amplitudes of the differential absorption structures of the cross sections (one parameter).
 - A wavelength shift to correct for differences in the wavelength calibration (one parameter).
 - A cubic polynomial to account for baseline drifts (four parameters).
- The revised data was compared to BMD, Bass and Paur and SCIAMACHY FM version 3.0 data (Bogumil et al., 2003) in the wavelength range 325–335 nm and at 225 and 240 K. The cross sections at the selected temperatures are calculated using the Bass-Paur temperature parameterization (Eq. 2). The literature data are convolved with the SCIAMACHY instrumental slit function. Sample fits are shown in Figs. 9 and 10 and the results are summarized in Table 4.

10 4 Retrieval tests

The retrieval of total ozone column is carried out using the Weighting Function Differential Optical Absorption Spectroscopy (WFDOAS) algorithm in the Huggins band (326.6–334.5 nm). This method uses a wavelength dependent weighting function of ozone and temperature that describes the relative radiance change due to a vertical profile change. The Bass-Paur temperature parameterization (Eq. 2) and temperature climatology are used in the radiation transfer code to express the vertical change of ozone absorption.

The WFDOAS algorithm as presented by Coldewey-Egbers et al. (2005), was successfully applied and validated for GOME ozone retrieval (Weber et al., 2005). The precision of the total ozone retrieval is better than 3 % for solar zenith angles below 80°. Weber et al. (2005) presented an elaborate global validation study of GOME WFDOAS with groundbased data from the WOUDC (World Ozone and UV Radiation Data Centre), an agreement within 1 % was observed, at high latitudes and high solar zenith angles the differences can reach few percents. The algorithm was also used in SCIAMACHY data processing to retrieve total ozone columns (Bracher et al., 2005) and a relative differences to within 1 % between SCIAMACHY WFDOAS and collocated

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GOME WFDOAS data was obtained at low and mid latitudes. Convolved GOME FM absorption cross section data (Burrows et al., 1999a) were used in the retrieval.

SCIAMACHY FM ozone cross-sections (Bogumil et al., 2003) differentially scaled by 5.3 % and shifted by 0.008 nm, is the cross section data used currently in the standard

SCIAMACHY WFDOAS retrieval (Weber et al., 2007). The total ozone amounts are within 0.5 % to that retrieved using GOME FM data (Weber et al., 2011).

In order to use the revised FM cross section data in the retrieval, the optimum wavelength shift has to be found. The optimum shift minimises the ozone fit residuals (RMS) as shown in Fig. 11. Shifting the SCIAMACHY cross section data by 0.018 nm minimizing the fit residuals and reduces total ozone by roughly 5 DU (−1.6 %).

Figures 12 and 13 show the total ozone column retrieved using the revised cross sections with the optimum wavelength shift applied for selected arbitrary SCIAMACHY orbits in 24 September 2008 (orbit 34339) and 20 March 2009 (orbit 36873), together with columns retrieved using the SCIAMACHY FM version 3.0 data. The total ozone values retrieved are roughly 1 % higher compared to the total ozone currently retrieved. The re-analysis of the FM data corrected total ozone amounts by 3–4 %, which is in agreement with results obtained from the direct comparisons (Sect. 3.3). Fit residuals remain unchanged using Bogumil et al. (2003) and the revised cross section data.

5 Conclusions

The re-analysis of SCIAMACHY temperature dependent FM ozone absorption cross section data is presented in this work. The re-analysis consists of calculating new optical density spectra (230–1070 nm) and scaling them to absolute values after concatenation. The revised SCIAMACHY FM cross section data show now the correct temperature dependence

The revised SCIAMACHY FM data agrees well with literature data (BMD and Bass Paur). In the DOAS ozone retrieval window, an overall agreement to within 1 % is obtained after proper spectral resolution adjustment and wavelength shifts when using the

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revised SCIAMACHY FM cross section data. A clear difference in the absorption structures between the revised data and Bogumil et al. (2003) version 3.0 data is observed, leading to a scaling difference in the differential structure of the Huggins band.

The revised data obtained in this study was successfully tested in the SCIAMACHY data processing. The application of the revised SCIAMACHY FM cross section data in the WFDOAS retrieval yields total ozone column in agreement to within 1 % of the values currently retrieved with SCIAMACHY.

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Table 1. Comparison of integrated cross-sections in the Hartley band (245–340 nm) in units of $10^{-16} \text{ cm}^2 \text{ nm molecule}^{-1}$, the second column indicates the mean from all available literature.

Temperature [K]	Mean value	Bass and Paur	BMD	Burrows	Bogumil	SCIA. revised
203	$3.53 \pm 1.2\%$	3.54	–	3.56	3.56	3.53
223	$3.53 \pm 1.1\%$	3.53	3.50	3.56	3.56	3.53
243	$3.54 \pm 1.1\%$	3.54	3.50	3.58	3.56	3.54
273	$3.55 \pm 1.0\%$	3.54	–	3.58	3.56	3.55
293	$3.55 \pm 0.6\%$	3.55	3.52	3.57	3.56	3.56

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Table 2. Comparison of integrated cross-sections in the Huggins band (325–340 nm) in units of $10^{-20} \text{ cm}^2 \text{ nm molecule}^{-1}$.

Temperature [K]	Mean value	Bass and Paur	BMD	Burrows	Bogumil	SCIA. revised
203	$5.64 \pm 3.7\%$	5.44	–	5.93	5.44	5.19
223	$5.89 \pm 3.3\%$	5.70	5.65	6.16	5.96	5.69
243	$6.30 \pm 1.8\%$	6.21	6.23	6.41	6.46	6.28
273	$7.42 \pm 2.9\%$	7.27	7.16	7.73	7.51	7.23
293	$8.30 \pm 0.7\%$	8.20	8.32	8.35	8.33	8.13

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Table 3. Comparison of integrated cross-sections in the Chappuis band (410–690 nm) in units of $10^{-19} \text{ cm}^2 \text{ nm molecule}^{-1}$.

Temperature [K]	Mean value	BMD	Burrows	Burk. Taluk.	Bogumil	SCIA revised
203	$6.48 \pm 1.6\%$	–	6.62	–	6.42	6.40
223	$6.35 \pm 2.4\%$	–	6.55	6.15	6.33	6.43
243	$6.35 \pm 1.7\%$	–	6.44	6.17	6.36	6.44
273	$6.44 \pm 2.3\%$	–	6.58	6.20	6.43	6.45
293	$6.38 \pm 1.6\%$	6.29	6.45	6.21	6.41	6.48

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Table 4. Direct comparison of SCIAMACHY FM revised data to literature data using a non-linear least square fitting program in the DOAS fitting window (325–335). The scaling factor and wavelength shifts indicated are the one that should be applied to the revised SCIAMACHY data in order to match the reference data.

Bass and Paur		BMD		SCIAMACHY FM		
	shift	ratio	shift	ratio	shift	ratio
225 K	−0.014	1.002	0.009	1.002	—	1.035
240 K	−0.012	1.003	0.008	1.006	—	1.036

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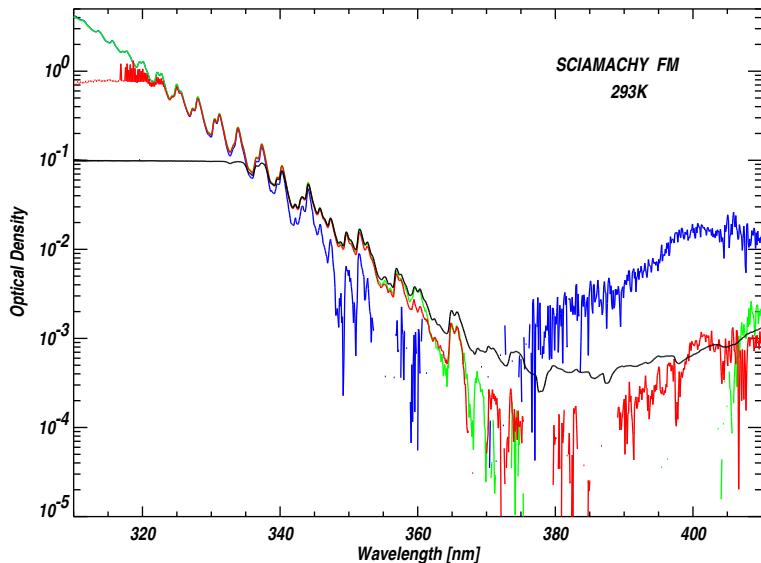


Fig. 1. Spectra of optical density obtained from four measurements in the Huggins band using different ozone concentrations and optical path lengths. Only limited regions of each spectrum are useful, as in most parts saturation is present or the optical density calculated is below the detection limit.

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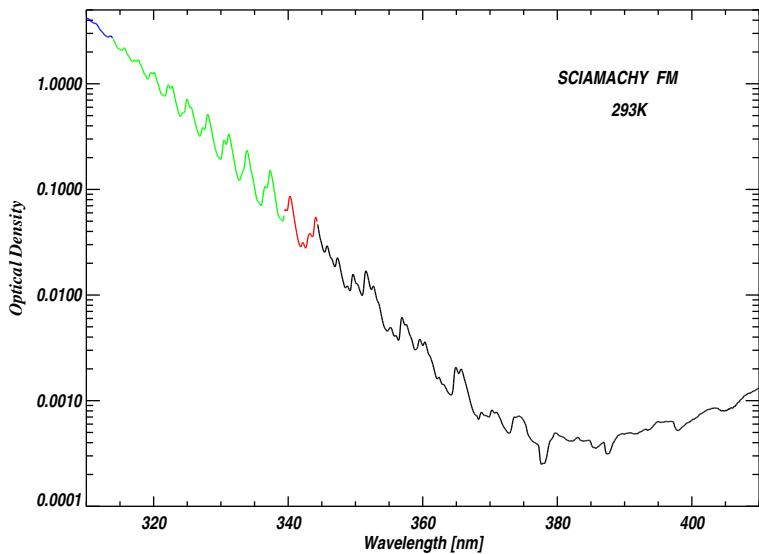


Fig. 2. Full spectra of ozone optical density (channel 2) obtained by concatenating the useful parts of each absorption measurement as indicated by different colors.

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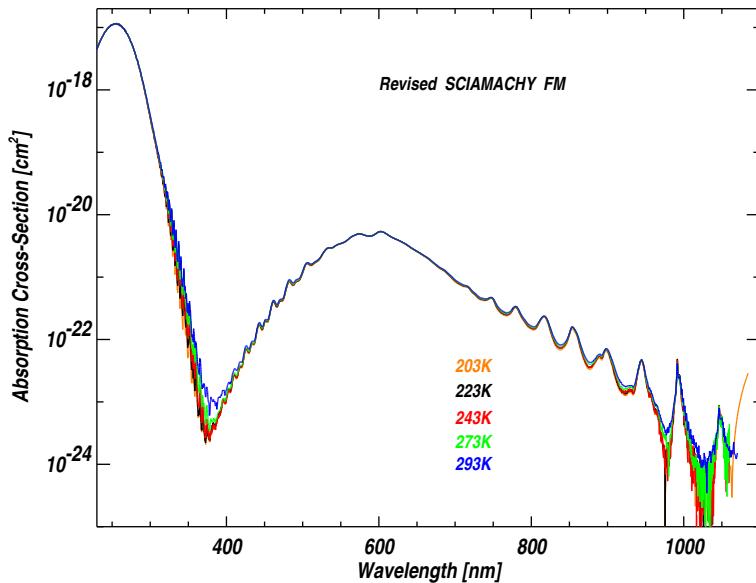


Fig. 3. Revised temperature dependent ozone absorption cross section spectra measured with the SCIAMACHY spectrometer (230–1070 nm). The cross section data cover the Hartley, Huggins Chappuis and the Wulf bands and were recorded at 203, 223, 243, 273, and 293 K.

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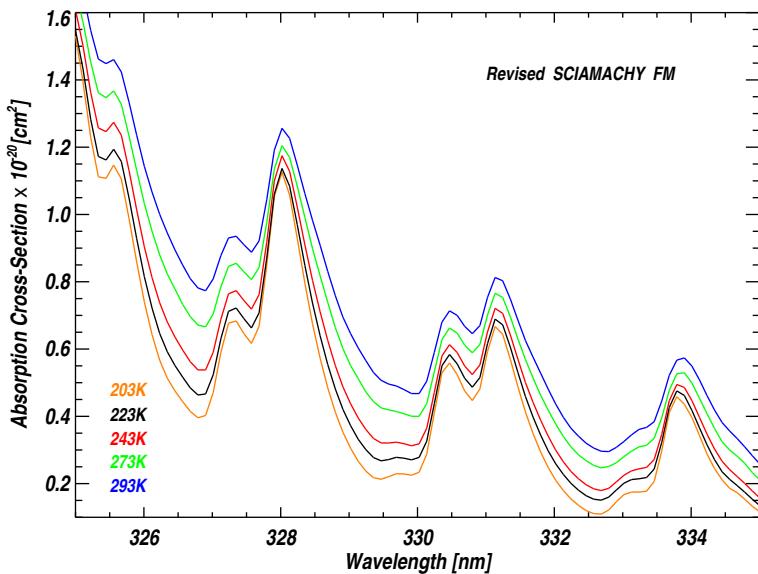


Fig. 4. Revised temperature dependent SCIAMACHY FM ozone absorption cross section spectra in the Huggins band.

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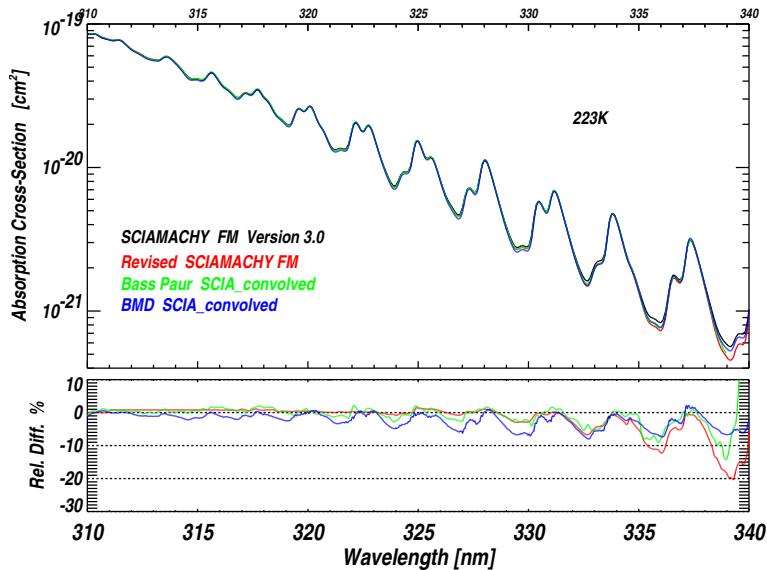


Fig. 5. Comparison between Bogumil et al. (2003) version 3.0 (black), revised (red), Bass and Paur (green) and BMD (blue) in the Huggins band (DOAS region). The amplitudes of the Bogumil et al. (2003) data are smaller compared to Bass and Paur, BMD and revised data. The lower sub-panels show the difference to the Bogumil et al. (2003) data.

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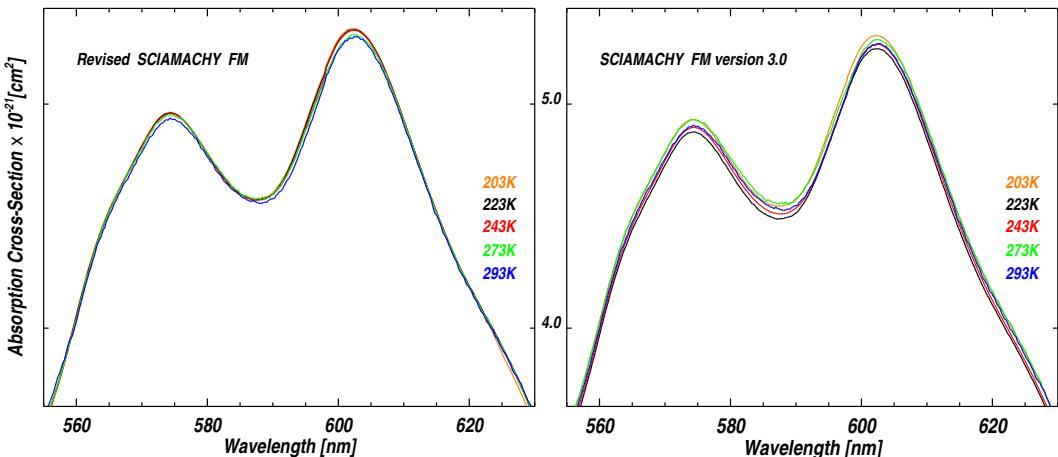


Fig. 6. Left panel: revised temperature dependent SCIAMACHY FM ozone absorption cross section spectra in the Chappuis band. Right panel: SCIAMACHY FM Version 3.0. The revised spectra preserve the correct temperature dependence.

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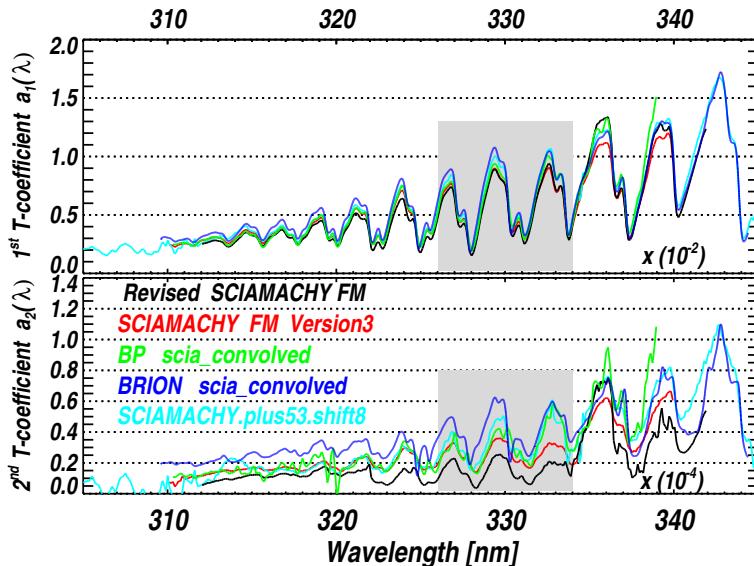


Fig. 7. Quadratic temperature coefficients ($a_1(\lambda)$ and $a_2(\lambda)$) in Eq. 2) for different ozone absorption spectra: SCIAMACHY revised and literature data convolved to SCIAMACHY slit function. The grey shaded area is the DOAS retrieval window. The cross-section labeled “SCIAMACHY.plus53.shift8” is the Bogumil spectra scaled by +5.3 % and shifted by 0.008 nm as used in the current SCIAMACHY WFDOAS retrieval (Weber et al., 2011).

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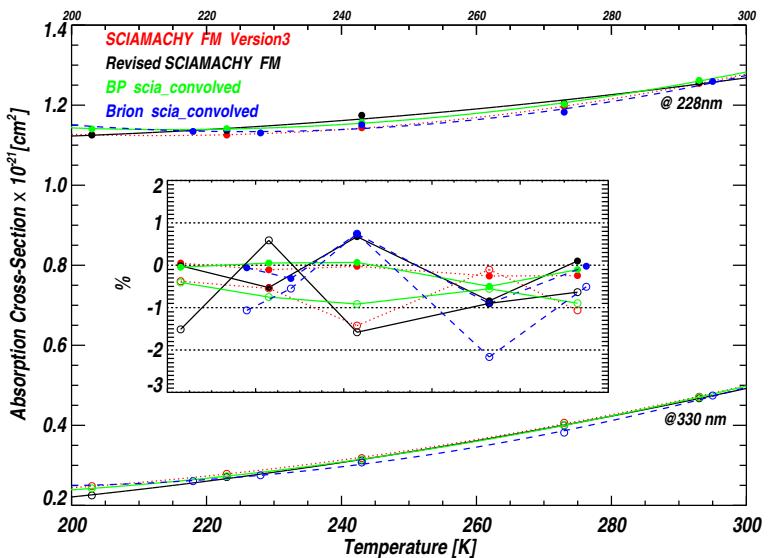


Fig. 8. Measured absorption cross-sections of SCIAMACHY FM and literature data convolved to SCIAMACHY spectral resolution at 328 and 330 nm. The differences between both are shown in the inlet.

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Fig. 9. Left panel: comparison of SCIAMACHY FM revised data with Bogumil et al. (2003) data (reference) at 225 K. Right panel: the revised SCIAMACHY FM data Bogumil et al. (2003) data and the residuals (orange) and the retrieved baseline polynomial (green) both shifted vertically for clarity.

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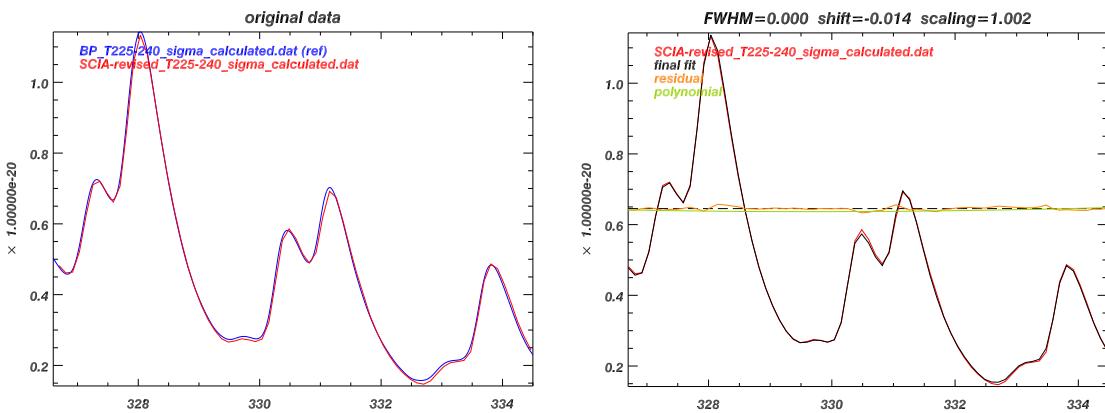


Fig. 10. Left panel: comparison of SCIAMACHY FM revised data with Bass and Paur data convolved with SCIAMACHY slit function at 225 K. Right panel: the revised SCIAMACHY FM revised data after proper wavelength shift and scaling together with Bass and Paur data and the residuals (orange) and the retrieved baseline polynomial (green).

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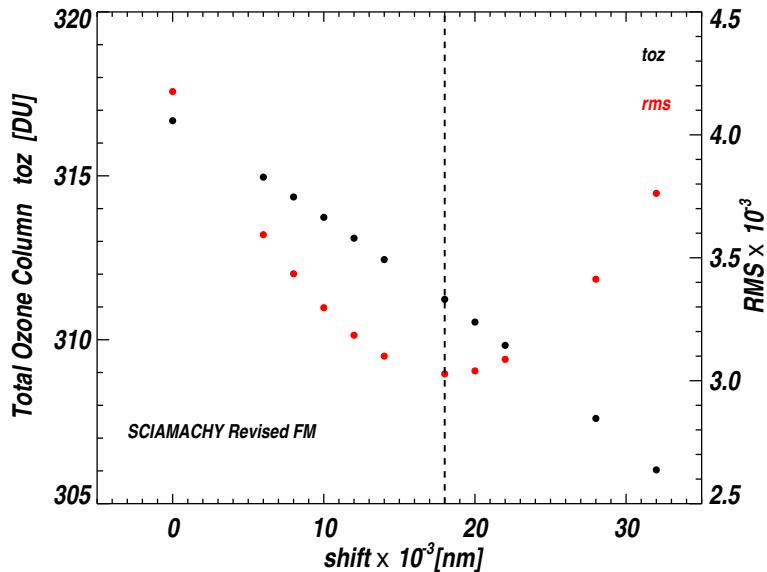


Fig. 11. Retrieved SCIAMACHY total ozone column and fit residuals (RMS) as a function of applied wavelength shifts to the revised SCIAMACHY FM cross sections. Minimum RMS is obtained at a shift of +0.018 nm.

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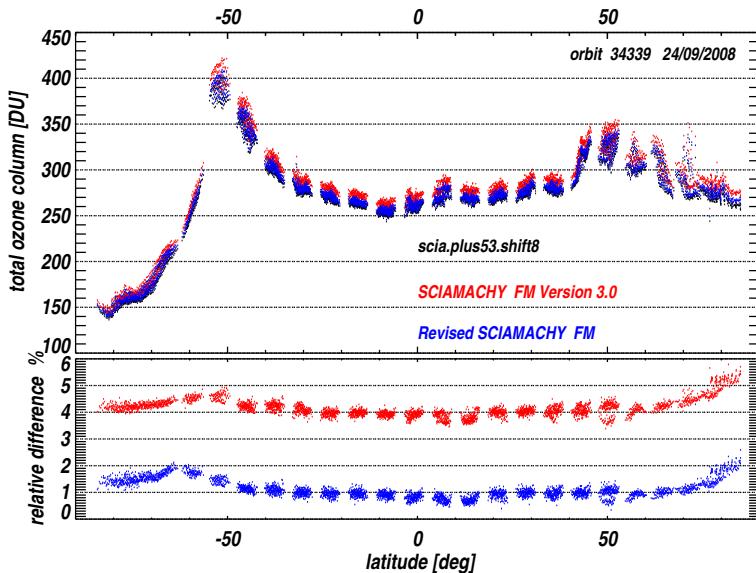


Fig. 12. SCIAMACHY's total ozone column retrievals with different cross section data for orbit 34339 (24 September 2008). Scia.plus53.shift8 is the SCIAMACHY FM data (Bogumil et al., 2003) with a differential scaling of +5.3 % and shift of 0.08 nm from a direct comparison to GOME FM cross-sections (Weber et al., 2011) as used in the current standard retrieval. The lower sub-panels show the difference to the retrieved ozone using scia.plus53.shift8 cross-sections.

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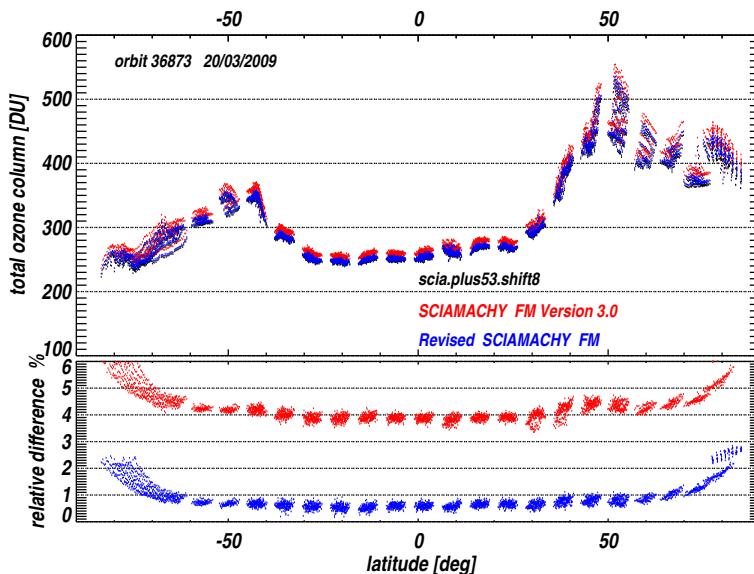


Fig. 13. Same as Fig. 12 for the orbit 36873 (20 March 2009).

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