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Spectroscopic parameters for ozone and its isotopes: recent measurements, outstanding issues, and prospects for improvements to HITRAN

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Abstract

In this article we review ozone spectroscopy from the microwave to the ultraviolet since the release of the 1996 HITRAN database. Uncertainties, deficiencies, areas of potential improvement, and anticipated new spectral line parameters datasets are highlighted.

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1. Introduction

Spectroscopic parameters for ozone are a key component of the High-resolution TRANsmission (HITRAN) database due to the importance of the molecule for remote sensing of the Earth's atmosphere at tropospheric to mesospheric altitudes and its impact on climate change [1–4]. Many past, currently operating, and planned experiments are designed for measuring O₃ from ground-based, airborne, and satellite-based platforms. The status of ozone spectroscopic parameters on the HITRAN compilation was last reviewed by Rinsland et al. [5] for the 1996 database [6]. Although spectroscopic parameters for ozone included in the HITRAN compilation have not changed since that time [7], there have been important studies reported in the literature. The goal of this paper is to summarize the work, discuss key aspects of the new data, describe areas of uncertainty in measurement and theory, identify remaining gaps, and provide a list of suggested updates and their availability for future HITRAN editions.

2. Recent thermal infrared studies

Since the release of the 1996 HITRAN edition, several groups have reported new sets of spectroscopic parameters for the thermal infrared region. The fundamental bands have been measured recently at high spectral resolution by Smith et al. [8], Claveau et al. [9], De Backer-Barilly and Barbe [10], and Wagner et al. [11]. A synthesis of these results was made by Flaud et al. [12], and the O₃ parameters derived from this synthesis appear in a database [13] used for analysis of the Michelson interferometer for passive atmospheric sounding (MIPAS) limb emission measurements [14]. Those measurements are recorded at 0.025 cm⁻¹ spectral resolution onboard the European ENVISAT platform launched in March 2002.

The measurements by Wagner et al. [11] cover the three ozone fundamentals and were recorded with a Bruker 120-HR Fourier transform spectrometer operating at spectral resolutions of 0.0011–0.0022 cm⁻¹, where resolution is defined as one divided by twice the maximum optical path difference of the interferometer. A total of 16 spectra were recorded at room temperature and 200 K with pure O₃-, N₂-, and O₂-broadened samples contained in a 24.9 cm path absorption cell. Scan time for recording individual spectra ranged from 100 to 200 min. A HgCdTe detector was used in the experiment with very small corrections applied to nearly eliminate the contribution of a weak out of band signal. The spectra were analyzed with the Fit Molecular Absorption Spectra (FitMAS) algorithm [15] to determine positions and intensities from the low pressure spectra and broadening coefficients from the pressure-broadened spectra.

The high spectral resolution and good signal-to-noise achieved ([11], Table 1) allowed improved Hamiltonian constants to be determined for the ¹⁶O₃ (0 1 0) and (1 0 0), (0 0 1) levels by combining the infrared measurements with precise microwave data from the literature. Measurements of the ¹⁶O₃ (0 2 0), (1 2 0), (0 2 1) and (2 0 0), (1 0 1), (0 0 2) states for the ¹⁶O¹⁶O¹⁸O and ¹⁶O¹⁸O¹⁶O isotopes were too limited to improve the previously determined molecular constant for the levels, and hence the generated linelist was determined from earlier studies. The list includes lines of ¹⁶O¹⁶O¹⁸O, ¹⁶O¹⁸O¹⁶O, ¹⁶O¹⁶O¹⁷O, and ¹⁶O¹⁷O¹⁶O, which are observable at high spectral resolution in the ν₃ region over long atmospheric paths (see [5], Section 4 for a summary of heavy ozone far infrared and infrared isotopic atmospheric measurements prior to 1998).

Table 1
Summary of $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ lines in the 4.8- μm region [37,38]

Band	$^{16}\text{O}^{18}\text{O}^{16}\text{O}$			$^{16}\text{O}^{16}\text{O}^{18}\text{O}$		
	$2\nu_3$	$\nu_1 + \nu_3$	$2\nu_1$	$2\nu_3$	$\nu_1 + \nu_3$	$2\nu_1$
Band centers ^a	1993	2049	2143	2028	2090	2172
J_{max}	56	60	47	52	57	55
$K_a \text{ max}$	17	18	12	15	16	13
Number of transitions	414	821	221	689	1063	1912

^aBand centers (cm^{-1}) do not coincide with the spectroscopic parameter E_{vv} in case of Darling–Dennison resonance according to theory in S&MPO [56].

In contrast to the theoretically calculated O_3 air-broadening coefficients on both HITRAN 1996 [6] and HITRAN 2000 [7] for the infrared bands [6,16], Wagner et al. [11] chose to model their measured broadening coefficients and their temperature-dependence assuming subbands follow a smooth variation in m , where $m = -J$ for P -branch transitions, and $m = J + 1$ for R -branch transitions. Their justification for the approach was the absence of a K_a dependence in their broadening coefficients larger than their measurement uncertainty, contrary to theoretical predictions [16], which are based on quantum Fourier transform theory. The large difference between the $J - K_a - K_c$ subbands in HITRAN was not found in the measured spectra [11]. Calculated air-broadening coefficients on HITRAN 1996 [6] for lines with rotational quantum numbers up to 35 were obtained by scaling calculated N_2 -broadening coefficients by a factor of 0.95, as recommended by Smith et al. [17] whereas the Wagner et al. [11] measurements suggest a scale factor ranging from 0.98 at low m to 0.96 at high m to reproduce their measured broadening coefficients.

Approximately 500, 400, and 1100 pressure-broadening coefficient measurements and 250, 200, and 500 measured temperature exponent coefficients were obtained for the ν_1 , ν_2 , and ν_3 bands, respectively, for both nitrogen and oxygen [11]. The dataset was least-squares fitted with statistical weightings based on measurement uncertainties to derive the database from the Bruker spectra. Details of the analysis are described by Wagner et al. [11], Section 6. Self-broadening was taken into account as part of the global fitting procedure. Differences between the HITRAN 1996 and Wagner et al. [11] air-broadening coefficients at 296 K are as large as 15%. The temperature dependence of the broadening coefficients was modeled as a function of m assuming the temperature dependence is smooth. The nitrogen- and oxygen-broadened spectra were fitted separately for the individual bands. HITRAN currently assumes 0.76 for the temperature dependence of the air-broadening coefficient of all lines, a mean recommended by Gamache et al. [18] from his calculations for 126 transitions for temperatures of 200–500 K. Values for this coefficient in the Wagner et al. [11] database range from 0.71 to 0.84.

Broadening coefficients for common sets of quantum numbers with respect to measurements obtained with the Fourier transform spectrometer on Kitt Peak in the ν_1 [19] and ν_2 bands [20] show agreement to within two-sigma uncertainty, though the widths from the Kitt Peak measurements are systematically smaller than those measured by Wagner et al. [11]. These discrepancies remain unexplained as the Kitt Peak instrument function is precisely known. Wagner et al. [11] noted better

agreement between their new laboratory results with respect to diode laser measurements [17] than the Kitt Peak Fourier transform measurements.

Measurements of self-, air-, and oxygen-broadening coefficients of pure rotation ozone lines and the temperature dependence of the coefficients have been reported recently from 14 pure rotational spectra recorded at 0.004-cm^{-1} resolution with a Fourier transform spectrometer at temperature between 212 and 296 K by Larsen et al. [21]. After accounting for effects of systematic errors, mean relative uncertainties of the 296 K broadening coefficients were $\sim 2\%$ for self-, air-, and N_2 -broadening. The authors conclude that the 296 K air-broadening coefficients on the HITRAN 2000 database (same as those from 1996) agree with the results of their study only for values of $J \leq 8$ and values of $J \geq 25$. For the range $8 \leq J \leq 25$ the HITRAN values are 13% lower than the pure rotation measurements. The HITRAN values average 6% lower than the pure rotation measurements. Although not discussed extensively, the K dependence of the air-broadening coefficients at fixed J was observed to be small (see their Fig. 5). Aside from small systematic deviations of the order of 2% the agreement with the ν_1 and ν_2 (same selection rules as rotational transitions) broadening parameters of Wagner et al. [11] is quite good, indicating that the vibrational dependence of the pressure broadening parameters is rather weak.

The intensities reported by Wagner et al. [11] are the measured intensities and calculated values predicted with the model [22]. The average ratio of the integrated intensities for the $^{16}\text{O}_3$ lines in the overlapping ν_1/ν_3 region equaled 0.972 times the value reported on the HITRAN 1996 database [6]. The measured total intensities are consistent with the values by De Backer-Barilly and Barbe [10] and Claveau et al. [9] to 1.6%. As the line intensities generated recently at $10\text{-}\mu\text{m}$ (Flaud et al. [12]) equal 0.958 and 0.966 times the values reported on the HITRAN 1996 database [6] for the ν_1 and ν_3 bands, respectively, intensities of all lines in the shorter wavelength regions currently on HITRAN [6,22] need to be reduced by similar scale factors to maintain consistency throughout the infrared in the database.

In contrast, the intensities derived from the laboratory spectra analyzed by Smith et al. [8] average 1% higher than those on HITRAN 1996 [6]. These measurements were recorded at room temperature and 0.0027 cm^{-1} resolution with dual liquid-helium cooled As-doped silicon detectors with the Kitt Peak Fourier transform spectrometer. A cross cell was employed with a UV-absorption monitor of the same design as used by Pickett et al. [23] to monitor the absorption at 254 nm. Ozone pressures were maintained between 0.3 and 0.5 Torr to avoid saturation. Intensities for a total of 376 lines were reported based on a simultaneous nonlinear least-squares analysis [24] of the 4 measured spectra. Of the total, 366 were in the ν_3 band with the remainder in the ν_1 band. Estimated total uncertainties of 2% include the uncertainty in the assumed 254-nm UV cross section.

Differences in the integrated $10\text{-}\mu\text{m}$ intensities reported by the 3 groups [8–11] of up to several percent and similar differences in reported air-broadening coefficients for similar rotational transitions in the far- [21] and mid-infrared [19,20] raise concerns about systematic errors and highlight the difficulty in selecting parameters to incorporate into the HITRAN database. For the present, we recommend replacing the rotational and temperature dependence of the air-broadening coefficients at 296 K currently on HITRAN with the smooth best-fit values determined by Wagner et al. [11]. Further experiments are needed to understand and resolve discrepancies, and additional comparison of the intensities and air-broadening coefficients of pure rotation lines (with intensities that can be computed from theory) with infrared results (including when necessary correction for residual thermal emission) are needed to guide future HITRAN updates and quantify uncertainties.

Table 2
Summary of $^{16}\text{O}_3$ bands in the range 4000–6000 cm^{-1} analyzed by the University of Reims group

Band	Band center (cm^{-1})	Integrated intensity ^a	Spectral range (cm^{-1})	Reference
$2\nu_1 + 2\nu_3$	4141	11.75	4034–4207	Barbe and Plateaux [45]
$3\nu_1 + \nu_3$	4250	25.1	4178–4264	Barbe et al. [46]
$2\nu_2 + 3\nu_3$	4346	23.6	4276–4370	Barbe et al. [47]
$\nu_1 + \nu_2 + 3\nu_3$	4658	88.4	4562–4669	Mikhailenko et al. [48]
$2\nu_1 + 3\nu_3$	5077	13.3	4997–5086	Barbe et al. [49]
$\nu_1 + 2\nu_2 + 3\nu_3$	5291	6.3	5216–5301	Barbe et al. [50]
$4\nu_1 + \nu_3$	5307	8.5	5244–5320	Barbe et al. [50]
$\nu_2 + 5\nu_3$	5518	9.3	5444–5527	Barbe et al. [51]
$2\nu_1 + \nu_2 + 3\nu_3$	5697	3.1	5625–5705	Barbe and Chichery [52]
$\nu_1 + 5\nu_3$	5783	4.6	5708–5791	Chichery et al. [53]

^aIn units of $\text{cm}^{-1}/(\text{molecule cm}^{-2})$ at $296 \text{ K} \times 10^{23}$.

Air-broadened shift coefficients are set to zero for all lines in both the HITRAN 1996 [6] and the Wagner et al. [11] databases. Measurements of air-induced pressure-induced shift coefficients in the ν_2 ([20], Table 2) and ν_1 bands ([17], Table 2; [19], Table 4) are small at atmospheric temperatures (about $-0.001 \text{ cm}^{-1} \text{ atm}^{-1}$). Larger pressure-induced shift coefficients have been measured in the 3.3–3.6 μm region, where average room-temperature values are $-0.007 \text{ cm}^{-1} \text{ atm}^{-1}$ [25]. Hence, shifts should be included in future HITRAN updates at least for this shorter wavelength region.

Self-broadening coefficients for O_3 on HITRAN are based on an empirical polynomial expression derived from least-squares fits to 355 lines in 5 different infrared bands as a function of J'' and K_a'' [26]. Although there is no theoretical justification for the expression, Larsen et al. [21] found their pure rotation measurements agreed with the relation, averaging only 3.5% lower than their measured values.

New spectra of natural abundance ozone have been recorded with 0.003 cm^{-1} apodized resolution with path length of 12 m in the fundamental regions by the group at the University of Reims. The analysis has resulted in increased observed quantum numbers range (J from 65 to 82 and K_a up to 22, respectively, for ν_3 and ν_2 band). A more accurate modeling of high J , K_a levels and transitions is currently in progress [27]. The results will be made available for future editions of HITRAN and also will appear in the spectroscopy and molecular properties of ozone databank (S&MPO) maintained by the Reims group and their coworkers, which is devoted to ozone (see Sections 3–5).

3. The 1300–1500 cm^{-1} spectral region

A first analysis of $^{16}\text{O}_3$ lines in the 1300–1500 cm^{-1} region was derived from ATMOS stratospheric solar occultation spectra recorded at 0.01 cm^{-1} resolution [28], which were limited to $J=37$ and $K_a=8$ for the $2\nu_2$ band. Barbe et al. [29] analyzed this spectral range using long absorption path laboratory spectra recorded with a signal-to-noise of 500 at a spectral resolution of 0.007 cm^{-1} . The $2\nu_2$ band lines are now measured to J values up to 57 and K_a values up to 16, leading to

improvements in the Hamiltonian parameters for this band. A fit on 268 line intensities allows 3 transition moment parameters to be obtained. A complete calculation with J up to 65 and K_a up to 20 leads to the integrated band intensity $S(2\nu_2) = 5.328 \times 10^{-22} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ at 296 K, with a minimum cutoff of 2×10^{-26} (same units). In addition, the weak hot band $3\nu_2 - \nu_2$ was measured for the first time. The observed $\nu_1 + \nu_3 - \nu_2$ hot band confirms, within experimental accuracy, the values for intensities already included in HITRAN. All these files have been submitted to HITRAN for inclusion in a future database update.

4. Positions and intensities at 4.8 μm

As summarized by Rinsland et al. [5], the current HITRAN database covering 4.8 μm contains only lines of $^{16}\text{O}_3$ bands based on the analysis of laboratory spectra recorded at 0.005 cm^{-1} spectral resolution [30,31]. This spectral range was analyzed at Reims previously from spectra recorded at 0.0018 cm^{-1} resolution [32]: 638 measured intensities of non-blended lines of the $2\nu_1$, $\nu_1 + \nu_3$ and $2\nu_3$ bands have been modeled theoretically with a RMS deviation of 2.4% that represents a considerable improvement for ozone data in this region. The calculated list has been included into the GEISA-IASI data bank [33]. Note that a further improvement of the $^{16}\text{O}_3$ bands in this spectral range is in progress by the S&MPO group [27], accounting for extrapolated resonance perturbations and newly measured weak transitions.

The integrated intensity of the 3 interacting bands $\nu_1 + \nu_3$, $2\nu_1$, and $2\nu_3$ and their hot bands is about one third as strong as the combined intensity of the 10- μm bands. As lines of $^{16}\text{O}^{16}\text{O}^{18}\text{O}$, $^{16}\text{O}^{18}\text{O}^{16}\text{O}$, $^{16}\text{O}^{16}\text{O}^{17}\text{O}$, and $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ have been identified in 10- μm atmospheric spectra, the same isotopomer species can be expected to be detectable in high spectral resolution ground-based and limb 4.8- μm atmospheric spectra. Recent laboratory work and the reported atmospheric detections are discussed below.

4.1. $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ and $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ isotopomers

A first calculation of the $\nu_1 + \nu_3$ band of $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ and $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ [34] was followed by identification of atmospheric spectral features of these bands [35,36]. Since that time, a systematic study of ^{18}O -enriched isotopomers in the 4.8- μm region has been undertaken in the Reims laboratory to improve on previous studies. Spectra of various mixtures have been recorded recently at 0.003 cm^{-1} resolution using large pressure-path length products (path lengths of 31, 300 or 1200 cm). Assignment of the 3 interacting bands $2\nu_3$, $\nu_1 + \nu_3$ and $2\nu_1$ of all isotopomer species $^{16}\text{O}^{16}\text{O}^{18}\text{O}$, $^{16}\text{O}^{18}\text{O}^{16}\text{O}$, $^{18}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ have been obtained. The range of quantum numbers for observed transitions is given in Table 1 for the two isotopic species of atmospheric interest. Transition moment parameters have been derived from observed intensities for the 3 bands. This allows a complete calculation of the 3 interacting bands for $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ [37] and $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ [38] to be performed, which will be soon incorporated in the S&MPO data bank. The relative accuracy for intensity is about 4%. However, due to the difficulty of quantification of partial pressures for various isotopomers, the absolute uncertainty determination is estimated to be in the range 10–15%.

4.2. $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ and $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ isotopomers

New 0.002 cm^{-1} resolution laboratory spectra [39] have led to the assignment of $\nu_1 + \nu_3$ bands of both ^{17}O isotopomers. The calculation was performed taking account of the Coriolis resonance interactions coupling the observed (1 0 1) state and (0 0 2), (2 0 0) dark states, as the $2\nu_1$ and $2\nu_3$ bands have not yet been observed. The intensities of the isotopic transitions have been computed assuming the transition moments calculated for the main isotope since an approach transferring the transition moments from the main to the isotopic species is theoretically debatable. As a consequence those results are likely to be correct to within several percent for lines of $\nu_1 + \nu_3$. In fact the intensities calculated for individual transitions of the isotopic lines may have errors of up to 15–20%. For these isotopomers, a set of parameters has been generated [13] and will be included in future editions of HITRAN.

Lines of the $\nu_1 + \nu_3$ $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ and $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ bands have been identified recently by Goldman et al. [40] in the $5\text{-}\mu\text{m}$ region of the same set of University of Denver balloon-borne solar absorption spectra, which were recorded at a spectral resolution of 0.003 cm^{-1} . A few of the lines are also observed in ground-based solar absorption spectra. A best set of isolated $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ and $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ lines suitable for quantitative analysis from balloon-borne and ground-based solar spectra has been prepared (see [40], Table 1).

5. The $4.1\text{ }\mu\text{m}$ spectral range of $^{16}\text{O}_3$

This spectral range corresponds to the $2\nu_2 + \nu_3$ and $2\nu_2 + \nu_1$ bands. Spectra recorded and assigned in the GSMA laboratory, Reims [41,42], lead to improvement for positions and intensities with respect to the previous work of Rinsland et al. [43]. The new calculation and molecular parameters are now incorporated in the S&MPO databank.

6. Near infrared line-by-line studies

As summarized previously ([5], Table 1), the current set of HITRAN parameters for O_3 extends from the microwave to the $2.5\text{-}\mu\text{m}$ region based primarily in the infrared on laboratory spectra recorded with the Fourier transform spectrometer at the US National Solar Observatory (NSO) on Kitt Peak. However, since that time a systematic, high spectral resolution analysis has been performed for the bands of $^{16}\text{O}_3$ between 4000 and 6000 cm^{-1} . Except for the analysis of Perrin et al. [44], which relied in part on spectra from NSO, all subsequent results were obtained with the Reims high Fourier transform spectrometer.

Table 2 summarizes the band assignments, integrated intensities, and provides reference to the published S&MPO work [45–53]. The bands have been observed with large pressure-path length products. Results of this work are now available in the S&MPO databank. This data bank is accessible on two websites: <http://ozone.univ-reims.fr> and <http://ozone.iao.ru> [54–56]. A reference list of publications on high and low resolution spectra, related theory, molecular properties and applications are regularly updated at the S&MPO sites.

The analyses take into account the many rovibrational resonances with dark states, and the resulting calculated line parameters list has a minimum intensity cutoff of $3 \times 10^{-26} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ at 296 K. Note that, despite their weakness, many lines may interfere with other atmospheric trace gases. All these results will be later incorporated into the HITRAN database.

As an example of additional results from spectra recorded in Reims, the 2.1- μm region was analyzed based on 0.008-cm^{-1} resolution laboratory spectra [57]. These results together with those derived from the analysis of the $\nu_1 + 4\nu_3 - \nu_3$ hot band in the 2.5- μm region were used to derive a large set of energy levels for the vibrational states (0 0 5), (3 1 1), and (1 0 4), which were then fitted and used to generate a comprehensive list of line intensities and positions.

Similarly, as described by Mikhailenko et al. [58], an improved set of positions and intensities has been generated for $2600\text{--}2900 \text{ cm}^{-1}$ from Reims spectra recorded at a spectral resolution of 0.005 cm^{-1} . The measurements extend the range of J and K_a with respect to the previous assignments used to generate the HITRAN list for this region [59]. The new set of positions and intensities for the triad of interacting cold bands absorbing in the region has been supplied to HITRAN for inclusion in its next update.

7. Absorption cross sections

The 1996 HITRAN compilation did not include separate files of O_3 absorption cross sections ([5], Section 3.6). Recommendations were made to include absorption cross-section files of several sets of UV measurements, Huggins band measurements, several sets of Chappuis visible band measurements, Wulf band measurements, and sets of high sensitivity measurements extending beyond 2- μm . At this time, only a set of ultraviolet cross sections has been provided for a future HITRAN update.

Ultraviolet cross sections for HITRAN derived from the measurements of Bass and Paur [60,61] are further discussed by Orphal and Chance [62]. These high-resolution measurements cover all atmospheric temperatures and are in very good agreement with other data particularly above 218 K [63,64] (see [65] and references therein). However, while the latter measurements contain less systematic wavelength calibration errors, they are not available at lower temperatures. We next summarize the ultraviolet data for HITRAN.

The Bass and Paur data provide a quadratic parameterization for the cross sections from 245 to 343 nm (air wavelengths are given) with a spectral resolution of less than 0.025 nm and wavelength uncertainties given as 0.025 nm. This range covers most of the Hartley–Huggins bands. The cross sections are re-calibrated in wavelength by first converting to vacuum wavelengths using the Edlén [66] refractive index formula and then fitting to the Voigt et al. [67] FTS O_3 measurements to obtain an addition shift of +0.015 nm. Final wavelength uncertainties are 0.040 nm.

The temperature parameterized values on the measured wavelength grid are given in a supplemental file, with wavelength values in air and in vacuum. The primary HITRAN values are cross-sections calculated at a range of temperatures from 200 to 300 K interpolated to an even wavenumber increment.

We next consider the status of Chappuis band cross-sections. The available laboratory cross sections agree in showing very small or no changes in the peak cross sections between 550 and 650 nm with temperature, and there also is also good agreement concerning the increase in the differential structure with decreasing temperature [65]. However, the four temperature-dependent sets of cross

sections [67–70] are systematically higher than the data from two other studies [71,72]. The two latter datasets sets agree closely, but do not cover temperatures down to 203 K. Hence, we do not recommend a set of Chappuis band cross sections for inclusion in HITRAN at this time.

The recent cross section measurements with the SCIAMACHY pre-flight model [68] extend to the near-infrared and cover for the first time the Wulf bands (675–1075 nm) at more than two temperatures. This study is an example of important new work on O₃ cross sections at the longer wavelengths of relevance to ongoing remote sensing projects and potentially available for a future HITRAN update.

Re-measurement of ozone cross sections in the ultraviolet and visible remains the highest priority for atmospheric spectroscopy [73]. Accurate values for the atmospheric range of temperatures, at high spectral resolution and without systematic differences among values for the different electronic absorption bands are required particularly for the growing fleet of satellite-based ozone measuring instruments to provide accurate determination of stratospheric ozone trends.

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