O_3 UV-Vis absorption cross-sections

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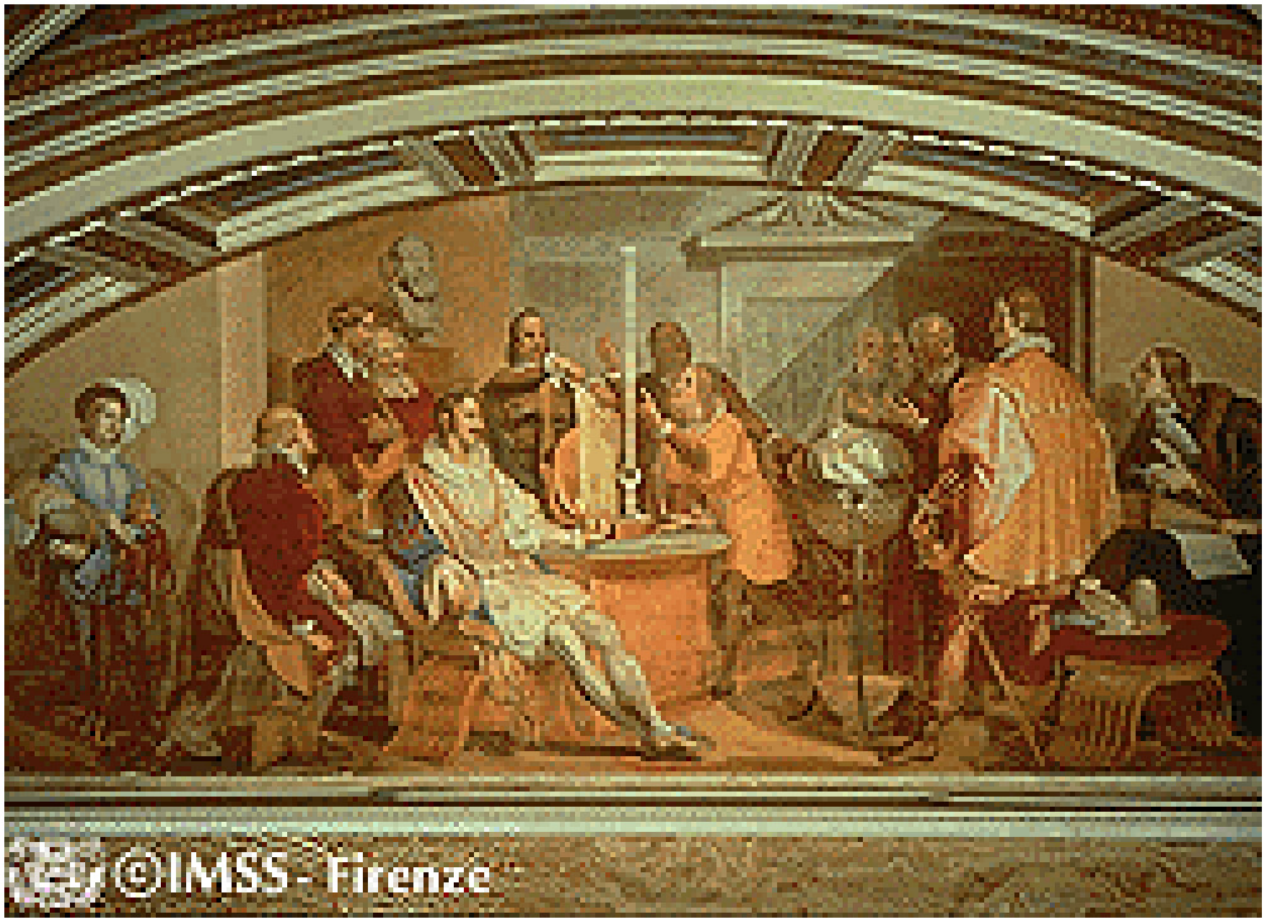
Topics

1. "New" O_3 cross-sections since 1999
2. "Critical Review" for ESA (2003)
3. Are the O_3 reference data consistent ?
4. Recommendations

It took nearly 250 years from the invention of the thermometer to the definition of a generally accepted temperature standard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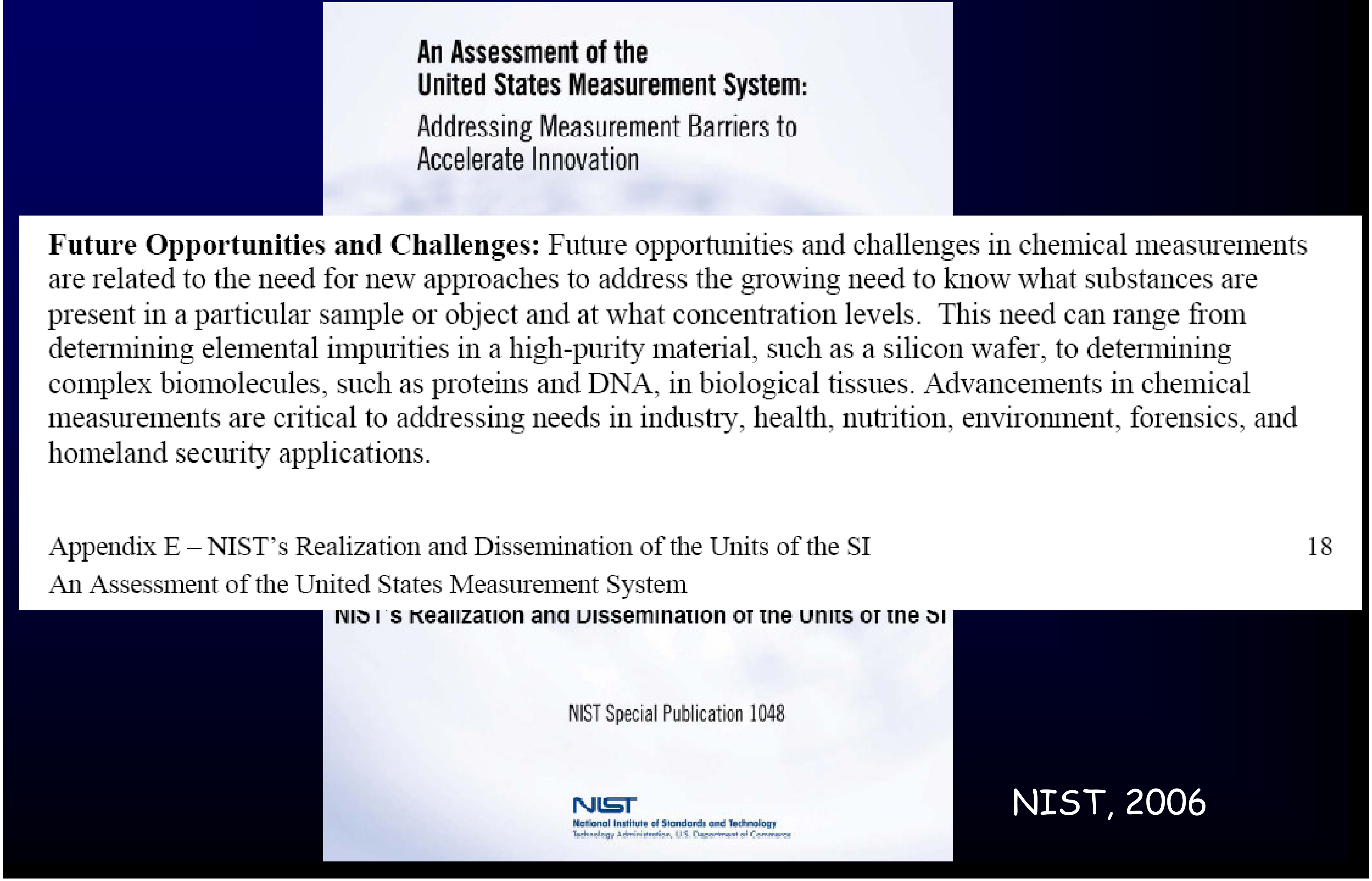
There is general need for chemical standards



An Assessment of the United States Measurement System:
Addressing Measurement Barriers to Accelerate Innovation

Future Opportunities and Challenges: Future opportunities and challenges in chemical measurements are related to the need for new approaches to address the growing need to know what substances are present in a particular sample or object and at what concentration levels. This need can range from determining elemental impurities in a high-purity material, such as a silicon wafer, to determining complex biomolecules, such as proteins and DNA, in biological tissues. Advancements in chemical measurements are critical to addressing needs in industry, health, nutrition, environment, forensics, and homeland security applications.

Appendix E – NIST's Realization and Dissemination of the Units of the SI 18
An Assessment of the United States Measurement System

NIST's Realization and Dissemination of the Units of the SI

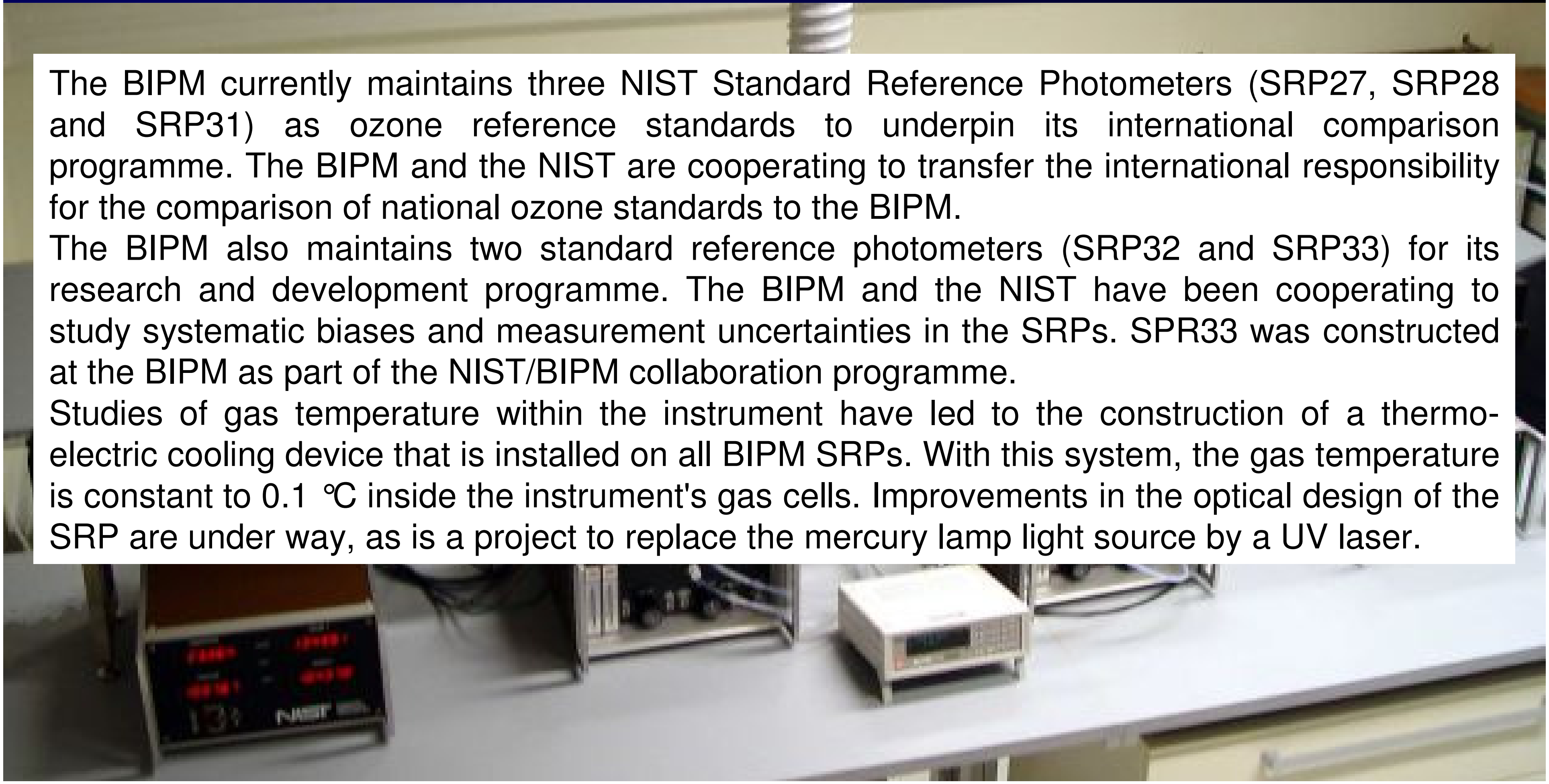
NIST Special Publication 1048

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

NIST, 2006

There is general need for chemical standards

The BIPM is establishing an international programme to ensure the equivalence of national ozone standards underpinning the international comparability of ground-level ozone measurements. Until March 2005 it was the coordinating laboratory for the CCQM pilot study CCQM-P28; it is now coordinating the key comparison BIPM.QM-K1 for ozone at ambient level.



The BIPM currently maintains three NIST Standard Reference Photometers (SRP27, SRP28 and SRP31) as ozone reference standards to underpin its international comparison programme. The BIPM and the NIST are cooperating to transfer the international responsibility for the comparison of national ozone standards to the BIPM.

The BIPM also maintains two standard reference photometers (SRP32 and SRP33) for its research and development programme. The BIPM and the NIST have been cooperating to study systematic biases and measurement uncertainties in the SRPs. SPR33 was constructed at the BIPM as part of the NIST/BIPM collaboration programme.

Studies of gas temperature within the instrument have led to the construction of a thermo-electric cooling device that is installed on all BIPM SRPs. With this system, the gas temperature is constant to 0.1 °C inside the instrument's gas cells. Improvements in the optical design of the SRP are under way, as is a project to replace the mercury lamp light source by a UV laser.

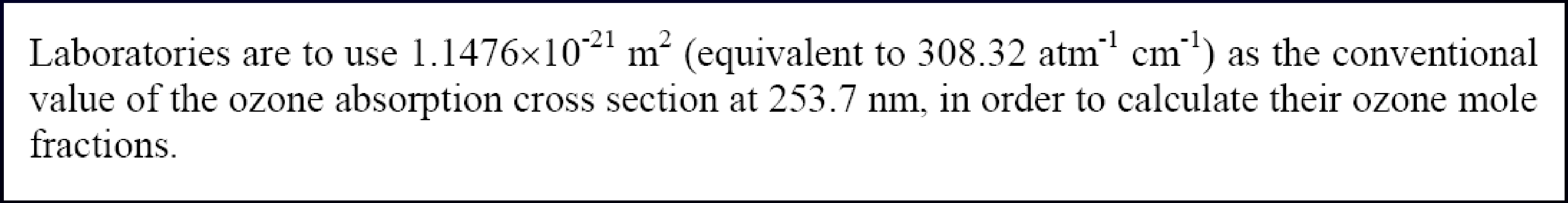
There is general need for chemical standards

The BIPM is establishing an international programme to ensure the equivalence of national ozone standards underpinning the international comparability of ground-level ozone measurements. Until March 2005 it was the coordinating laboratory for the CCQM pilot study CCQM-P28; it is now coordinating the key comparison BIPM.QM-K1 for ozone at ambient level.

Protocol for the Key Comparison BIPM.QM-K1, Ozone at ambient level

Coordinating laboratory: Bureau International des Poids et Mesures

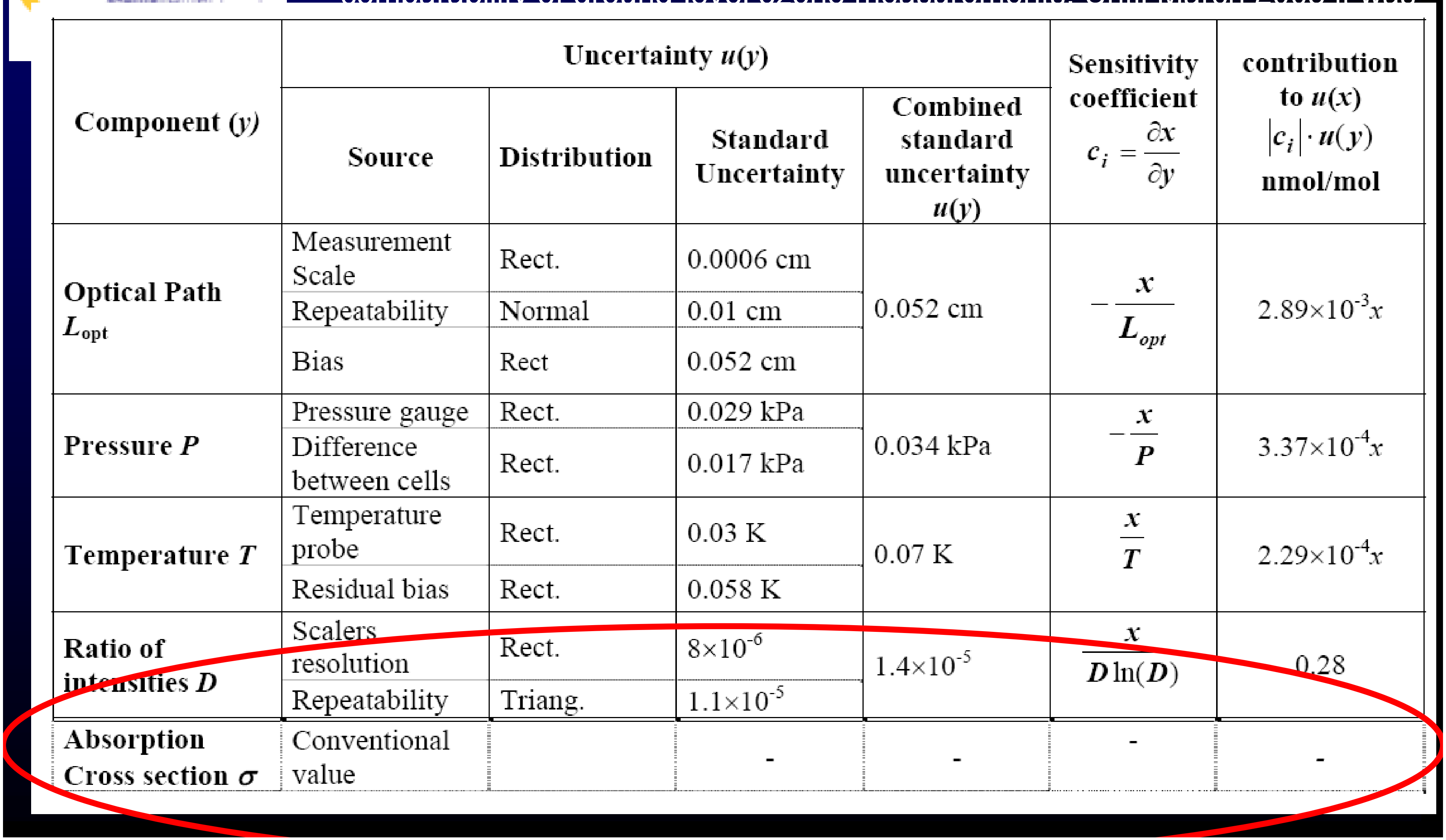
Contact person: Joële Viallon, BIPM, Pavillon de Breteuil, F-92312 France
email: jviallon@bipm.org, Tel: +33 1 45 07 62 70, Fax: +33 1 45 07 20 21.



Laboratories are to use 1.1476×10^{-21} m^2 (equivalent to 308.32 atm^{-1} cm^{-1}) as the conventional value of the ozone absorption cross section at 253.7 nm, in order to calculate their ozone mole fractions.

There is general need for chemical standards

The BIPM is establishing an international programme to ensure the equivalence of national ozone standards underpinning the international comparability of ground-level ozone measurements. Until March 2005 it was

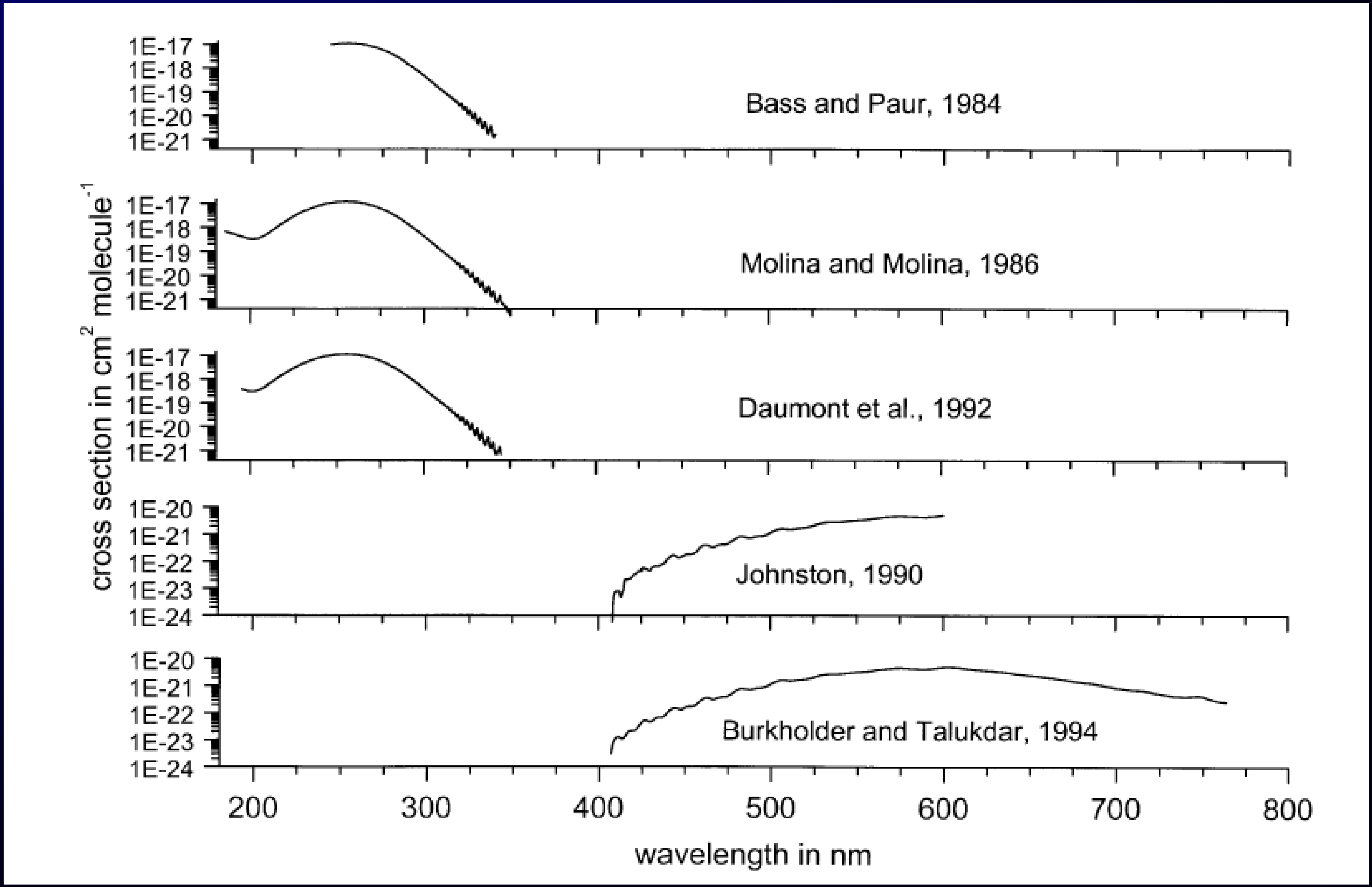


Component (y)	Uncertainty $u(y)$				Sensitivity coefficient $c_i = \frac{\partial x}{\partial y}$	contribution to $u(x)$ $\lvert c_i \rvert \cdot u(y)$ nmol/mol
	Source	Distribution	Standard Uncertainty	Combined standard uncertainty $u(y)$		
Optical Path L_{opt}	Measurement Scale	Rect.	0.0006 cm	0.052 cm	$-\frac{x}{L_{opt}}$	$2.89\times10^{-3}x$
	Repeatability	Normal	0.01 cm			
	Bias	Rect	0.052 cm			
Pressure P	Pressure gauge	Rect.	0.029 kPa	0.034 kPa	$-\frac{x}{P}$	$3.37\times10^{-4}x$
	Difference between cells	Rect.	0.017 kPa			
Temperature T	Temperature probe	Rect.	0.03 K	0.07 K	$\frac{x}{T}$	$2.29\times10^{-4}x$
	Residual bias	Rect.	0.058 K			
Ratio of intensities D	Scalers resolution	Rect.	8×10^{-6}	1.4×10^{-5}	$\frac{x}{D\ln(D)}$	0.28
	Repeatability	Triang.	1.1×10^{-5}			
Absorption Cross section σ	Conventional value		-	-	-	-

1. "New" O_3 cross-sections since 1999

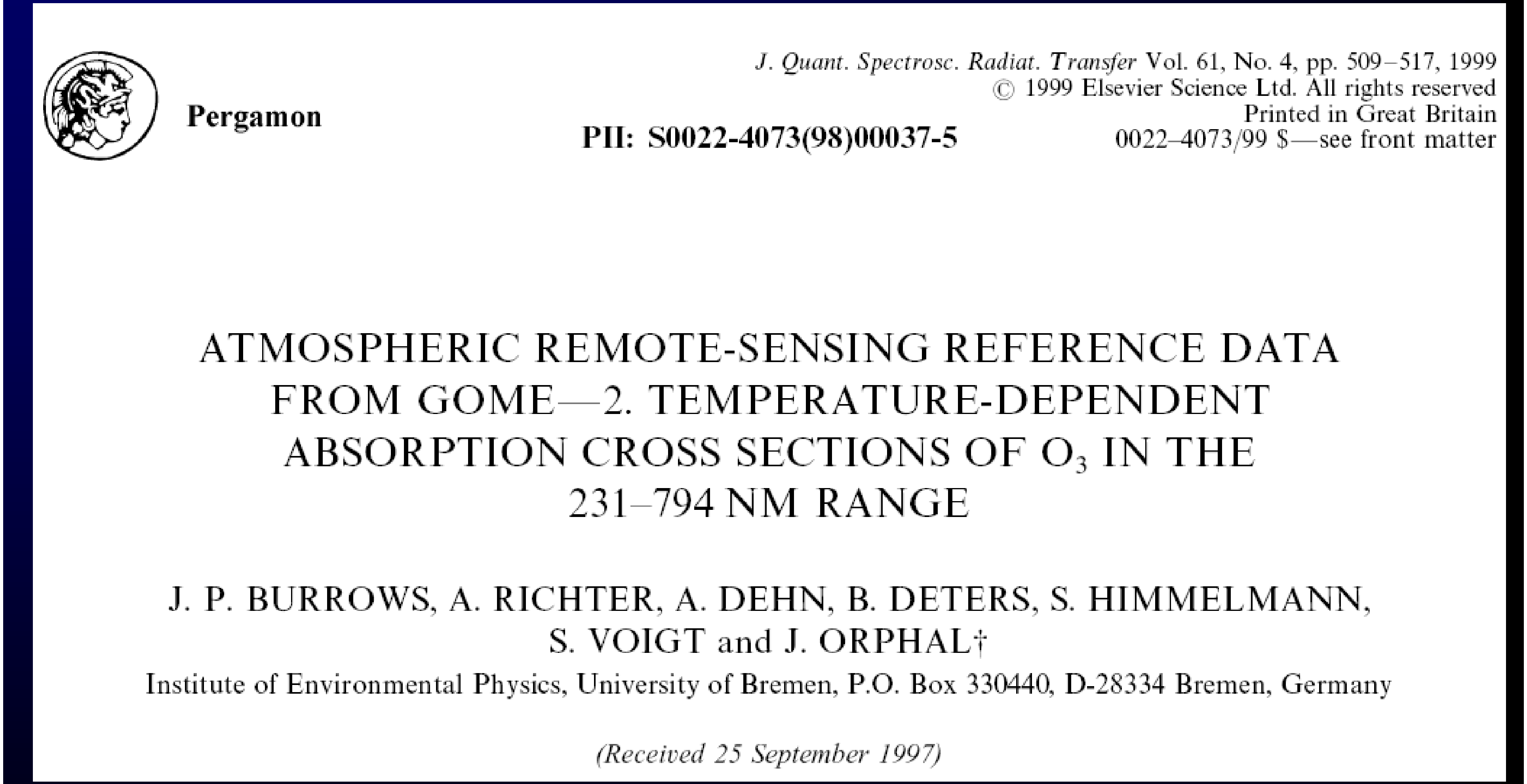
- GOME FM: Burrows et al., JQSRT 1999
- UV-FTS: Voigt et al., JPP-A 2001
- SCIAMACHY PFM: Bogumil et al., JPP-A 2003
- GOME-2 FMs: Gür et al., Report to ESA, 2005

O_3 broad-band cross-sections before 1995



O_3 cross-sections from GOME – FM (1999)

O_3 cross-sections from GOME (1999)



Pergamon

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0022–4073/99 $—see front matter

PII: S0022-4073(98)00037-5

ATMOSPHERIC REMOTE-SENSING REFERENCE DATA FROM GOME—2. TEMPERATURE-DEPENDENT ABSORPTION CROSS SECTIONS OF O_3 IN THE 231–794 NM RANGE

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(Received 25 September 1997)

O_3 cross-sections from GOME (1999)

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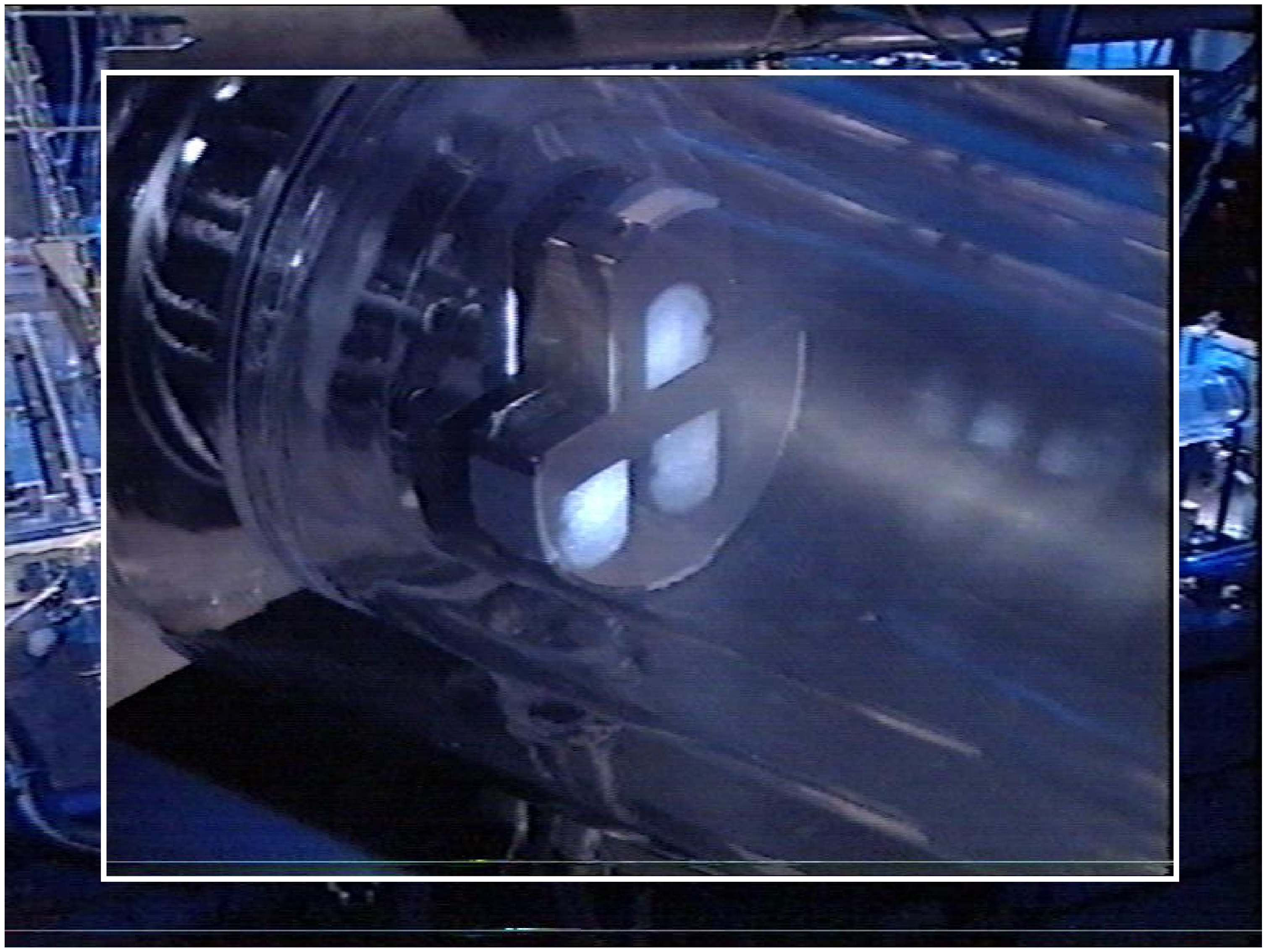
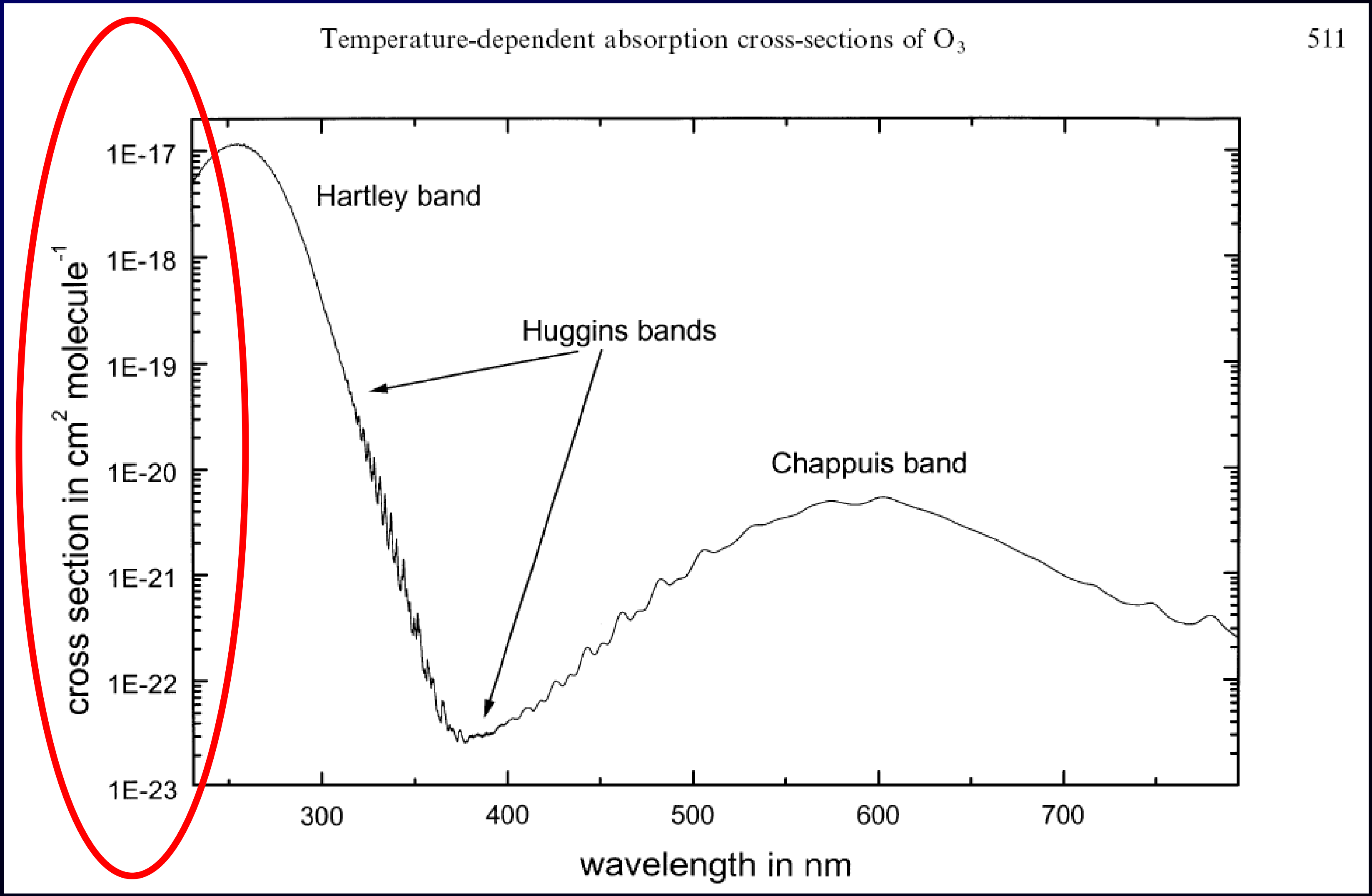


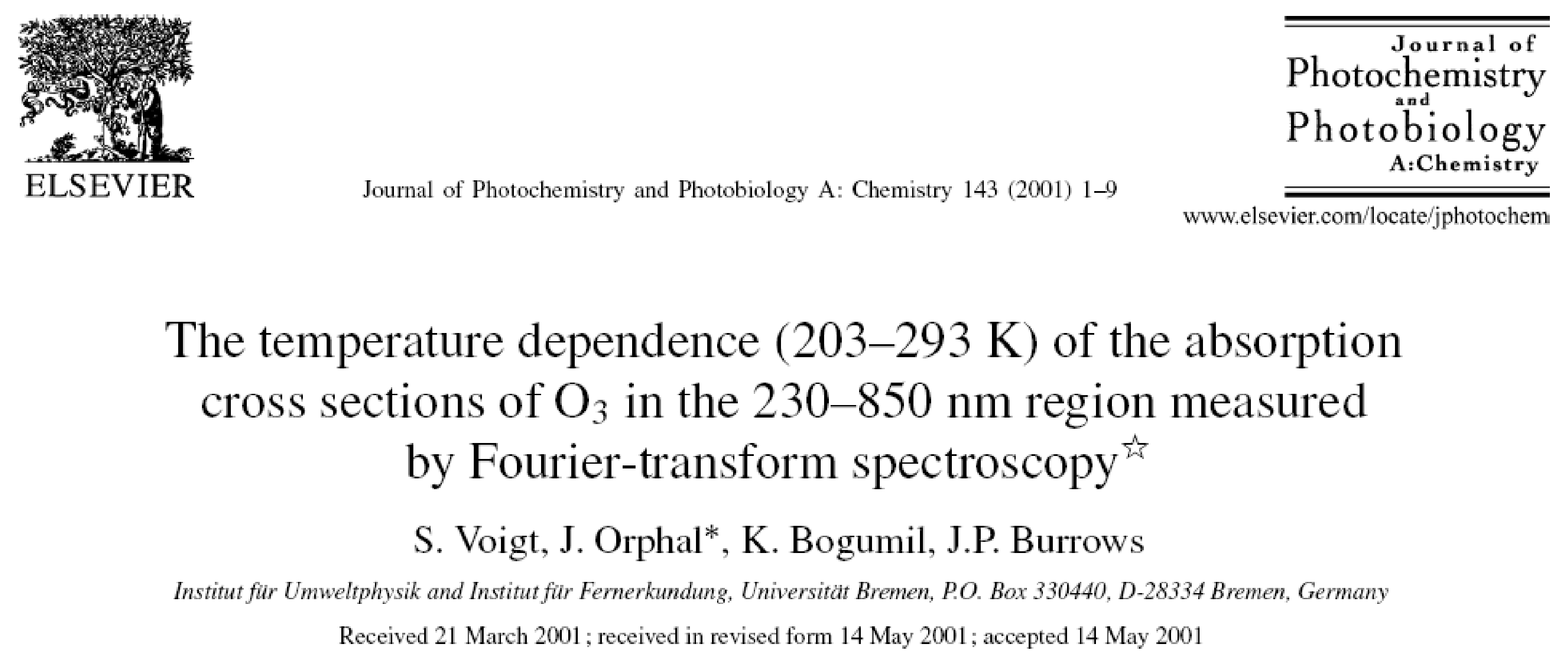
O_3 cross-sections from GOME (1999)



Temperature-dependent absorption cross-sections of O_3 511

O_3 cross-sections from FTS at IUP (2001)

O_3 cross-sections from FTS (2001)



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Journal of Photochemistry and Photobiology A: Chemistry 143 (2001) 1–9

Journal of Photochemistry and Photobiology A:Chemistry

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The temperature dependence (203–293 K) of the absorption cross sections of O_3 in the 230–850 nm region measured by Fourier-transform spectroscopy☆

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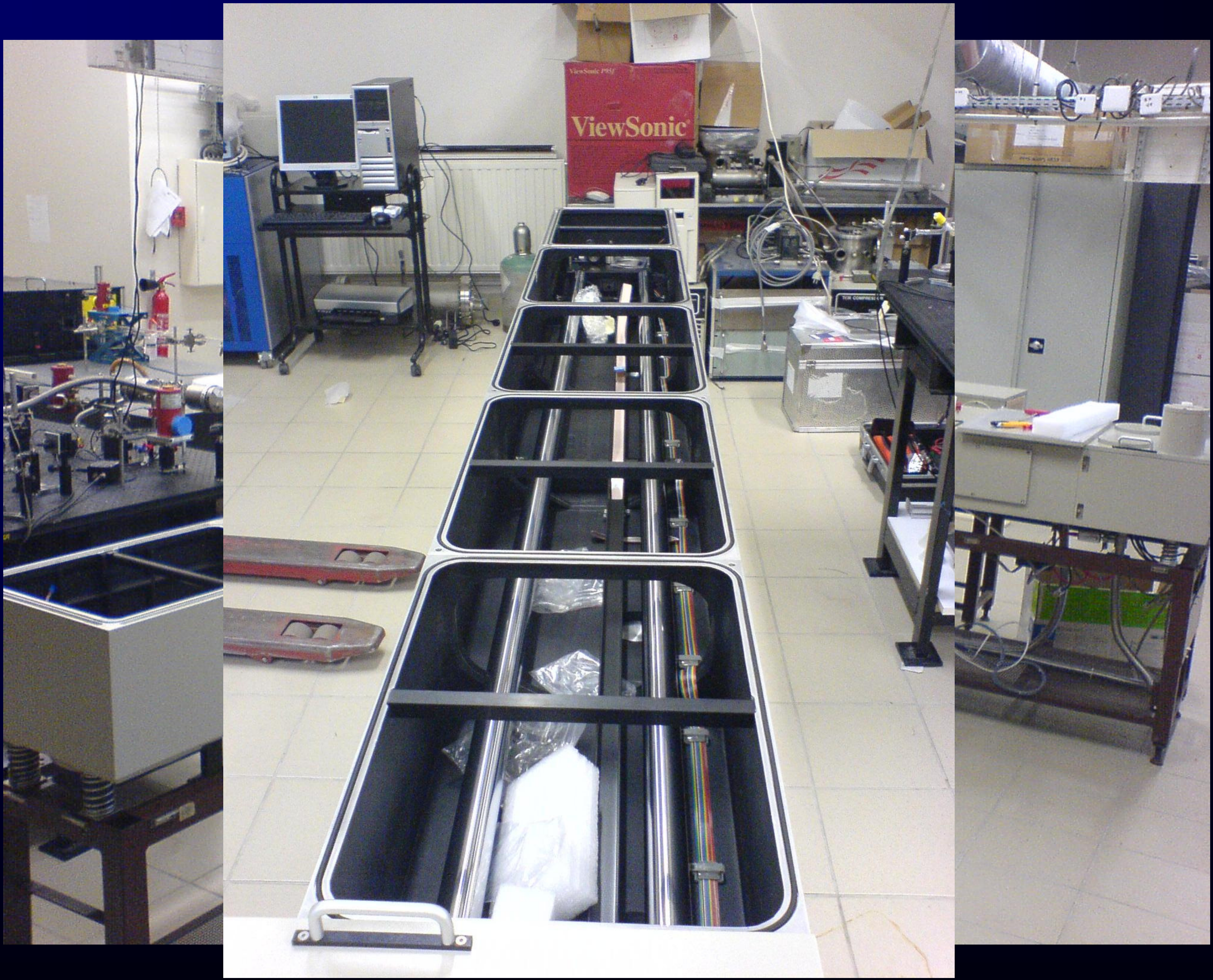
O_3 cross-sections from FTS (2001)



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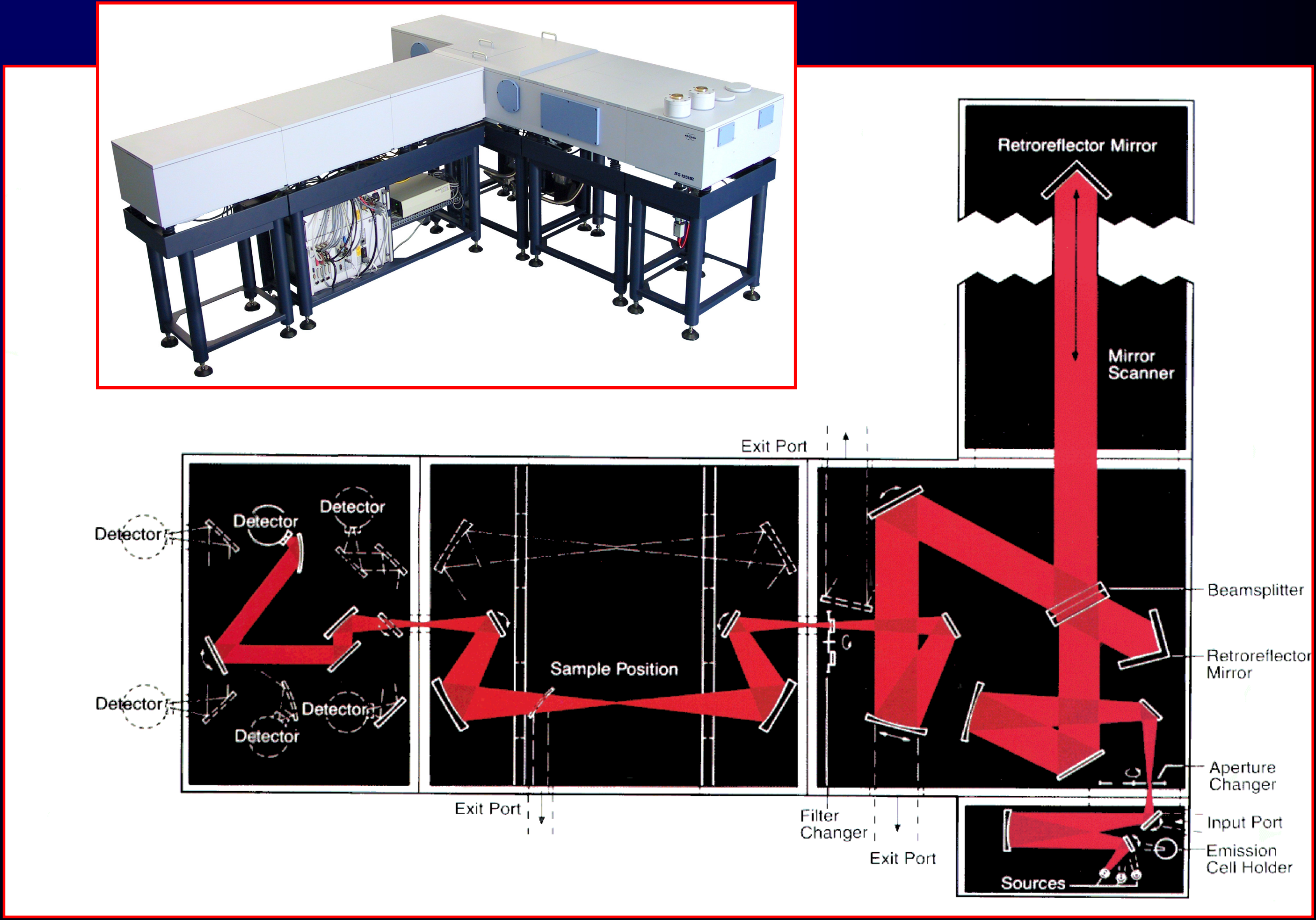

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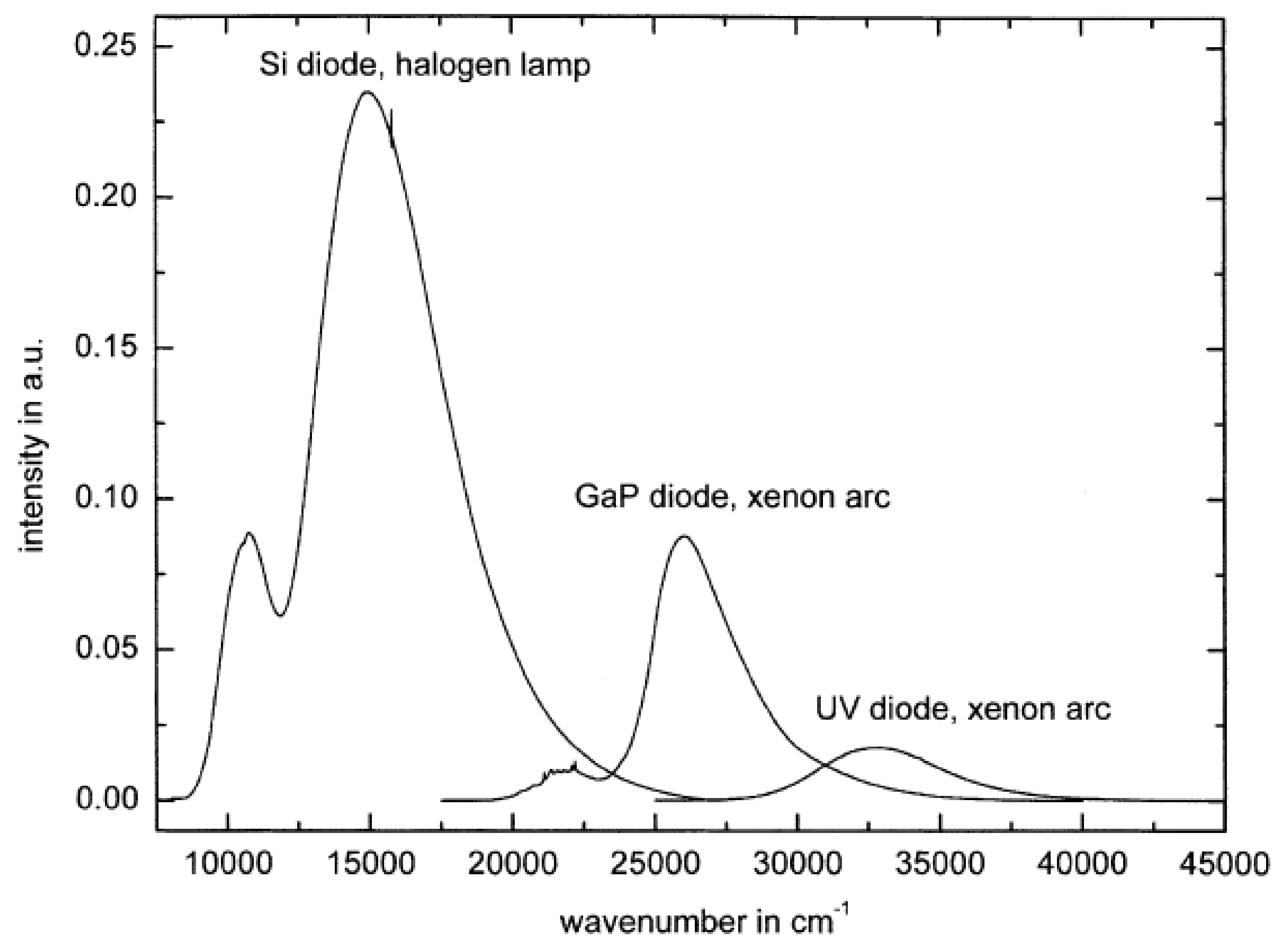

O_3 cross-sections from FTS (2001)

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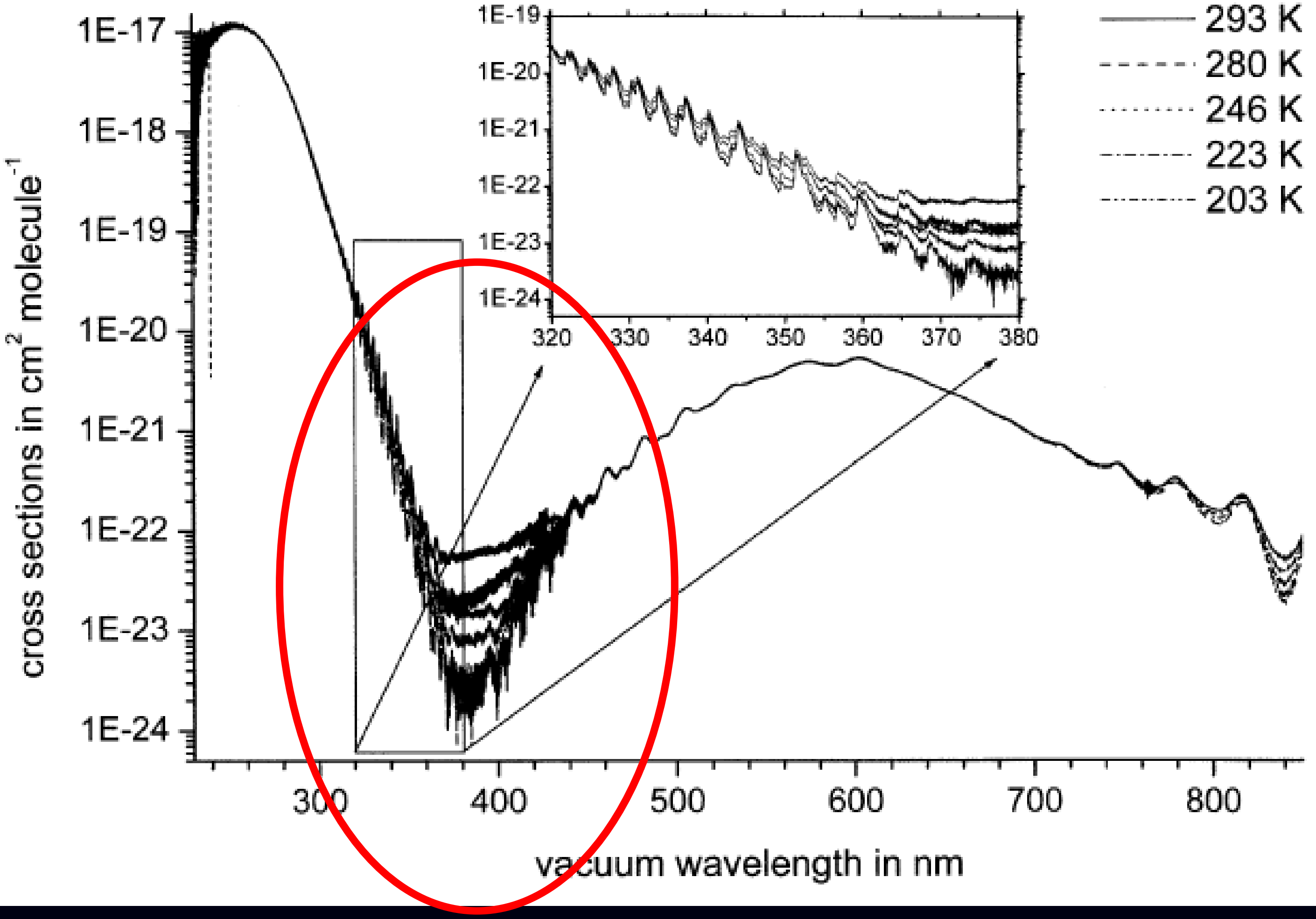
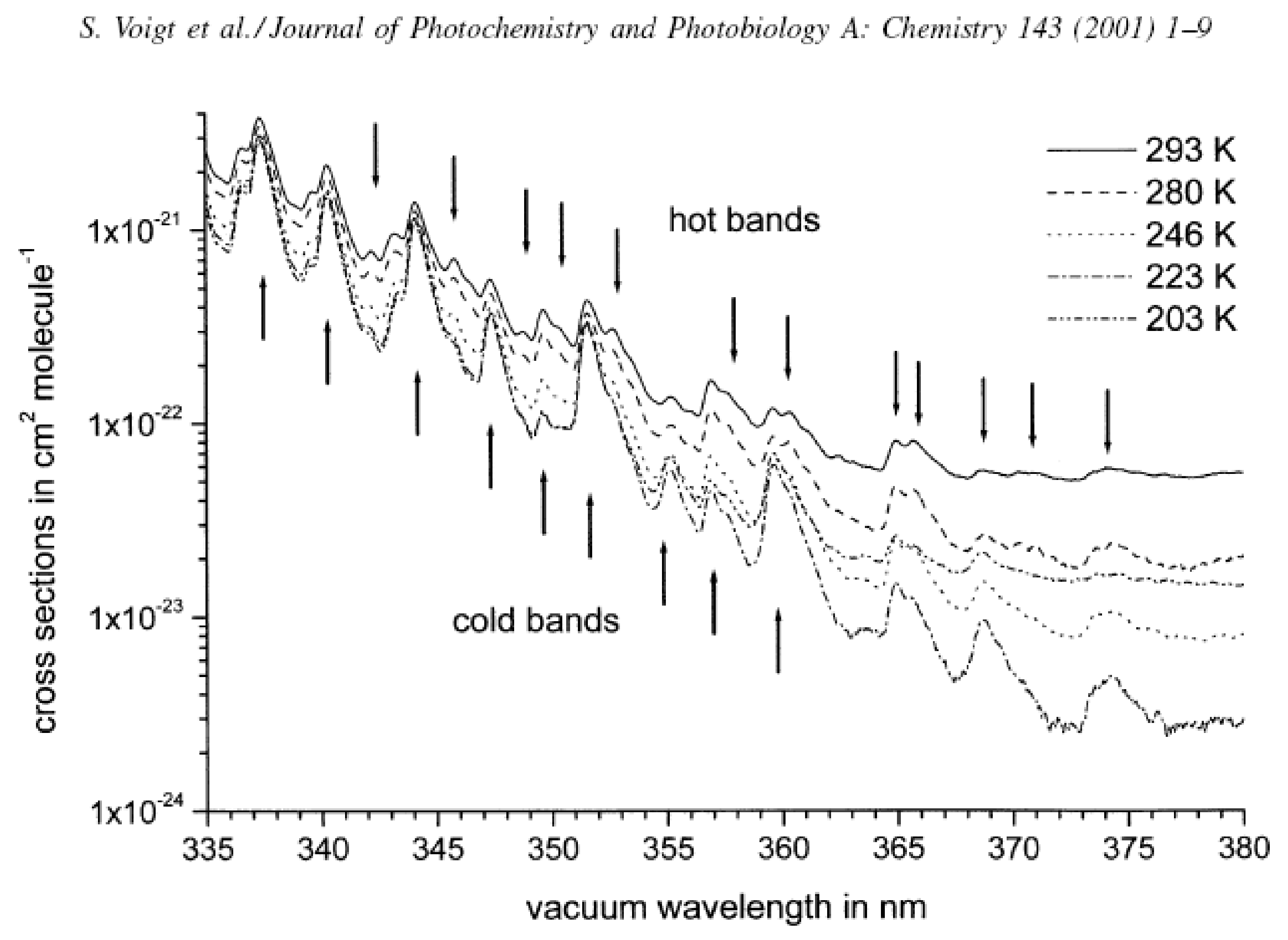


O_3 cross-sections from FTS (2001)



S. Voigt et al. / Journal of Photochemistry and Photobiology A: Chemistry 143 (2001) 1–9

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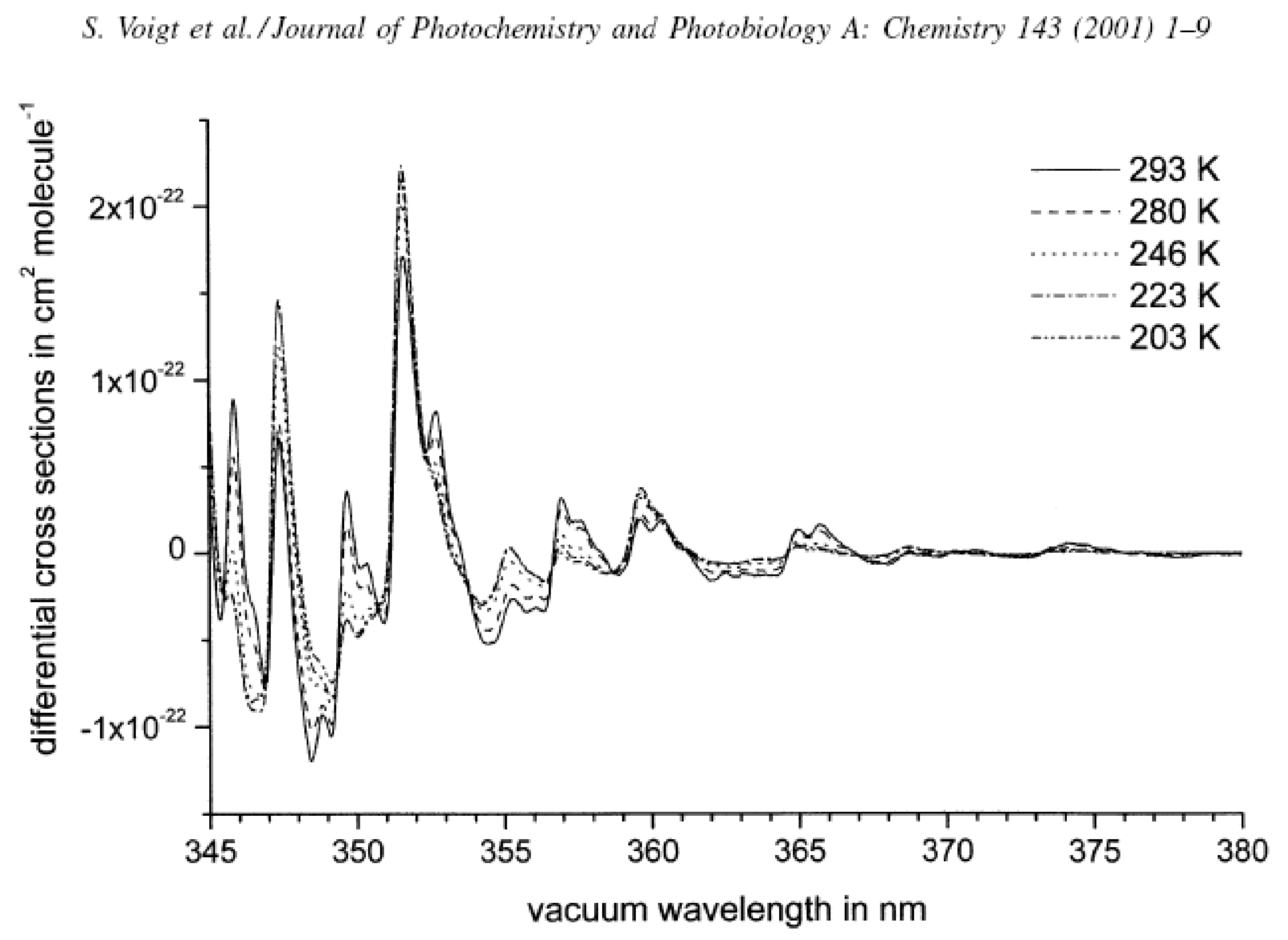
S. Voigt et al. / Journal of Photochemistry and Photobiology A: Chemistry 143 (2001) 1–9

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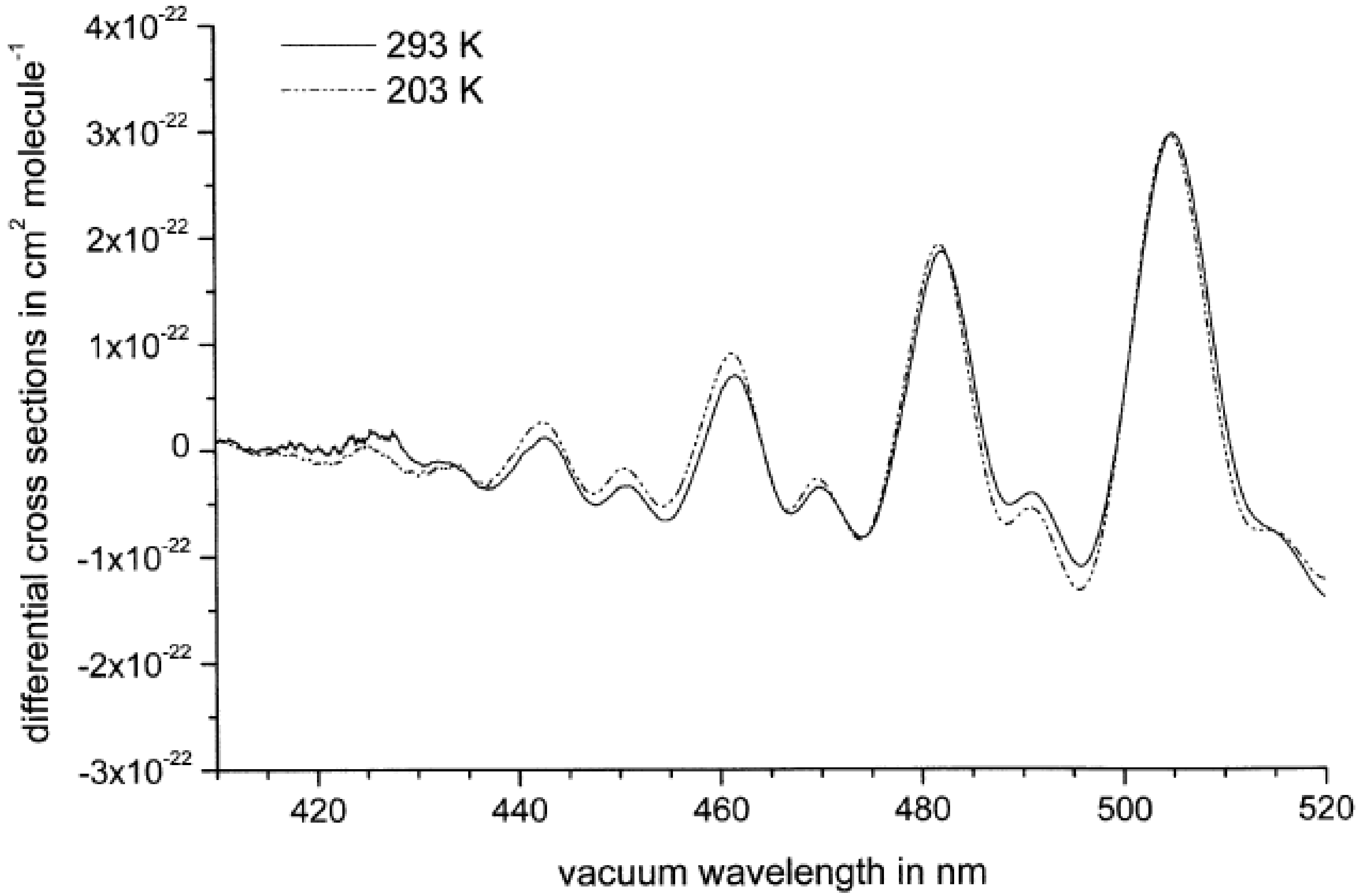
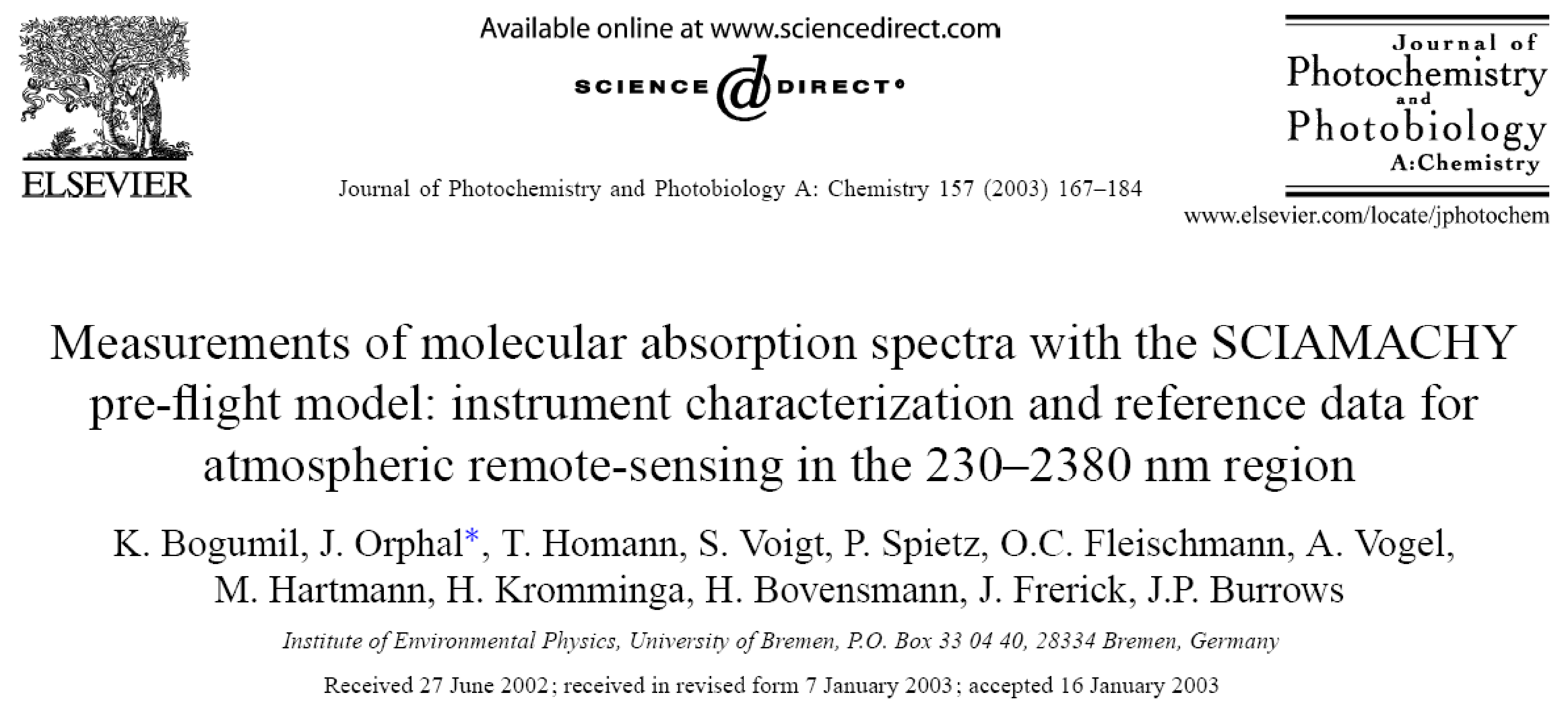


O_3 cross-sections from SCIAMACHY (2003)

O_3 cross-sections from SCIAMACHY (2003)



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Journal of Photochemistry and Photobiology A: Chemistry 157 (2003) 167–184

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Measurements of molecular absorption spectra with the SCIAMACHY pre-flight model: instrument characterization and reference data for atmospheric remote-sensing in the 230–2380 nm region

K. Bogumil, J. Orphal*, T. Homann, S. Voigt, P. Spietz, O.C. Fleischmann, A. Vogel, M. Hartmann, H. Kromminga, H. Bovensmann, J. Frerick, J.P. Burrows

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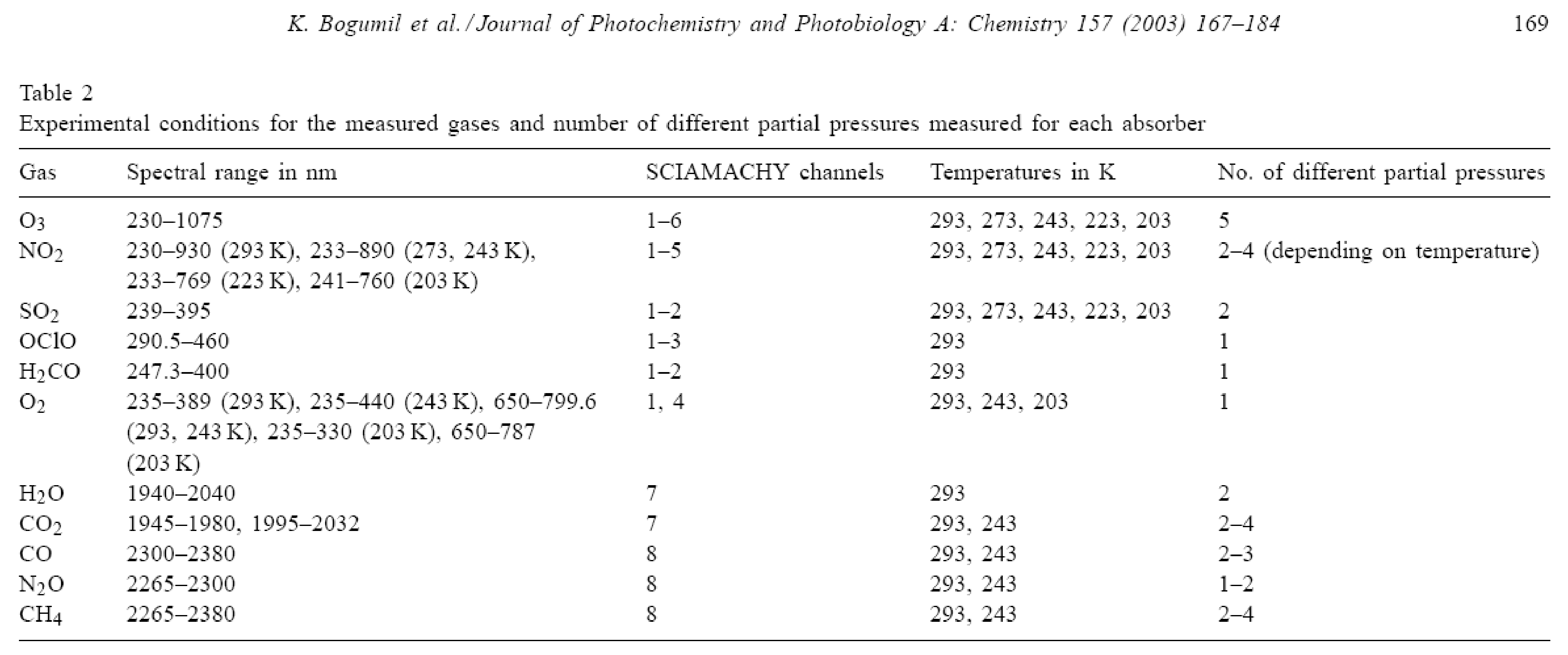
O_3 cross-sections from SCIAMACHY (2003)

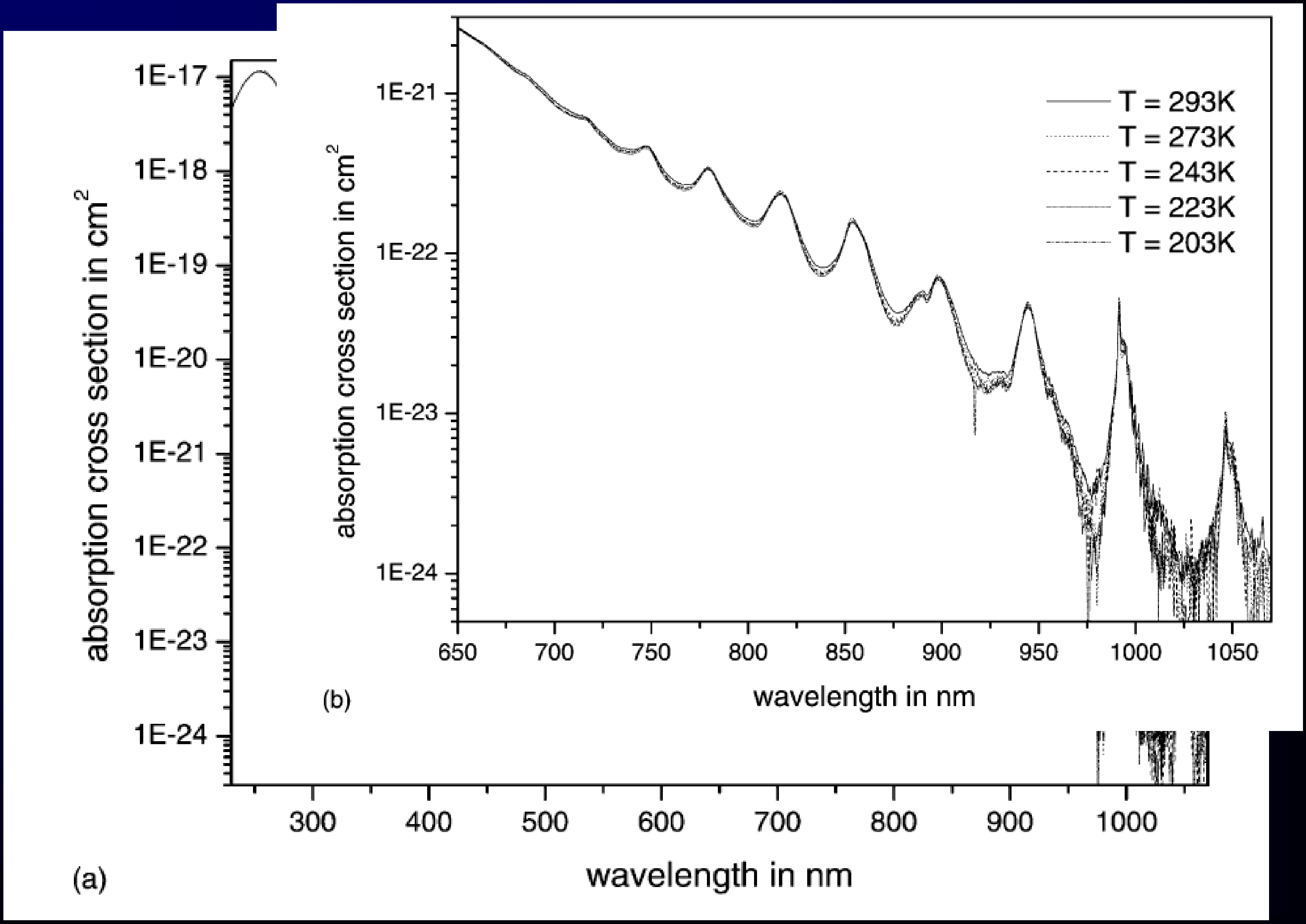


K. Bogumil et al. / Journal of Photochemistry and Photobiology A: Chemistry 157 (2003) 167–184 169

Table 2
Experimental conditions for the measured gases and number of different partial pressures measured for each absorber

Gas	Spectral range in nm	SCIAMACHY channels	Temperatures in K	No. of different partial pressures
O_3	230–1075	1–6	293, 273, 243, 223, 203	5
NO_2	230–930 (293 K), 233–890 (273, 243 K), 233–769 (223 K), 241–760 (203 K)	1–5	293, 273, 243, 223, 203	2–4 (depending on temperature)
SO_2	239–395	1–2	293, 273, 243, 223, 203	2
OClO	290.5–460	1–3	293	1
H_2CO	247.3–400	1–2	293	1
O_2	235–389 (293 K), 235–440 (243 K), 650–799.6 (293, 243 K), 235–330 (203 K), 650–787 (203 K)	1, 4	293, 243, 203	1
H_2O	1940–2040	7	293	2
CO_2	1945–1980, 1995–2032	7	293, 243	2–4
CO	2300–2380	8	293, 243	2–3
N_2O	2265–2300	8	293, 243	1–2
CH_4	2265–2380	8	293, 243	2–4

O_3 cross-sections from SCIAMACHY (2003)



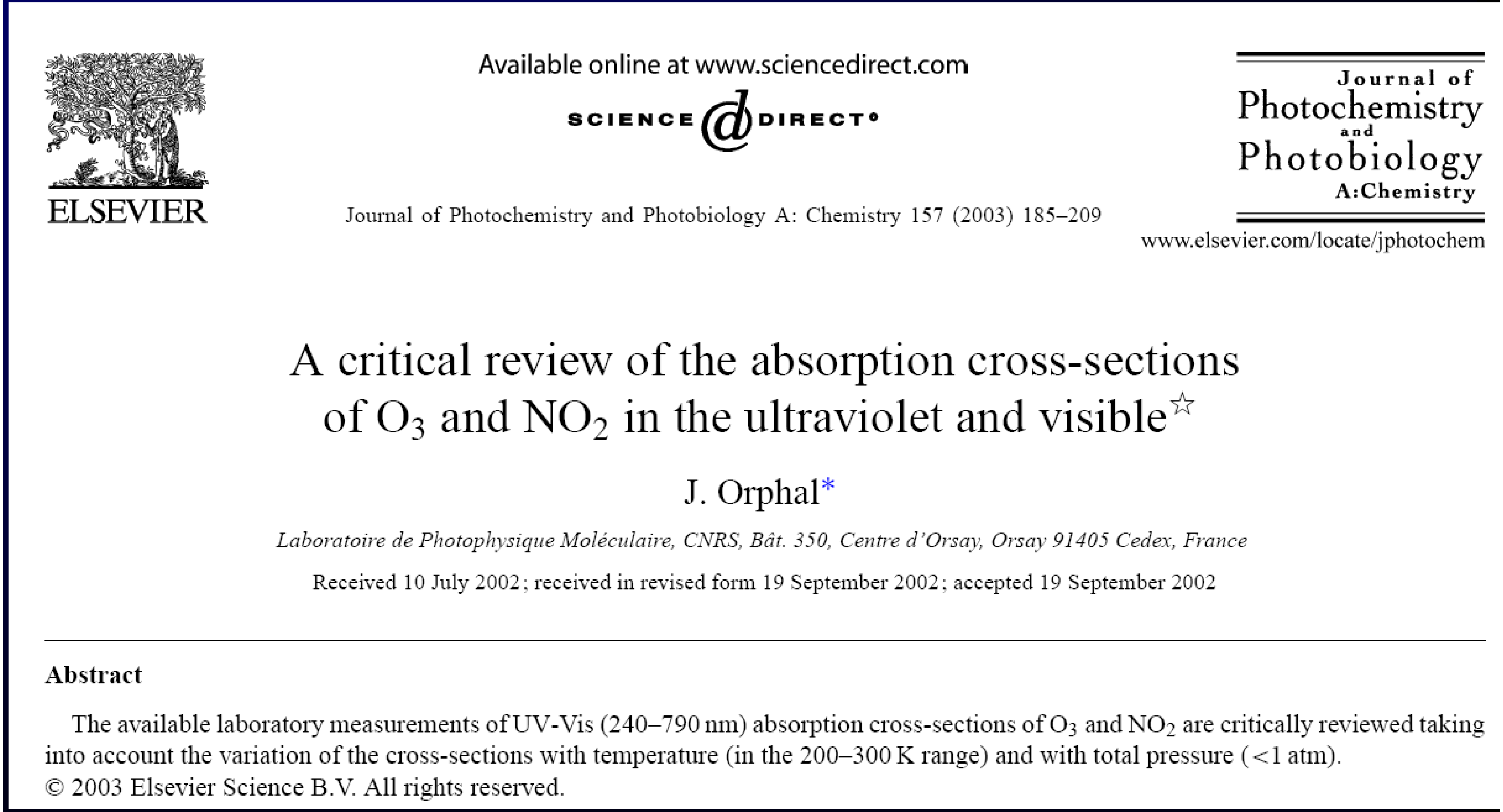
Conclusions for "new" O_3 cross-sections

- cover broad spectral range (0.2-1.2 μm)
- cover most atmospheric temperatures
- from different instruments
  - GOME-FM (resolution 0.2-0.4 nm)
  - FTS (resolution 0.01-0.10 nm)
  - SCIAMACHY (resolution 0.2-0.4 nm)
- but: they are still not "perfect"
  - straylight and "baseline" issues
  - consistency (differences)
  - temperature range (all above 200 K)

2. O_3 (and NO_2) "Critical Review" for ESA

- review by R. Hudson (about 1990)
- initiated by ESA/ESTEC (C. Readings)
- work started in 2000 (T.O. J. Callies)
- final presentation in 2001 (GOME SAG)
- published as ESA "Technical Report"
- shorter summary published in 2003 (JPP-A)
- over 60 times cited (> 10 per year)

ESA O_3 critical review



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A critical review of the absorption cross-sections of O_3 and NO_2 in the ultraviolet and visible☆

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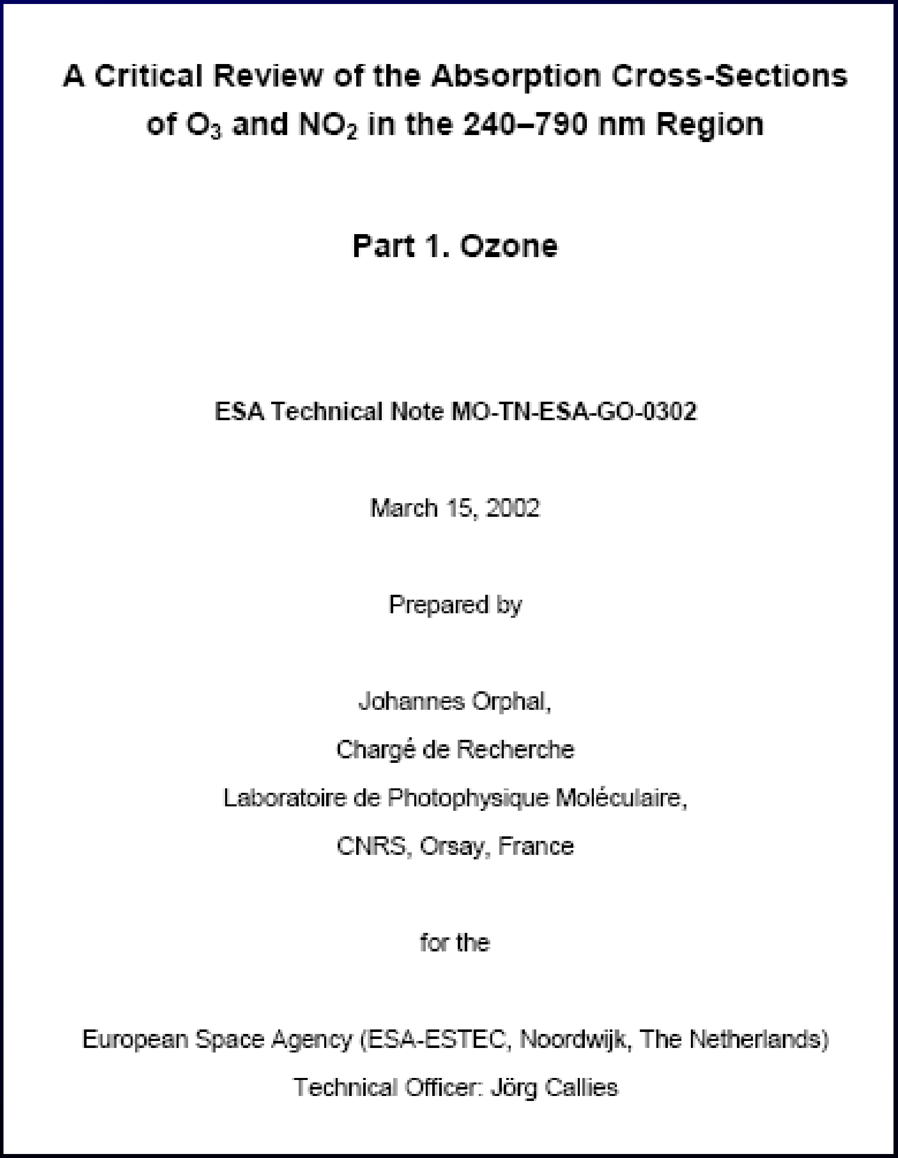
Received 10 July 2002; received in revised form 19 September 2002; accepted 19 September 2002

Abstract

The available laboratory measurements of UV-Vis (240–790 nm) absorption cross-sections of O_3 and NO_2 are critically reviewed taking into account the variation of the cross-sections with temperature (in the 200–300 K range) and with total pressure (<1 atm).

ESA O_3 critical review



A Critical Review of the Absorption Cross-Sections
of O_3 and NO_2 in the 240–790 nm Region

Part 1. Ozone

ESA Technical Note MO-TN-ESA-GO-0302

March 15, 2002

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European Space Agency (ESA-ESTEC, Noordwijk, The Netherlands)
Technical Officer: Jörg Callies

ESA O_3 critical review

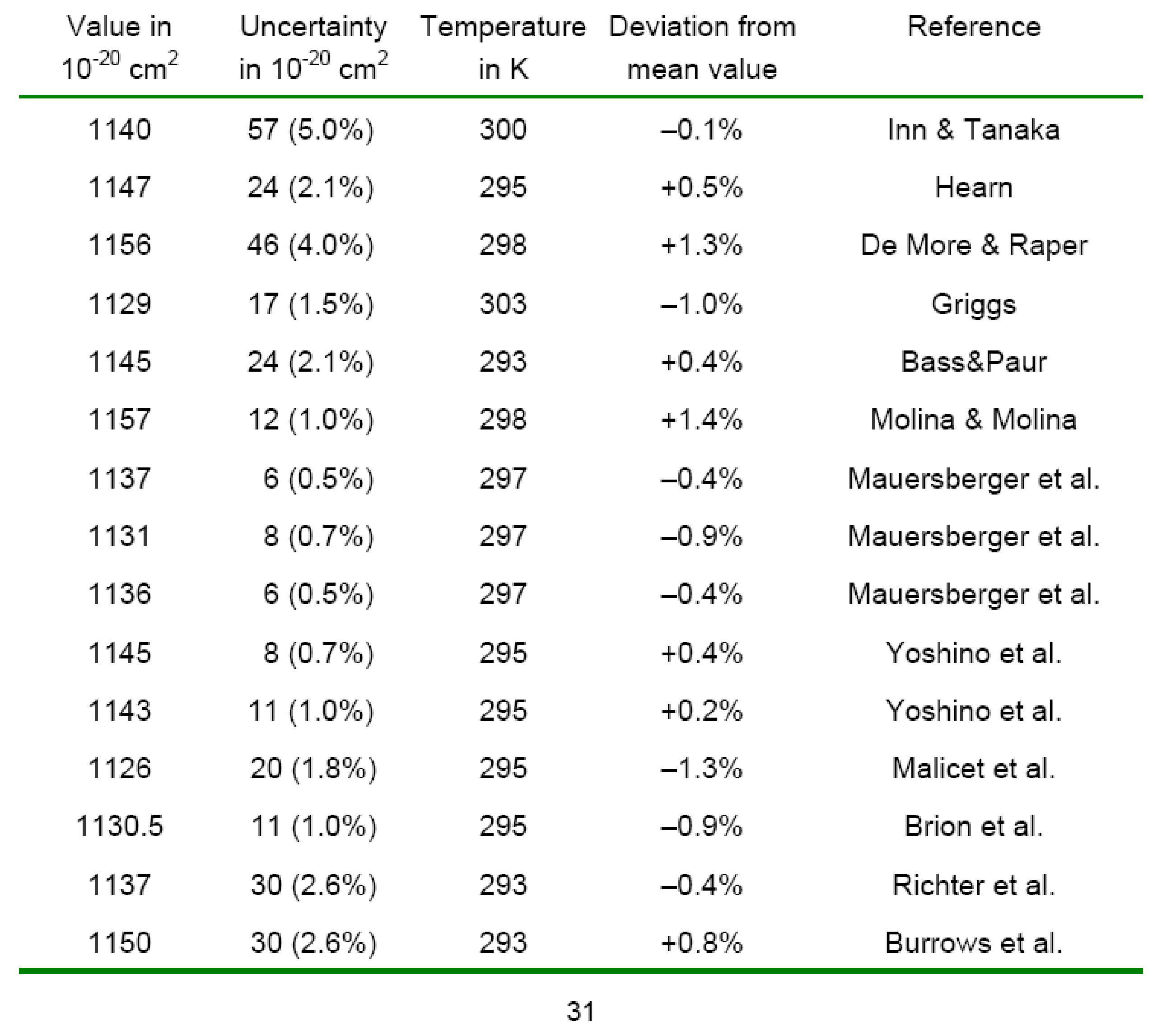
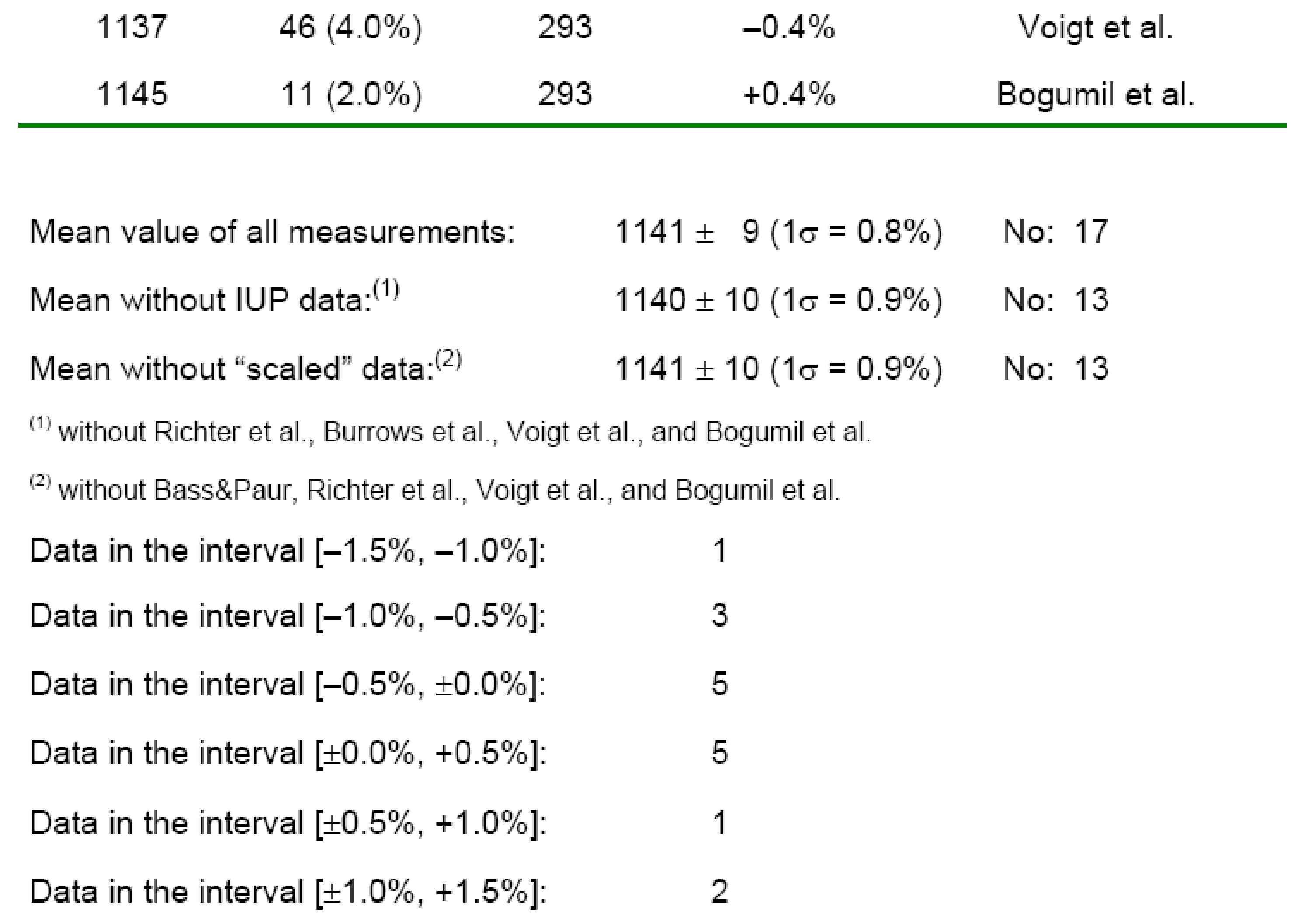


Table 6-1: Comparison of the O_3 cross-sections at 298±5K at 253.65 nm

Value in 10^{-20} cm^2	Uncertainty in 10^{-20} cm^2	Temperature in K	Deviation from mean value	Reference
1140	57 (5.0%)	300	–0.1%	Inn & Tanaka
1147	24 (2.1%)	295	+0.5%	Hearn
1156	46 (4.0%)	298	+1.3%	De More & Raper
1129	17 (1.5%)	303	–1.0%	Griggs
1145	24 (2.1%)	293	+0.4%	Bass&Paur
1157	12 (1.0%)	298	+1.4%	Molina & Molina
1137	6 (0.5%)	297	–0.4%	Mauersberger et al.
1131	8 (0.7%)	297	–0.9%	Mauersberger et al.
1136	6 (0.5%)	297	–0.4%	Mauersberger et al.
1145	8 (0.7%)	295	+0.4%	Yoshino et al.
1143	11 (1.0%)	295	+0.2%	Yoshino et al.
1126	20 (1.8%)	295	–1.3%	Malicet et al.
1130.5	11 (1.0%)	295	–0.9%	Brion et al.
1137	30 (2.6%)	293	–0.4%	Richter et al.
1150	30 (2.6%)	293	+0.8%	Burrows et al.

ESA O_3 critical review



1137	46 (4.0%)	293	–0.4%	Voigt et al.
1145	11 (2.0%)	293	+0.4%	Bogumil et al.

Mean value of all measurements: 1141 ± 9 ($1\sigma = 0.8\%$) No: 17

Mean without IUP data:(1) 1140 ± 10 ($1\sigma = 0.9\%$) No: 13

Mean without “scaled” data:(2) 1141 ± 10 ($1\sigma = 0.9\%$) No: 13

(1) without Richter et al., Burrows et al., Voigt et al., and Bogumil et al.

(2) without Bass&Paur, Richter et al., Voigt et al., and Bogumil et al.

Data in the interval [–1.5%, –1.0%]: 1

Data in the interval [–1.0%, –0.5%]: 3

Data in the interval [–0.5%, ±0.0%]: 5

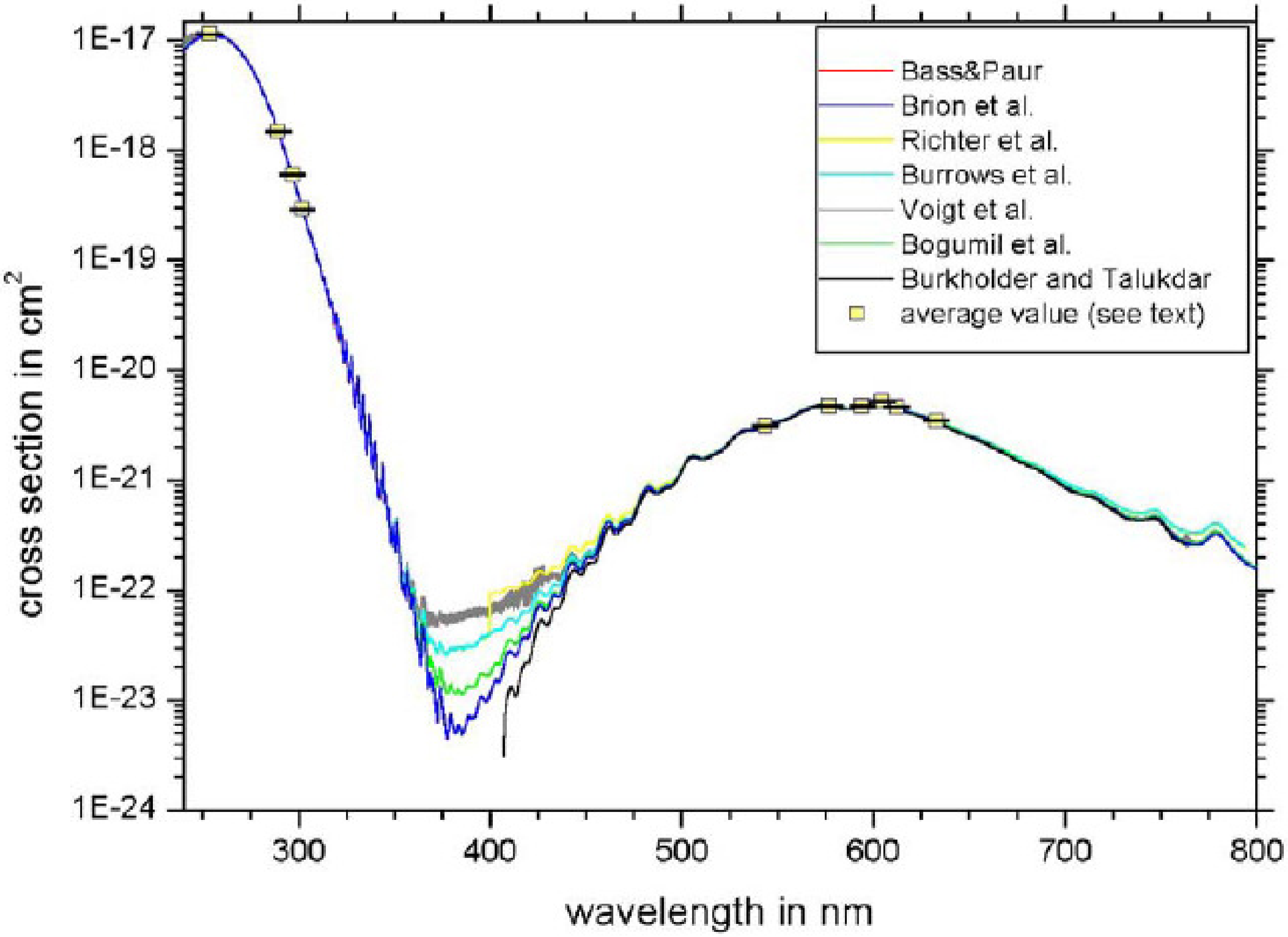
Data in the interval [±0.0%, +0.5%]: 5

Data in the interval [±0.5%, +1.0%]: 1

Data in the interval [±1.0%, +1.5%]: 2

ESA O_3 critical review

Figure 6-1: Comparison of O_3 absorption cross-sections at 298±5 K: 240–800 nm



ESA O_3 critical review

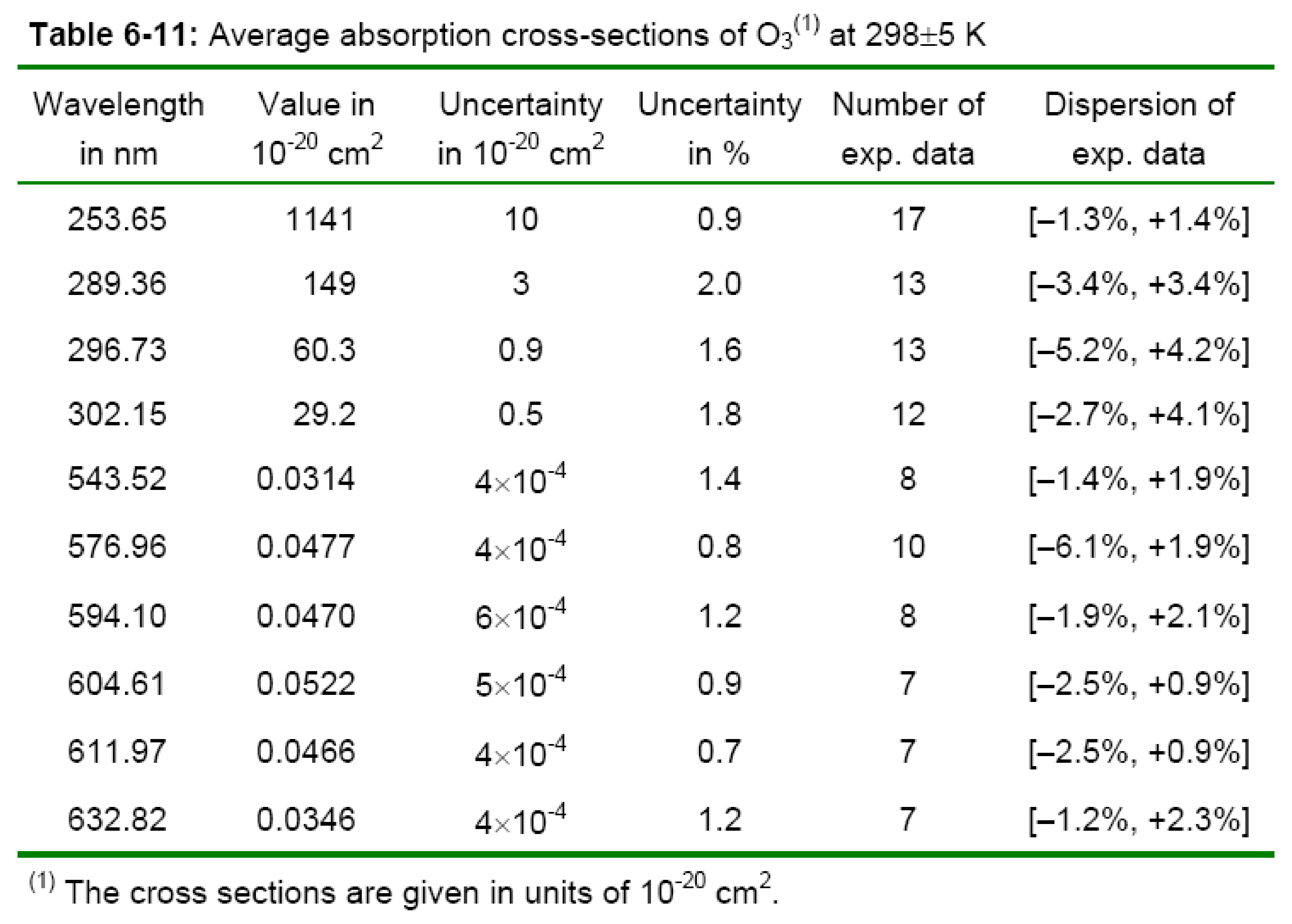


Table 6-11: Average absorption cross-sections of $O_3^{(1)}$ at 298±5 K

Wavelength in nm	Value in 10^{-20} cm^2	Uncertainty in 10^{-20} cm^2	Uncertainty in %	Number of exp. data	Dispersion of exp. data
253.65	1141	10	0.9	17	[–1.3%, +1.4%]
289.36	149	3	2.0	13	[–3.4%, +3.4%]
296.73	60.3	0.9	1.6	13	[–5.2%, +4.2%]
302.15	29.2	0.5	1.8	12	[–2.7%, +4.1%]
543.52	0.0314	4×10^{-4}	1.4	8	[–1.4%, +1.9%]
576.96	0.0477	4×10^{-4}	0.8	10	[–6.1%, +1.9%]
594.10	0.0470	6×10^{-4}	1.2	8	[–1.9%, +2.1%]
604.61	0.0522	5×10^{-4}	0.9	7	[–2.5%, +0.9%]
611.97	0.0466	4×10^{-4}	0.7	7	[–2.5%, +0.9%]
632.82	0.0346	4×10^{-4}	1.2	7	[–1.2%, +2.3%]

(1) The cross sections are given in units of 10^{-20} cm^2.

ESA O_3 critical review

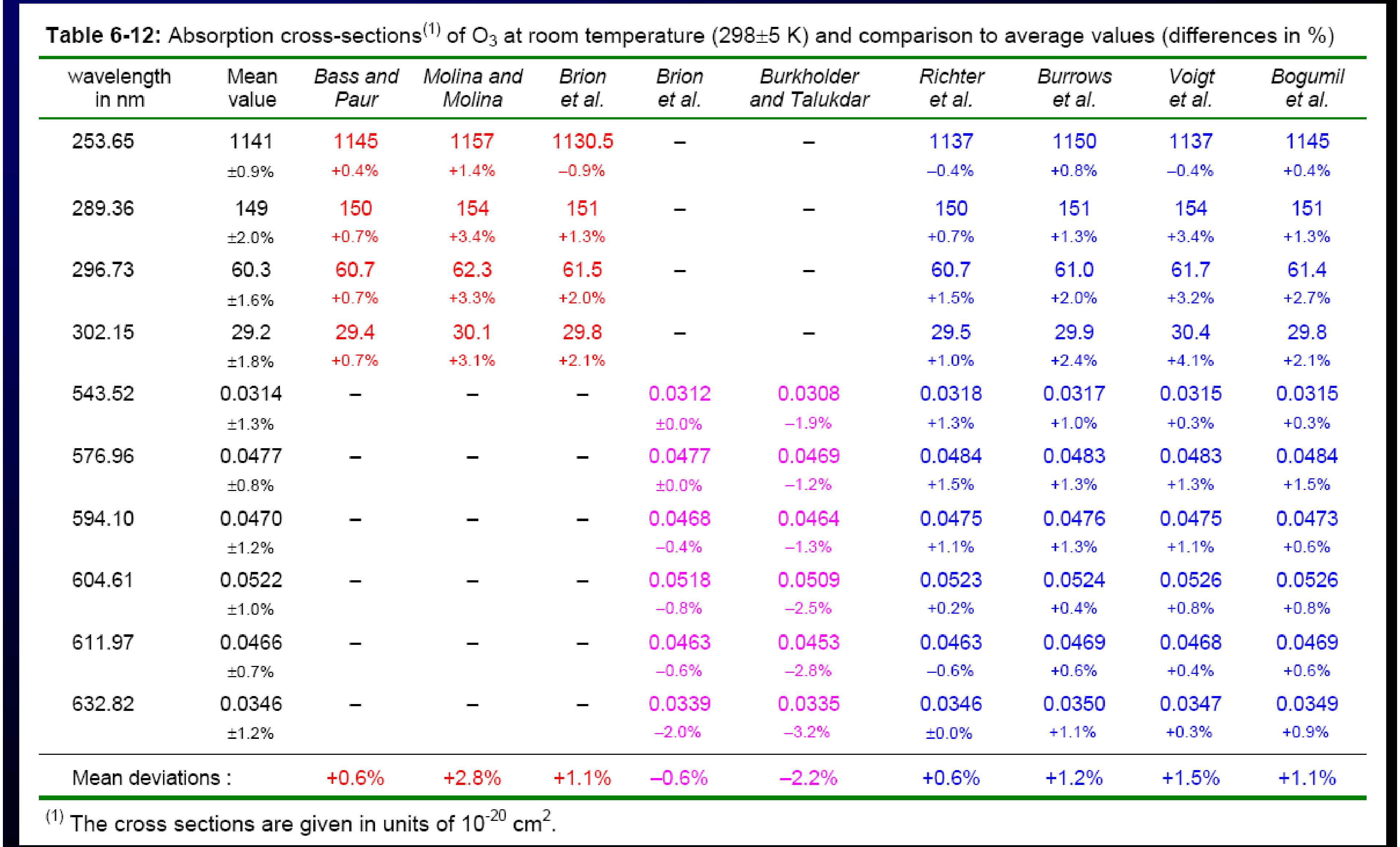


Table 6-12: Absorption cross-sections(1) of O_3 at room temperature (298±5 K) and comparison to average values (differences in %)

wavelength in nm	Mean value	*Bass and Paur*	*Molina and Molina*	*Brion et al.*	*Brion et al.*	*Burkholder and Talukdar*	*Richter et al.*	*Burrows et al.*	*Voigt et al.*	*Bogumil et al.*
253.65	1141 ±0.9%	1145 +0.4%	1157 +1.4%	1130.5 –0.9%	–	–	1137 –0.4%	1150 +0.8%	1137 –0.4%	1145 +0.4%
289.36	149 ±2.0%	150 +0.7%	154 +3.4%	151 +1.3%	–	–	150 +0.7%	151 +1.3%	154 +3.4%	151 +1.3%
296.73	60.3 ±1.6%	60.7 +0.7%	62.3 +3.3%	61.5 +2.0%	–	–	60.7 +1.5%	61.0 +2.0%	61.7 +3.2%	61.4 +2.7%
302.15	29.2 ±1.8%	29.4 +0.7%	30.1 +3.1%	29.8 +2.1%	–	–	29.5 +1.0%	29.9 +2.4%	30.4 +4.1%	29.8 +2.1%
543.52	0.0314 ±1.3%	–	–	–	0.0312 ±0.0%	0.0308 –1.9%	0.0318 +1.3%	0.0317 +1.0%	0.0315 +0.3%	0.0315 +0.3%
576.96	0.0477 ±0.8%	–	–	–	0.0477 ±0.0%	0.0469 –1.2%	0.0484 +1.5%	0.0483 +1.3%	0.0483 +1.3%	0.0484 +1.5%
594.10	0.0470 ±1.2%	–	–	–	0.0468 –0.4%	0.0464 –1.3%	0.0475 +1.1%	0.0476 +1.3%	0.0475 +1.1%	0.0473 +0.6%
604.61	0.0522 ±1.0%	–	–	–	0.0518 –0.8%	0.0509 –2.5%	0.0523 +0.2%	0.0524 +0.4%	0.0526 +0.8%	0.0526 +0.8%
611.97	0.0466 ±0.7%	–	–	–	0.0463 –0.6%	0.0453 –2.8%	0.0463 –0.6%	0.0469 +0.6%	0.0468 +0.4%	0.0469 +0.6%
632.82	0.0346 ±1.2%	–	–	–	0.0339 –2.0%	0.0335 –3.2%	0.0346 ±0.0%	0.0350 +1.1%	0.0347 +0.3%	0.0349 +0.9%
Mean deviations :		+0.6%	+2.8%	+1.1%	–0.6%	–2.2%	+0.6%	+1.2%	+1.5%	+1.1%

(1) The cross sections are given in units of 10^{-20} cm^2.

ESA O_3 critical review

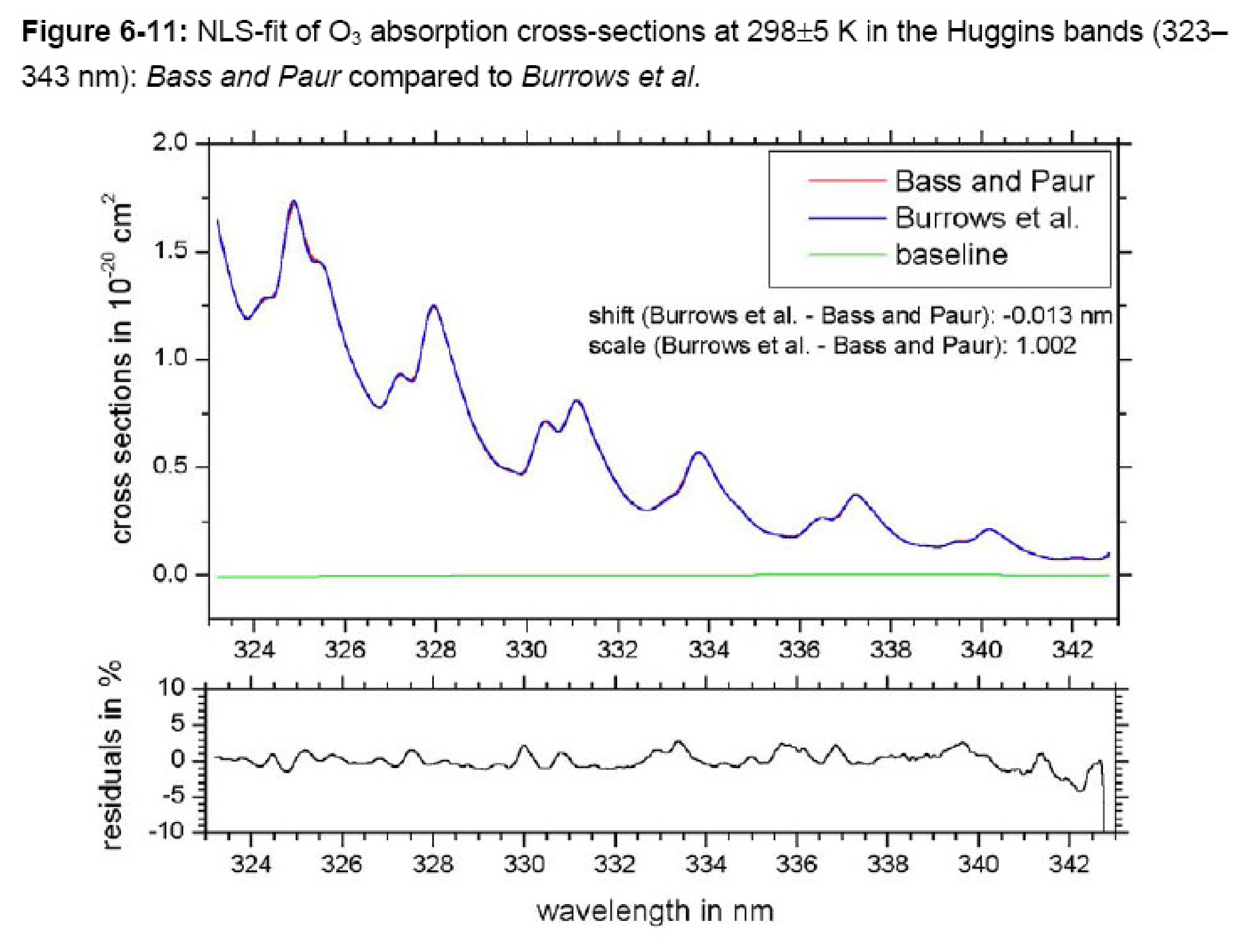
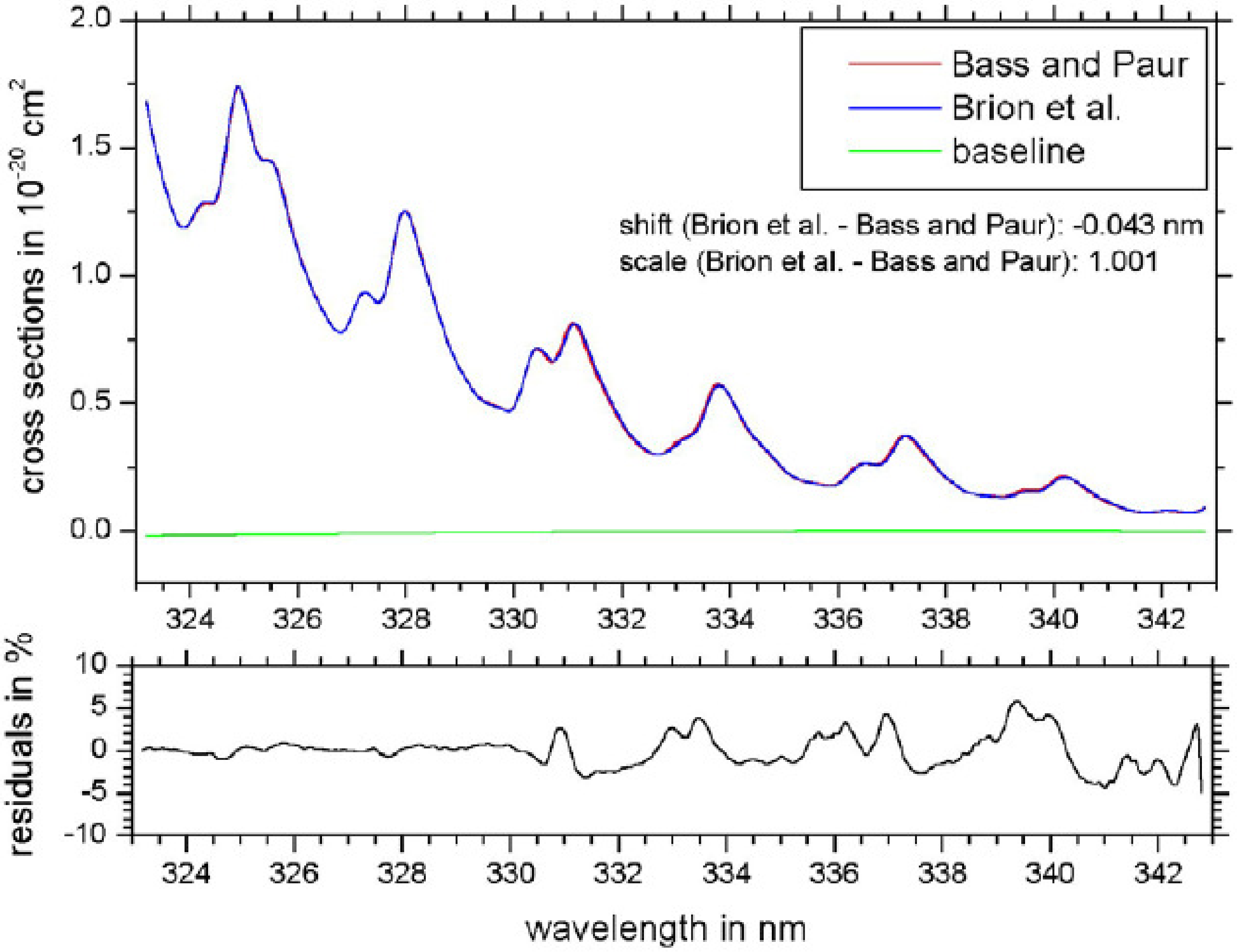


Figure 6-11: NLS-fit of O_3 absorption cross-sections at 298±5 K in the Huggins bands (323–343 nm): *Bass and Paur* compared to *Burrows et al.*

ESA O_3 critical review

Figure 6-9: NLS-fit of O_3 absorption cross-sections at 298±5 K in the Huggins bands (323–343 nm): *Bass and Paur* compared to *Brion et al.*



shift (Brion et al. - Bass and Paur): -0.043 nm
scale (Brion et al. - Bass and Paur): 1.001

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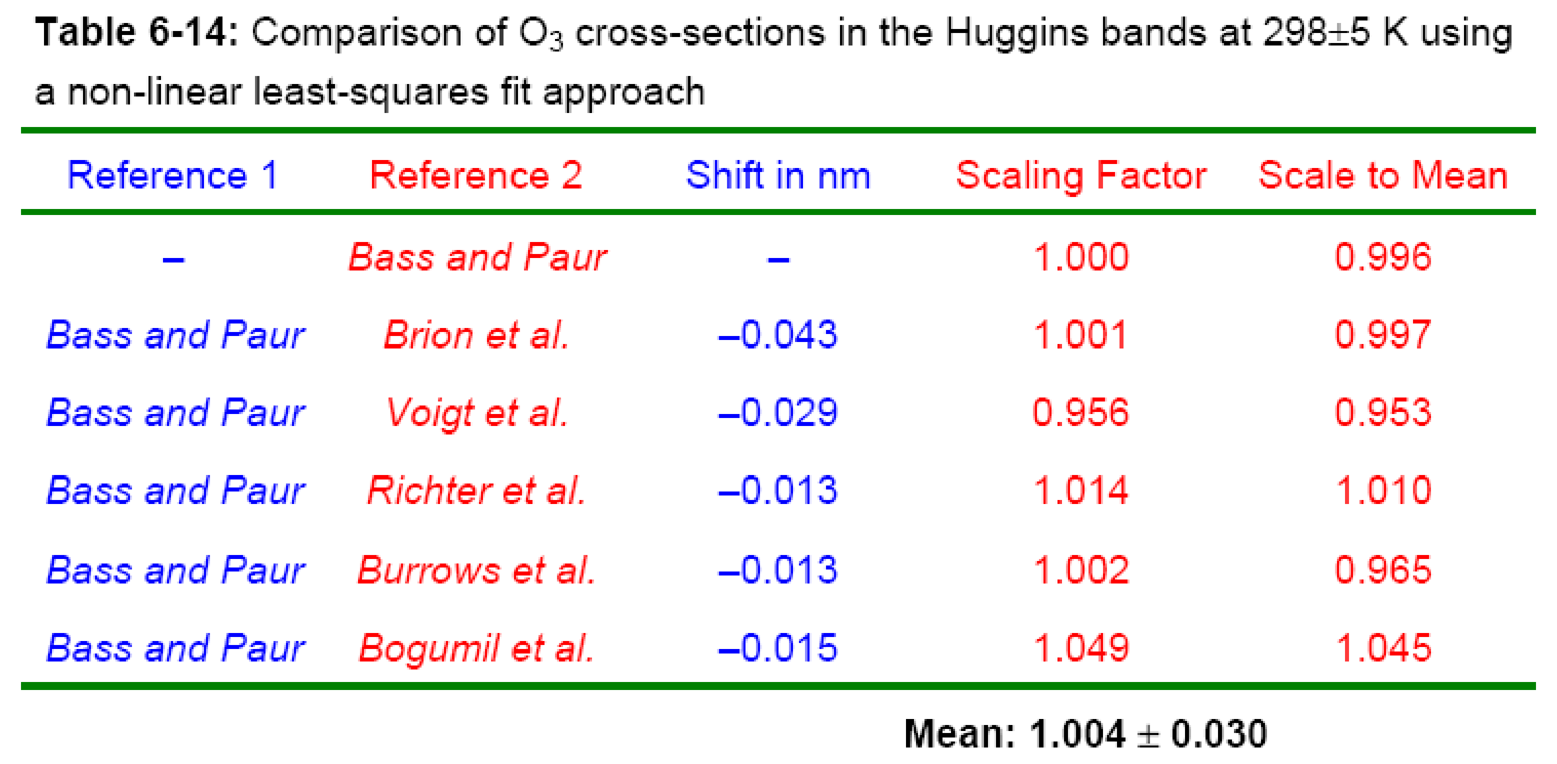


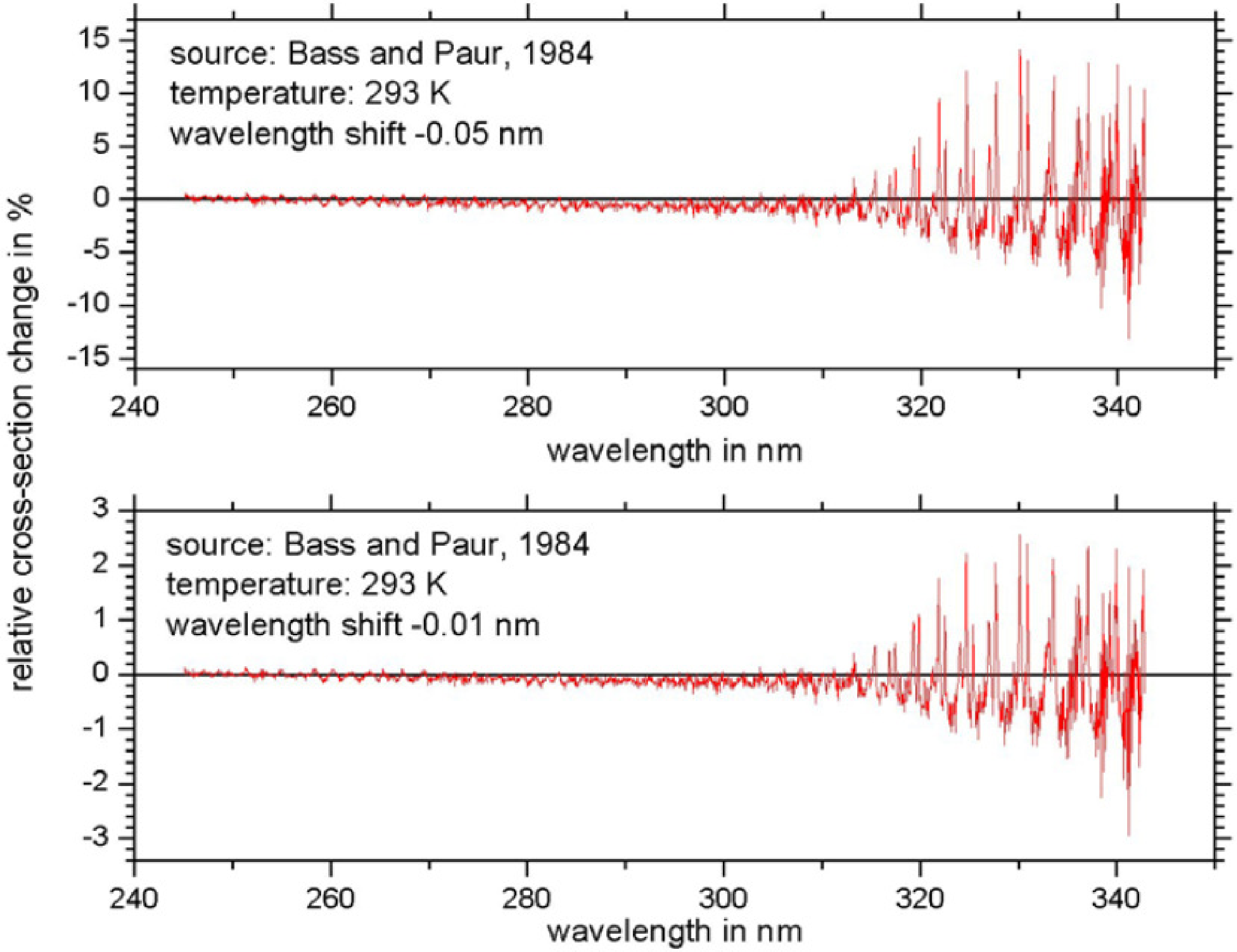
Table 6-14: Comparison of O_3 cross-sections in the Huggins bands at 298±5 K using a non-linear least-squares fit approach

Reference 1	Reference 2	Shift in nm	Scaling Factor	Scale to Mean
–	*Bass and Paur*	–	1.000	0.996
Bass and Paur	*Brion et al.*	–0.043	1.001	0.997
Bass and Paur	*Voigt et al.*	–0.029	0.956	0.953
Bass and Paur	*Richter et al.*	–0.013	1.014	1.010
Bass and Paur	*Burrows et al.*	–0.013	1.002	0.965
Bass and Paur	*Bogumil et al.*	–0.015	1.049	1.045

Mean: 1.004 ± 0.030

ESA O_3 critical review

Figure 5-3: relative change of the O_3 spectrum (source: *Bass and Paur*, spectral resolution less than 0.025 nm) after wavelength shifts of –0.05 nm and –0.01 nm, respectively



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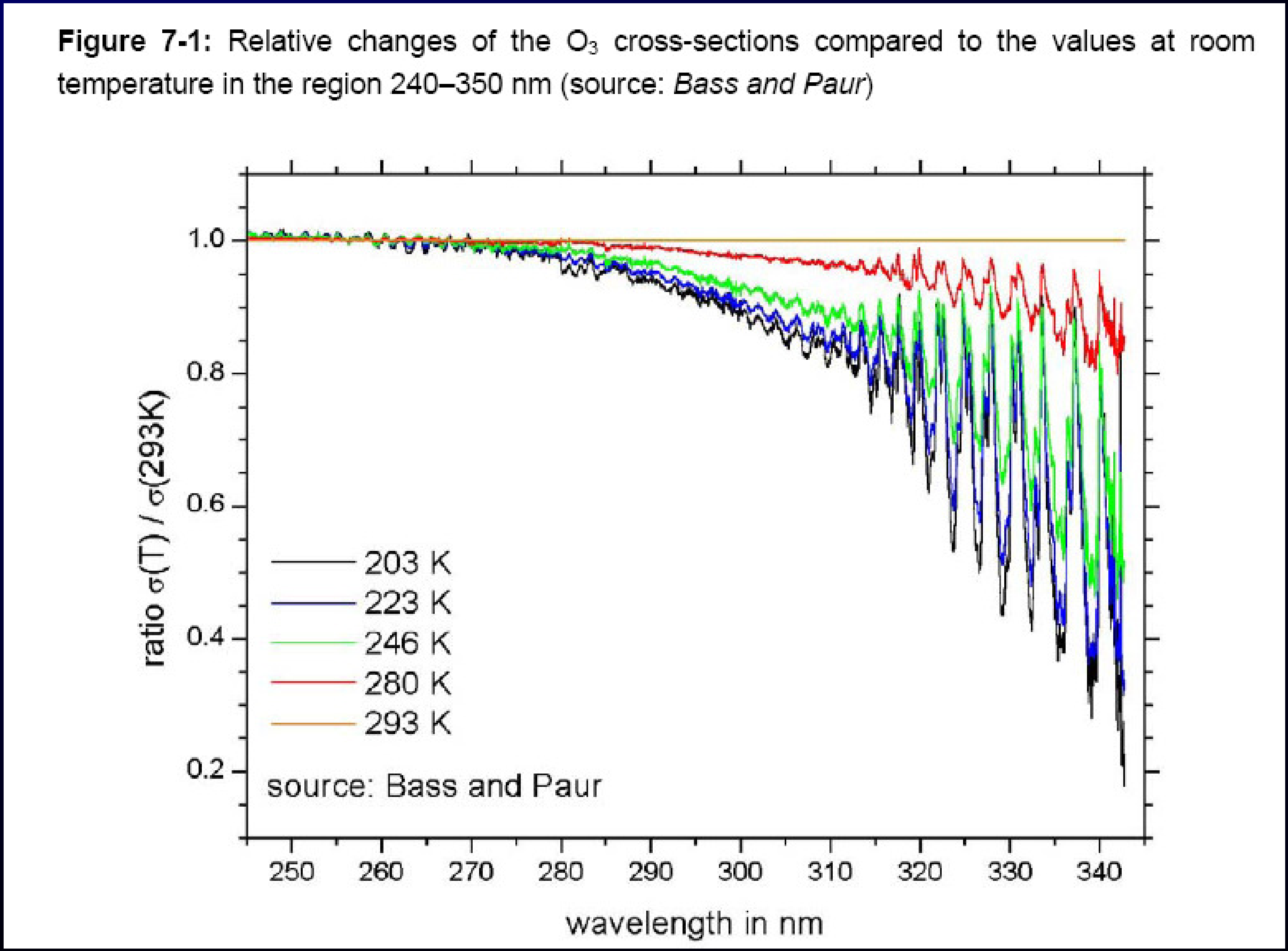

Figure 7-1: Relative changes of the O_3 cross-sections compared to the values at room temperature in the region 240–350 nm (source: *Bass and Paur*)

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Figure 7-4: Relative changes of the O_3 cross-sections compared to the values at room temperature in the region 240–350 nm (source: *Burrows et al.*)

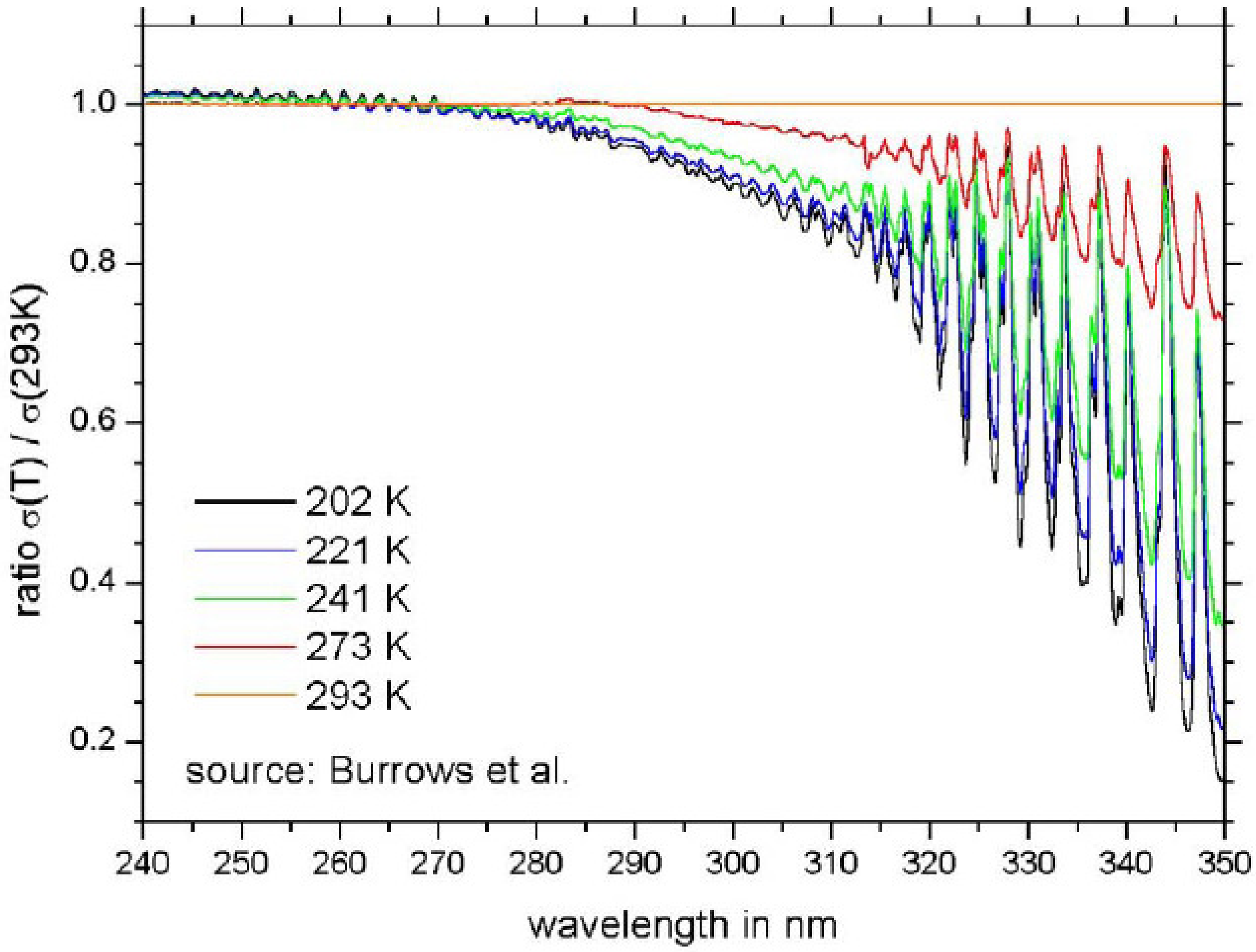

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Figure 7-7: Relative changes of the O_3 cross-sections compared to the values at room temperature in the region 400–790 nm (source: *Burkholder and Talukdar*)

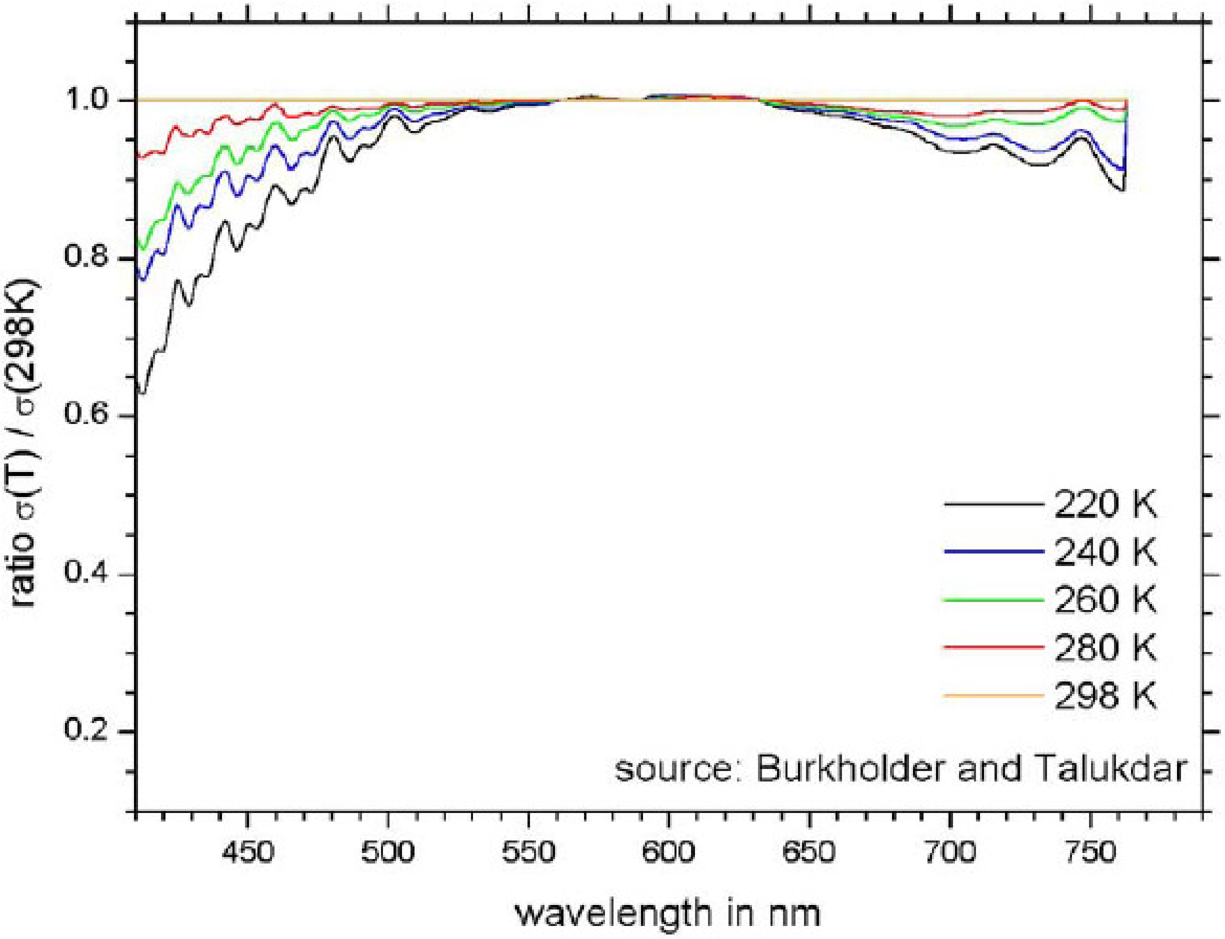

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Table 7-13: Relative differences in the cross-sections of O_3 at different temperatures in the Huggins bands (323–343 nm)

Reference 1	Reference 2	295 K	273 K	243 K	223 K	203 K
–	*Bass and Paur*	1.000	1.000	1.000	1.000	1.000
Bass and Paur	*Brion et al.*	1.001	0.998	0.995	0.992	–
Bass and Paur	*Voigt et al.*	0.956	1.040	1.063	1.070	1.195
Bass and Paur	*Richter et al.*	1.014	1.013	1.016	1.018	1.011
Bass and Paur	*Burrows et al.*	1.002	0.989	0.992	0.995	0.983
Bass and Paur	*Bogumil et al.*	1.049	1.050	1.065	1.080	1.077

Table 7-14: Wavelength shifts (in nm) in the cross-sections of O_3 at different temperatures in the Huggins bands (323–343 nm)

Reference 1	Reference 2	295 K	273 K	243 K	223 K	203 K
–	*Bass and Paur*	0.000	0.000	0.000	0.000	0.000
Bass and Paur	*Brion et al.*	–0.043	–0.027	–0.022	–0.026	–
Bass and Paur	*Voigt et al.*	–0.029	–0.030	–0.032	–0.037	–0.047
Bass and Paur	*Richter et al.*	–0.013	–0.007	–0.007	–0.012	–0.015
Bass and Paur	*Burrows et al.*	–0.013	–0.007	–0.007	–0.012	–0.015
Bass and Paur	*Bogumil et al.*	–0.015	–0.014	–0.017	–0.025	–0.021

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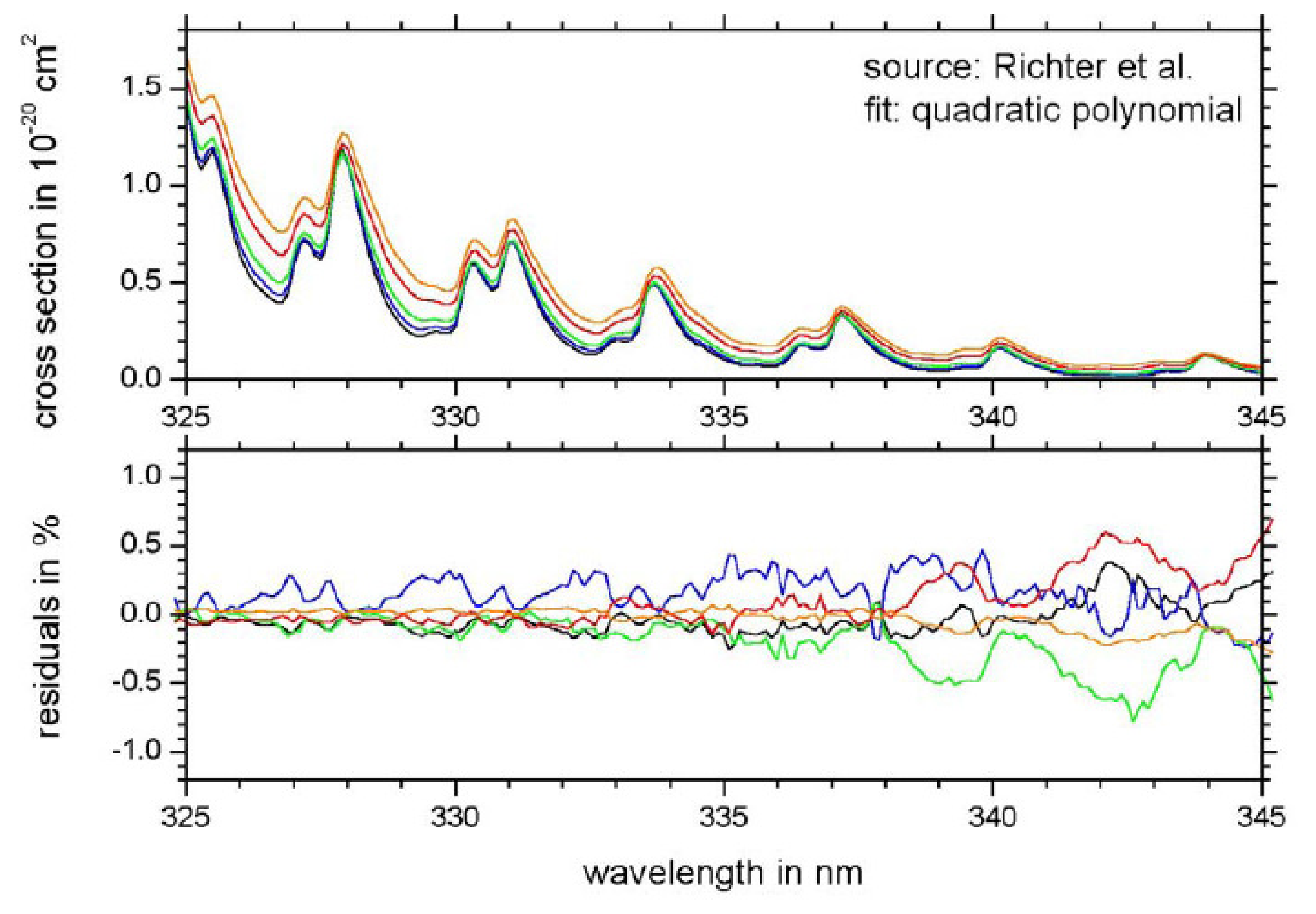


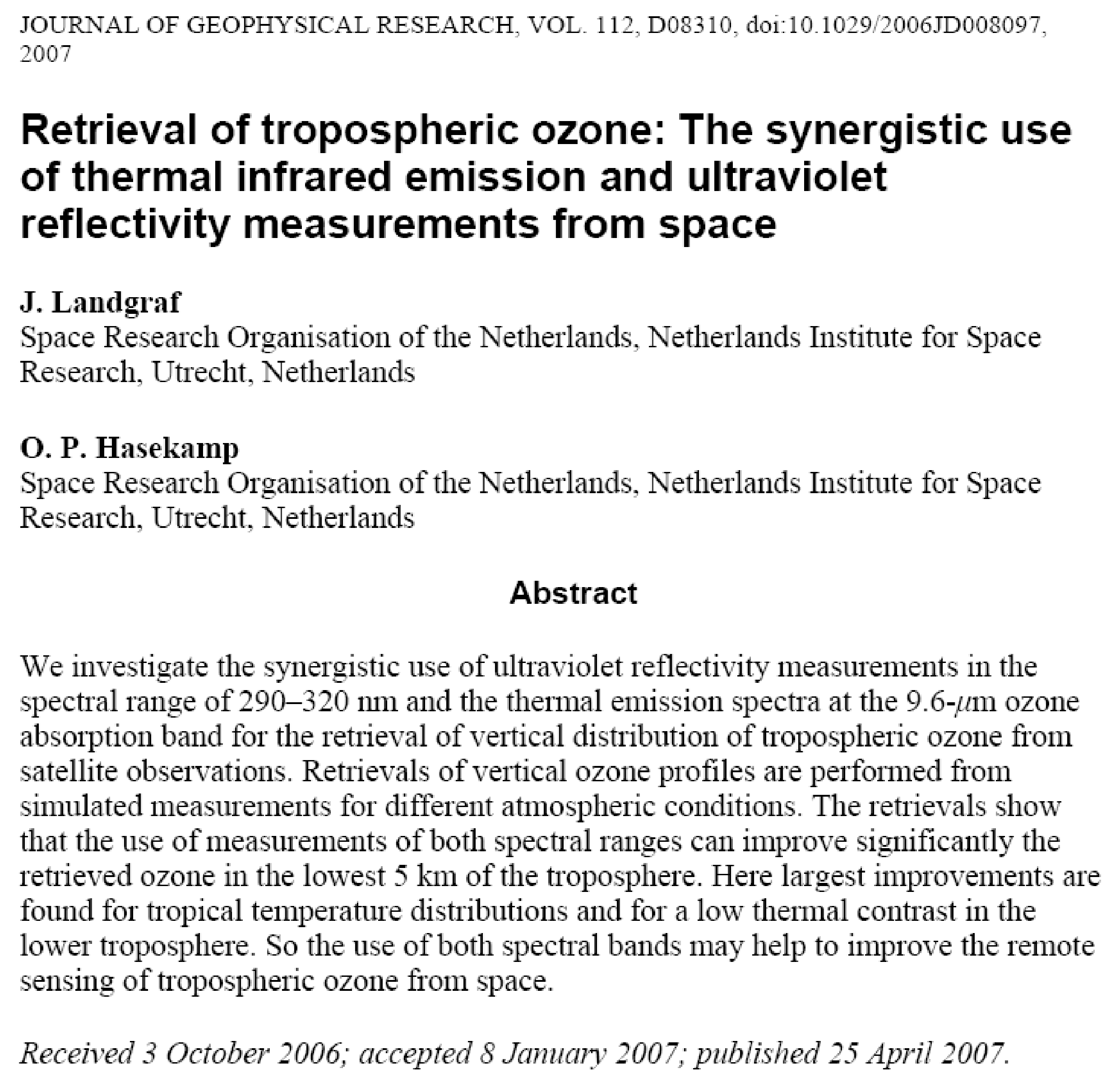
Recommendations from the ESA Review

- define an O_3 absorption standard
- take care of temperature dependence
- check resolution and λ calibration
- analyse field measurements for biases
- make new laboratory mesurements for
  - more accurate absolute values
  - temperature dependence of Chappuis
  - consistency of Huggins and Chappuis
  - consistency of UV/IR, UV/MW, etc.

3. Spectral consistency of O_3 cross sections

- UV/IR: Dufour et al., 2004
- UV/IR: Picquet-Varrault et al., 2005
- UV/IR: Ibrahim et al., 2006
- UV/VIS (GOME-2): Gür et al., 2006

O_3 IR/UV intercomparison: motivation



JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 112, D08310, doi:10.1029/2006JD008097, 2007

Retrieval of tropospheric ozone: The synergistic use of thermal infrared emission and ultraviolet reflectivity measurements from space

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Abstract

We investigate the synergistic use of ultraviolet reflectivity measurements in the spectral range of 290–320 nm and the thermal emission spectra at the 9.6-μm ozone absorption band for the retrieval of vertical distribution of tropospheric ozone from satellite observations. Retrievals of vertical ozone profiles are performed from simulated measurements for different atmospheric conditions. The retrievals show that the use of measurements of both spectral ranges can improve significantly the retrieved ozone in the lowest 5 km of the troposphere. Here largest improvements are found for tropical temperature distributions and for a low thermal contrast in the lower troposphere. So the use of both spectral bands may help to improve the remote sensing of tropospheric ozone from space.

Received 3 October 2006; accepted 8 January 2007; published 25 April 2007.

O_3 IR/UV intercomparison: motivation

806, 2007

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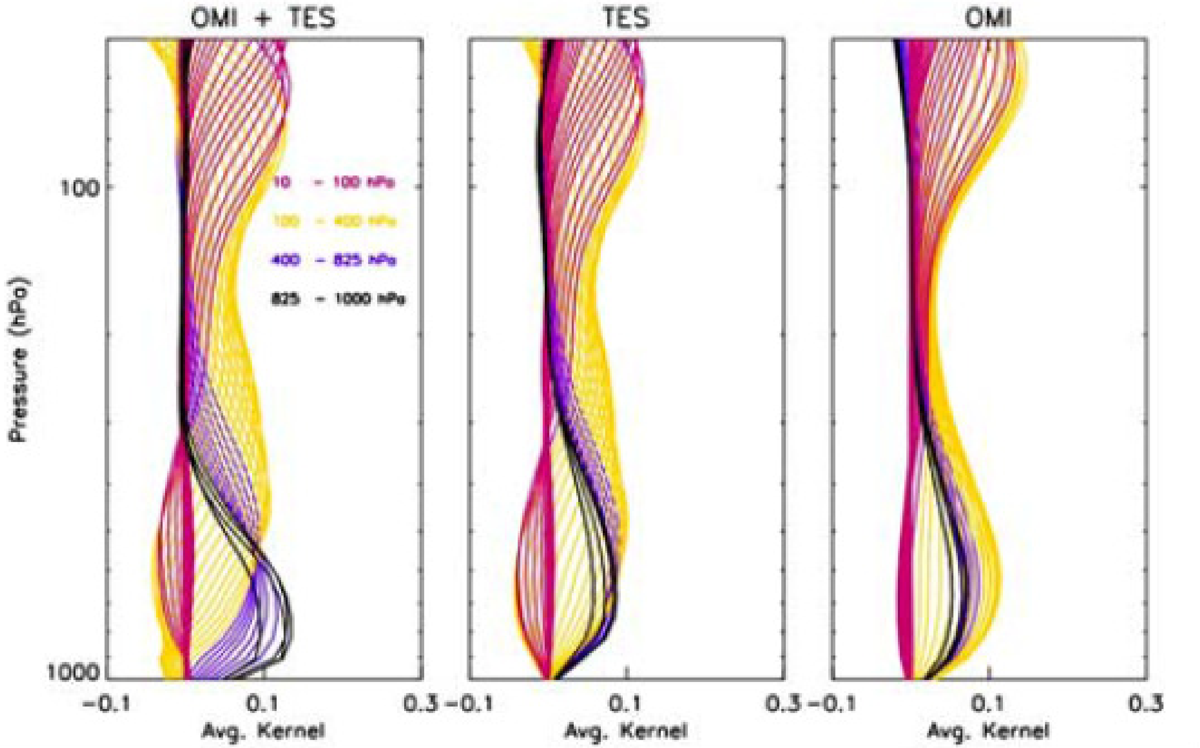
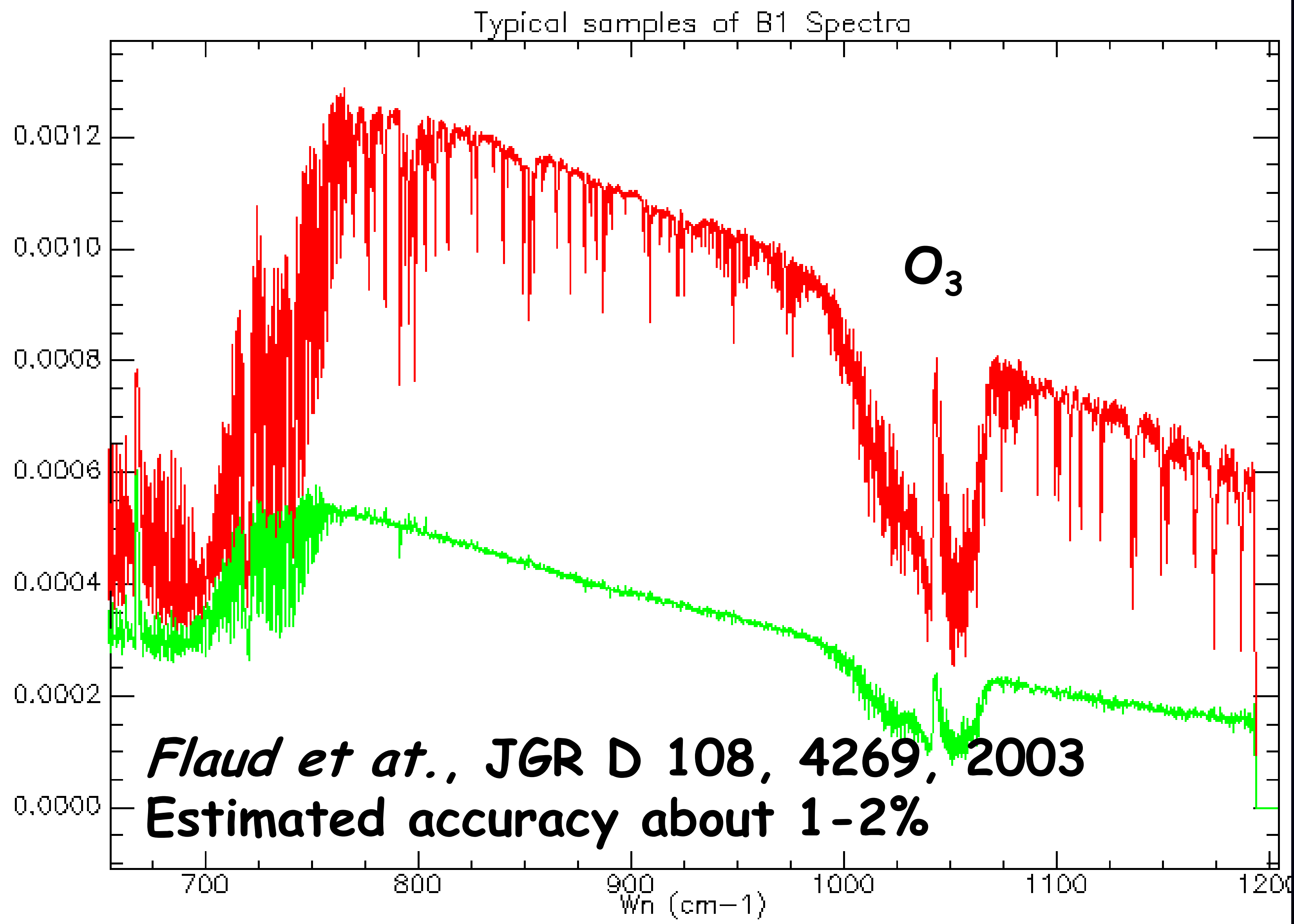


Figure 2. Examples of averaging kernels. (left) Averaging kernels for an OMI and TES synthetic ozone profile retrieval for the ozone estimate at 30.5 degrees latitude shown in Figure 1. (middle, right) Averaging kernels for this same scene but assuming a TES and OMI sounding of this scene, respectively.

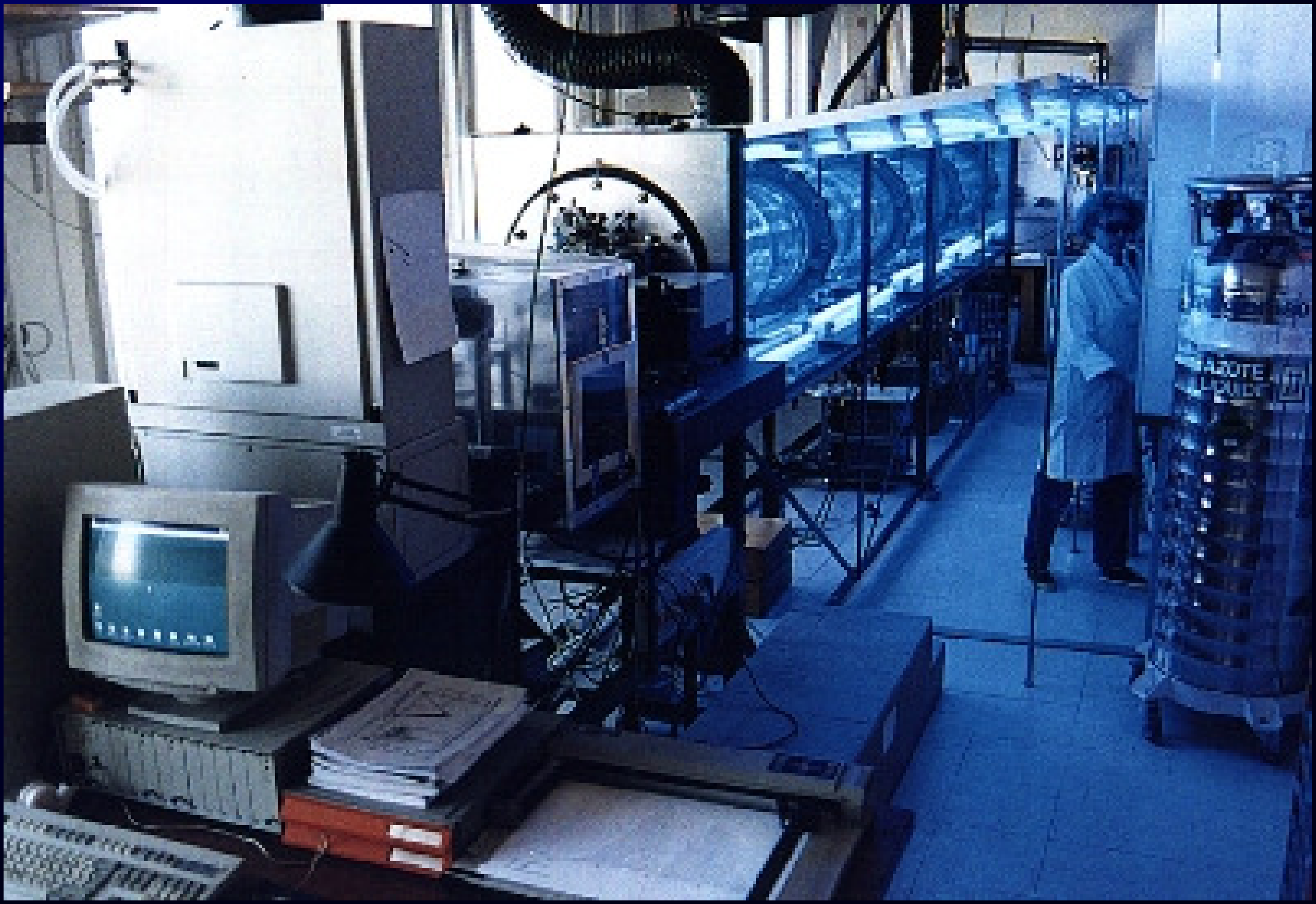
O_3 IR/UV intercomparison: motivation



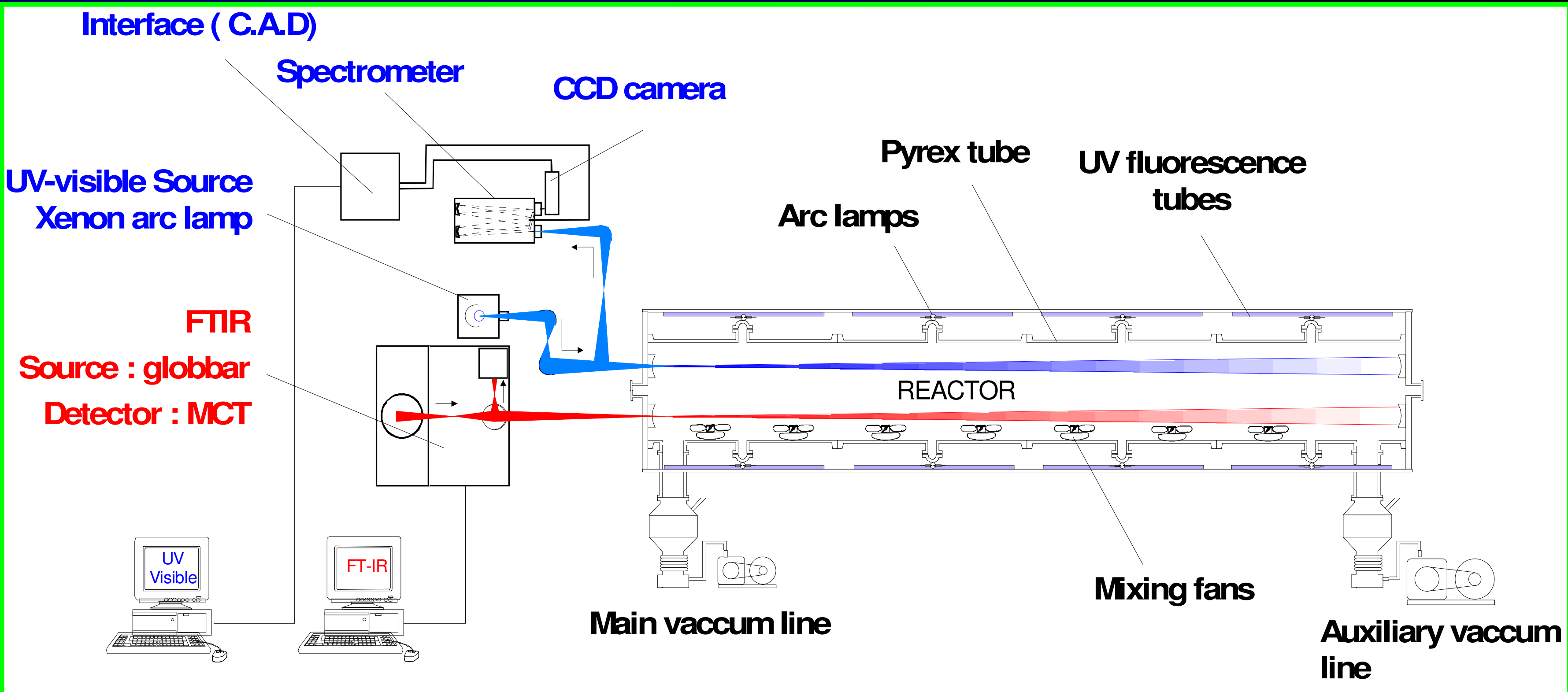
***Flaud et at.*, JGR D 108, 4269, 2003**

Estimated accuracy about 1-2%

O_3 IR/UV intercomparison: experimental set-up



O_3 IR/UV intercomparison: experimental set-up



Reactor :

Pyrex tube

Volume : 0.977 m^3

Mixing : 8 teflon fans

Vaccum :2 turbomolecular pumps
2 rotary pumps
Max vaccum : 10^{-3} mbar

Irradiation :

48 UV fluorescence tubes centred on 360 nm

48 UV fluorescence tubes centred on 420 nm

16 arc lamps

UV-Visible spectrometry :

DOAS system

Multipass White cell

Optical path length : 12 - 72 m

Source : XBO lamp

Spectral range : 290-650 nm

resolution 0.15 nm

FTIR spectrometry :

Stabilised multipass cell

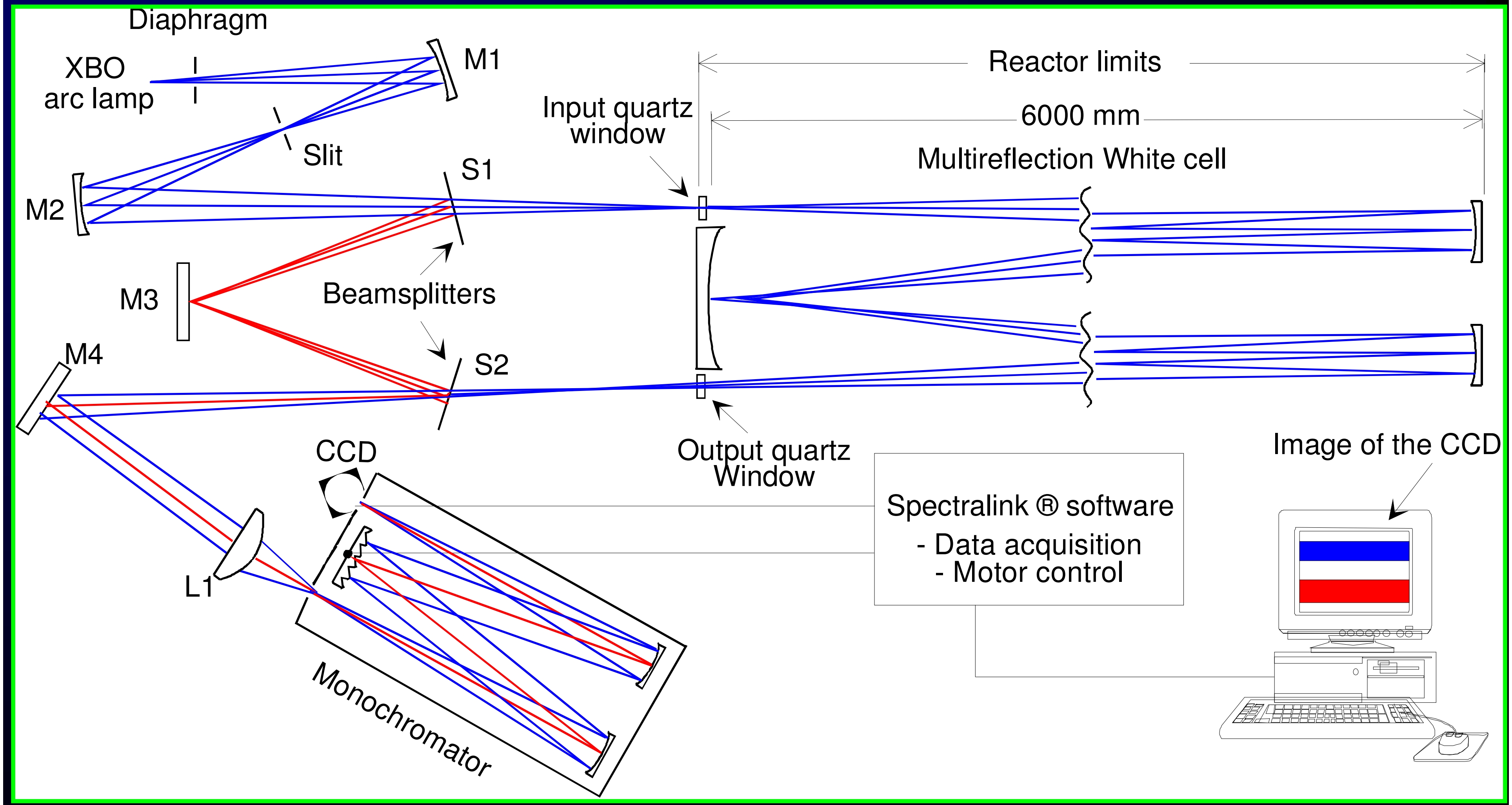
Optical path length : 12 - 672 m

Bomem DA 8 system

Spectral range : 500-5000 cm^{-1}

resolution 0.04 cm^{-1}

O_3 IR/UV intercomparison: experimental set-up



O_3 IR/UV intercomparison: results

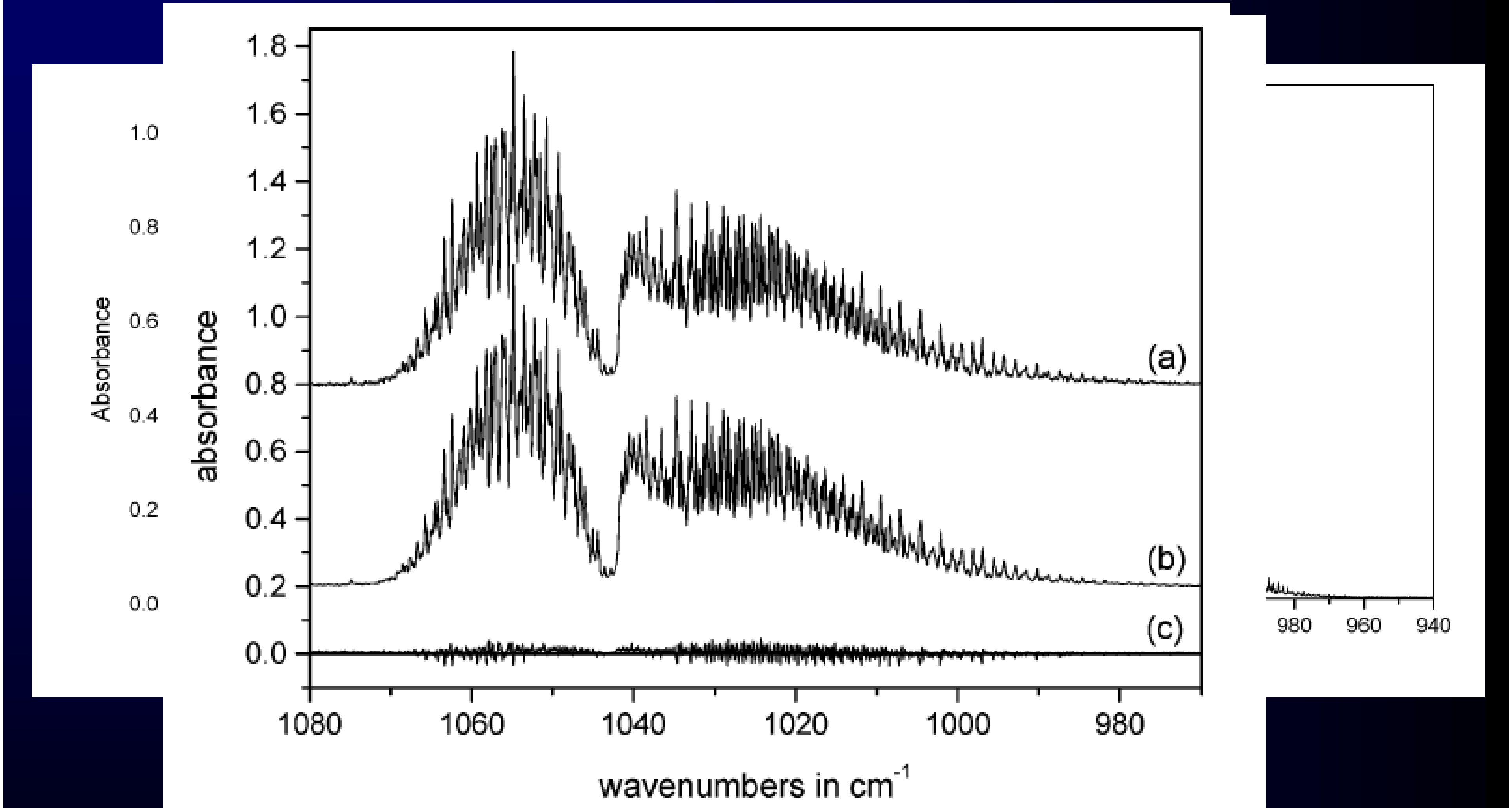
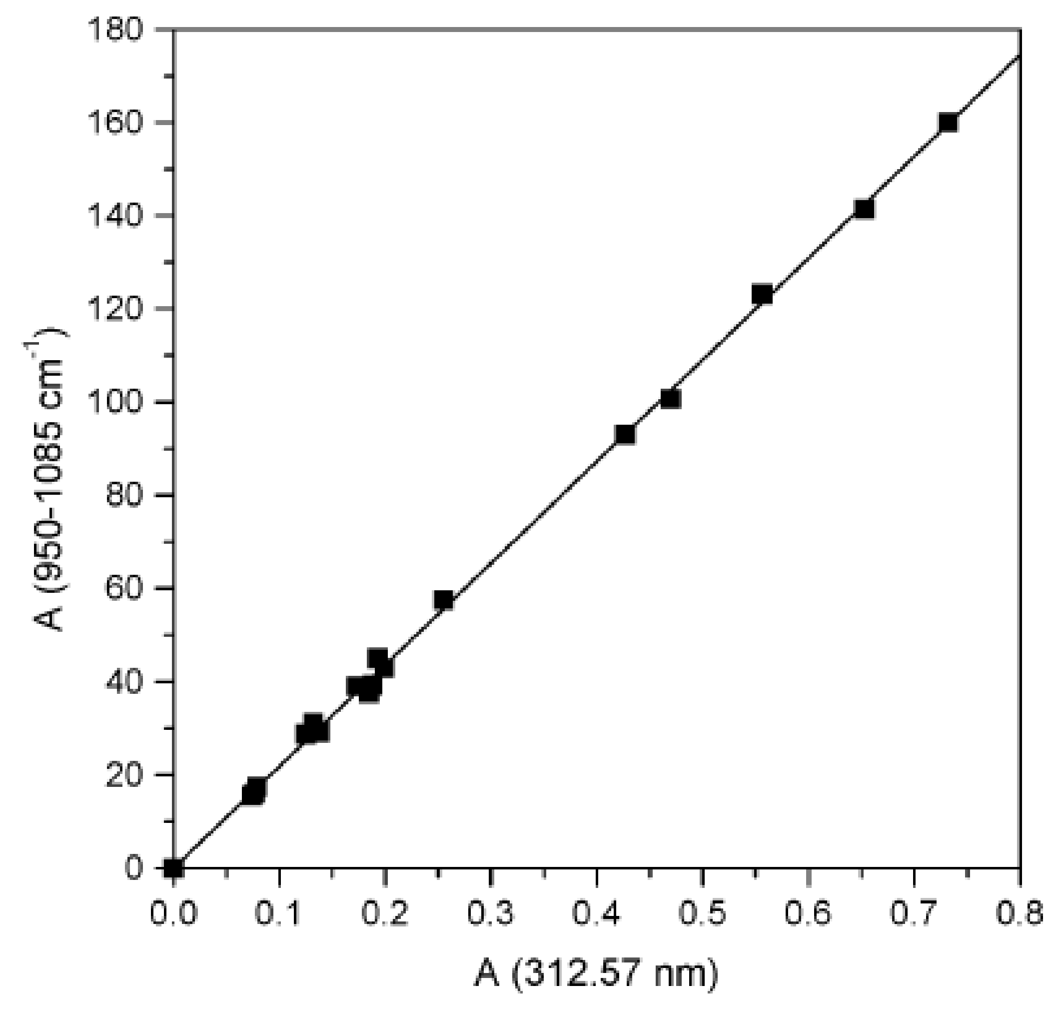


Figure 7. Comparison of IR spectrum acquired by this work (a) with theoritical spectrum calculated from the HITRAN database (b). Plot c corresponds to a − b.

O_3 IR/UV intercomparison: results



O_3 IR/UV intercomparison: results

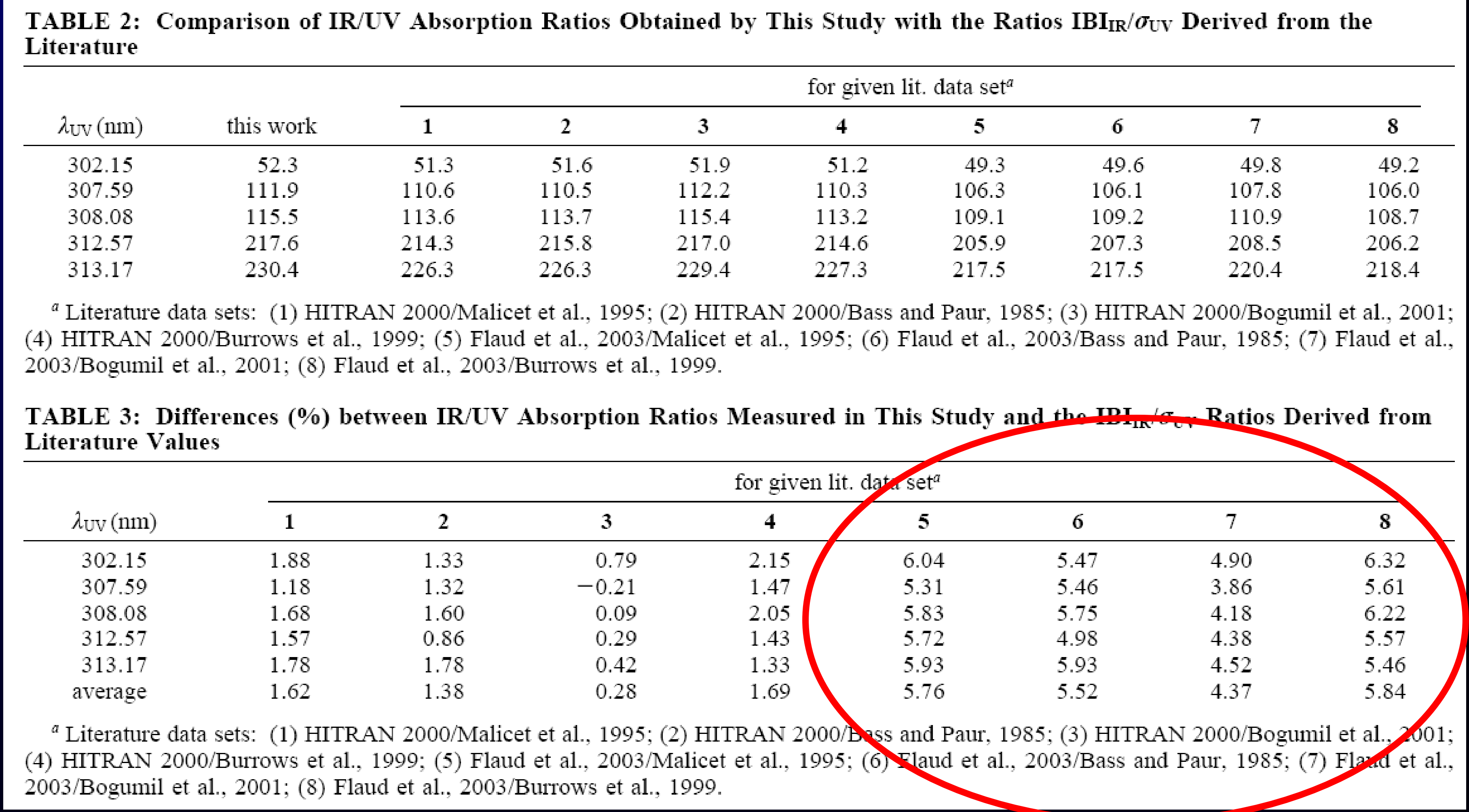


TABLE 2: Comparison of IR/UV Absorption Ratios Obtained by This Study with the Ratios IBI_{IR}/σ_{UV} Derived from the Literature

		for given lit. data set[a]							
λ_{UV} (nm)	this work	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
302.15	52.3	51.3	51.6	51.9	51.2	49.3	49.6	49.8	49.2
307.59	111.9	110.6	110.5	112.2	110.3	106.3	106.1	107.8	106.0
308.08	115.5	113.6	113.7	115.4	113.2	109.1	109.2	110.9	108.7
312.57	217.6	214.3	215.8	217.0	214.6	205.9	207.3	208.5	206.2
313.17	230.4	226.3	226.3	229.4	227.3	217.5	217.5	220.4	218.4

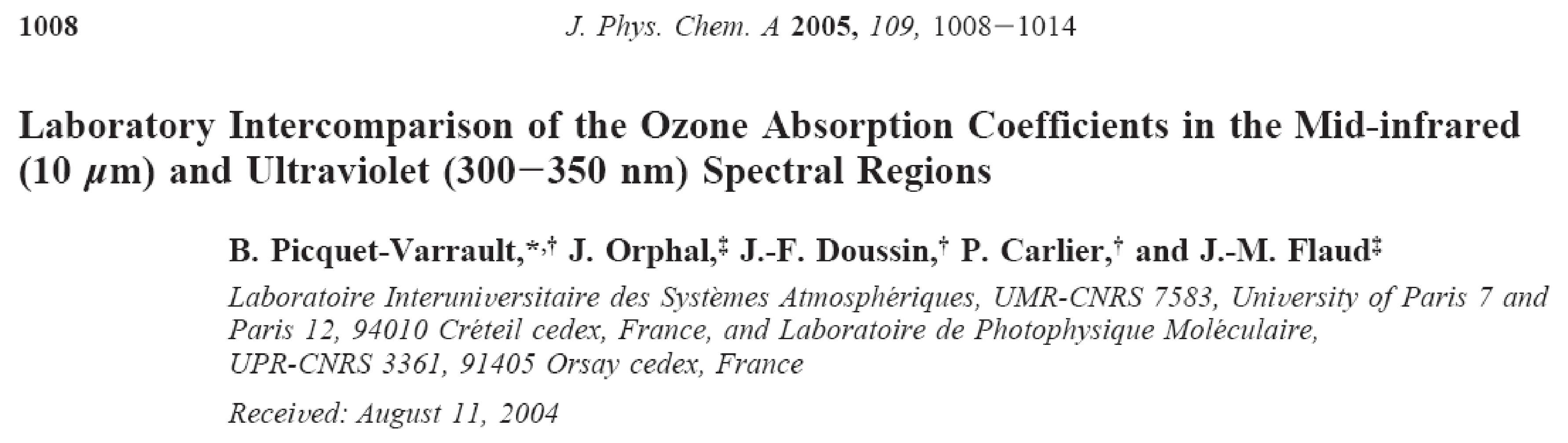
[a] Literature data sets: (1) HITRAN 2000/Malicet et al., 1995; (2) HITRAN 2000/Bass and Paur, 1985; (3) HITRAN 2000/Bogumil et al., 2001; (4) HITRAN 2000/Burrows et al., 1999; (5) Flaud et al., 2003/Malicet et al., 1995; (6) Flaud et al., 2003/Bass and Paur, 1985; (7) Flaud et al., 2003/Bogumil et al., 2001; (8) Flaud et al., 2003/Burrows et al., 1999.

TABLE 3: Differences (%) between IR/UV Absorption Ratios Measured in This Study and the IBI_{IR}/σ_{UV} Ratios Derived from Literature Values

	for given lit. data set[a]							
λ_{UV} (nm)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
302.15	1.88	1.33	0.79	2.15	6.04	5.47	4.90	6.32
307.59	1.18	1.32	−0.21	1.47	5.31	5.46	3.86	5.61
308.08	1.68	1.60	0.09	2.05	5.83	5.75	4.18	6.22
312.57	1.57	0.86	0.29	1.43	5.72	4.98	4.38	5.57
313.17	1.78	1.78	0.42	1.33	5.93	5.93	4.52	5.46
average	1.62	1.38	0.28	1.69	5.76	5.52	4.37	5.84

[a] Literature data sets: (1) HITRAN 2000/Malicet et al., 1995; (2) HITRAN 2000/Bass and Paur, 1985; (3) HITRAN 2000/Bogumil et al., 2001; (4) HITRAN 2000/Burrows et al., 1999; (5) Flaud et al., 2003/Malicet et al., 1995; (6) Flaud et al., 2003/Bass and Paur, 1985; (7) Flaud et al., 2003/Bogumil et al., 2001; (8) Flaud et al., 2003/Burrows et al., 1999.

O_3 IR/UV intercomparison: results



1008 *J. Phys. Chem. A* **2005,** *109,* 1008−1014

Laboratory Intercomparison of the Ozone Absorption Coefficients in the Mid-infrared (10 μm) and Ultraviolet (300−350 nm) Spectral Regions

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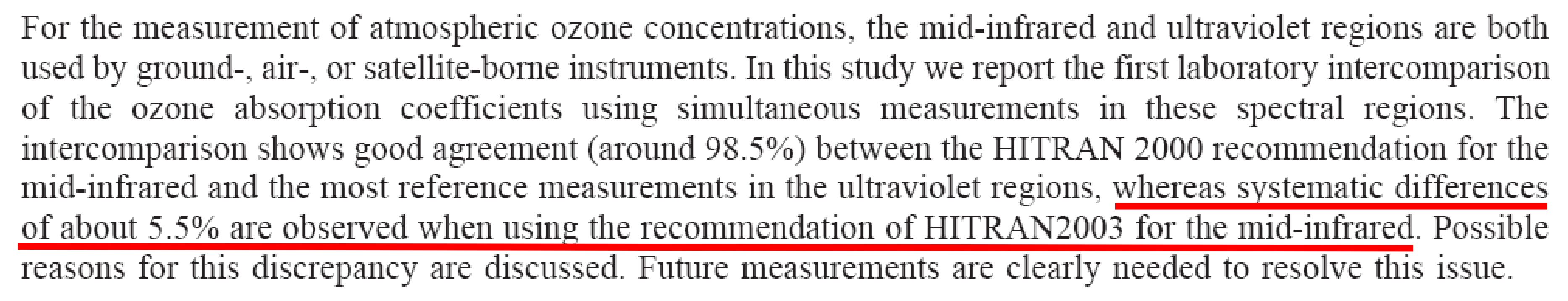
Laboratoire Interuniversitaire des Systèmes Atmosphériques, UMR-CNRS 7583, University of Paris 7 and Paris 12, 94010 Créteil cedex, France, and Laboratoire de Photophysique Moléculaire, UPR-CNRS 3361, 91405 Orsay cedex, France

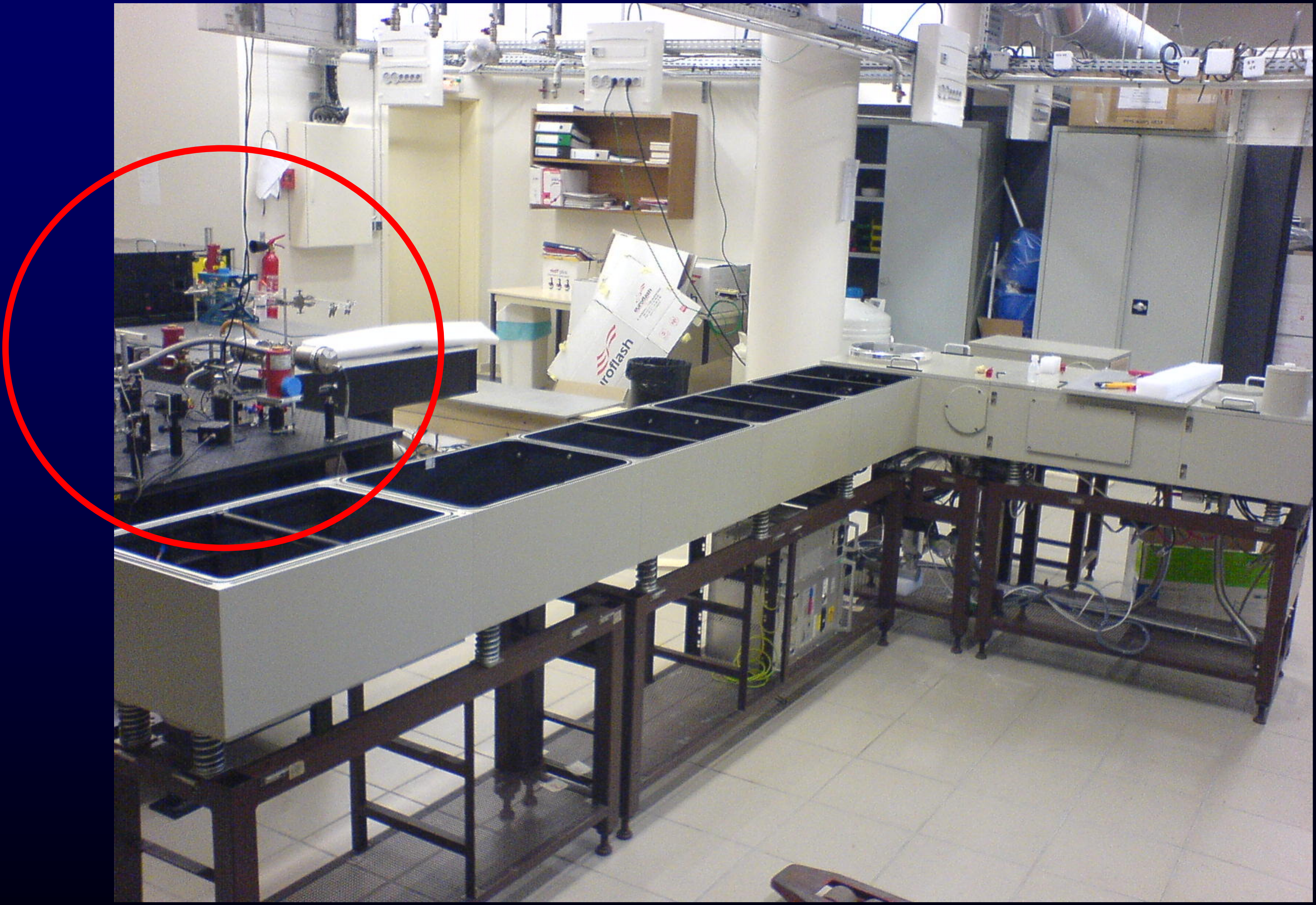
Received: August 11, 2004



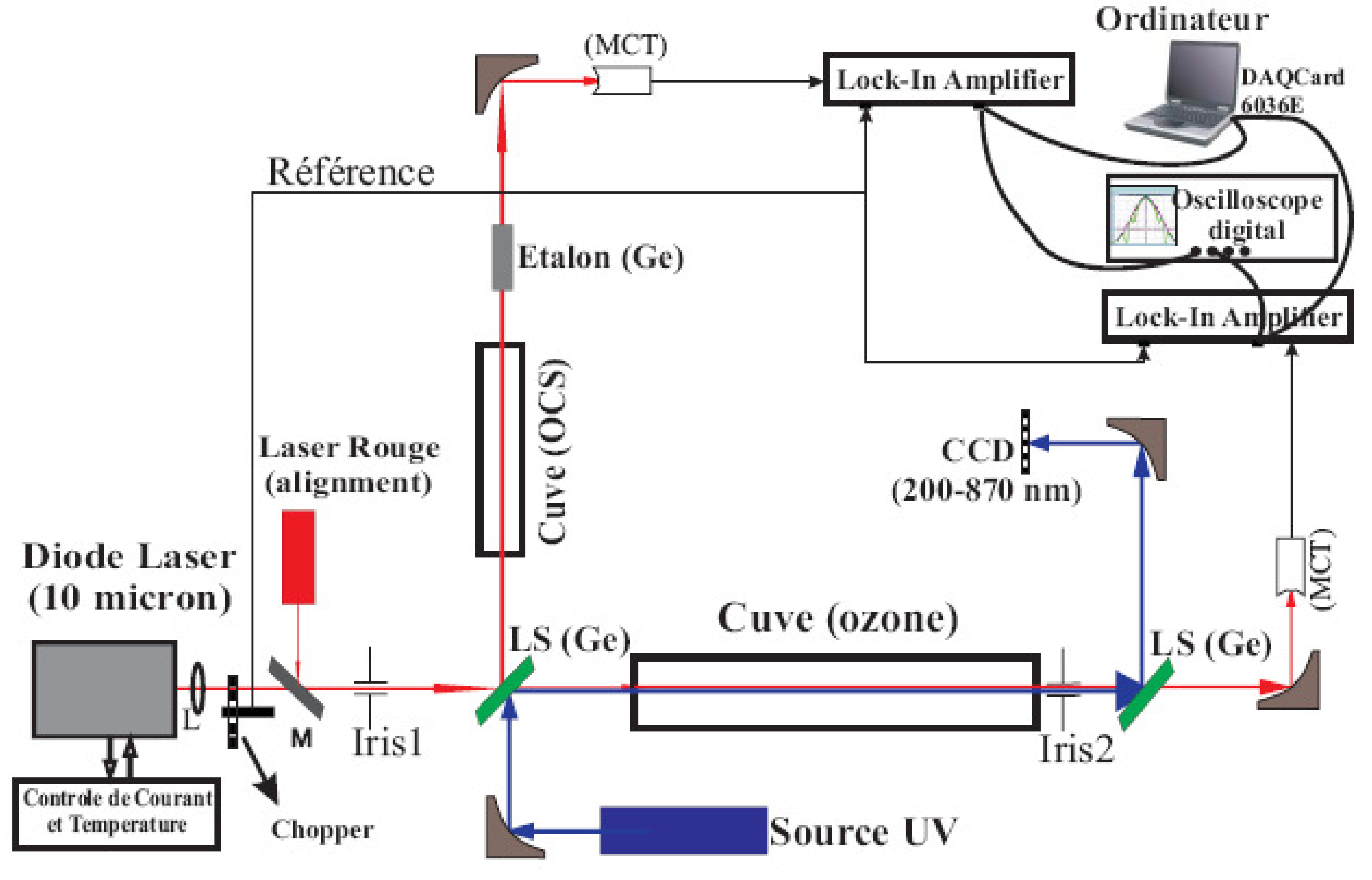
For the measurement of atmospheric ozone concentrations, the mid-infrared and ultraviolet regions are both used by ground-, air-, or satellite-borne instruments. In this study we report the first laboratory intercomparison of the ozone absorption coefficients using simultaneous measurements in these spectral regions. The intercomparison shows good agreement (around 98.5%) between the HITRAN 2000 recommendation for the mid-infrared and the most reference measurements in the ultraviolet regions, whereas systematic differences of about 5.5% are observed when using the recommendation of HITRAN2003 for the mid-infrared. Possible reasons for this discrepancy are discussed. Future measurements are clearly needed to resolve this issue.

Difference of about 5 %: new measurements needed!

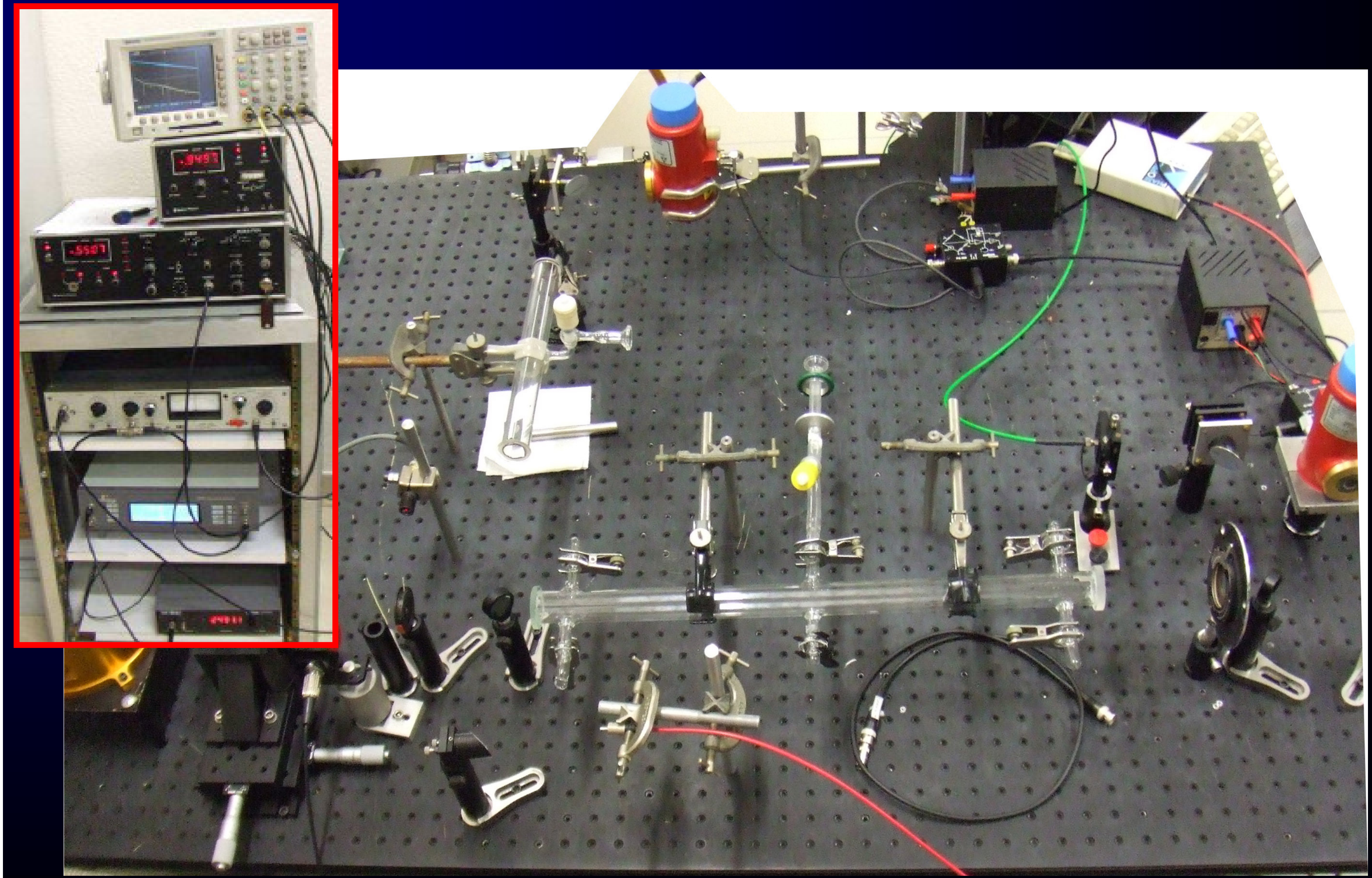
O_3 intercomparison using laser/CCD



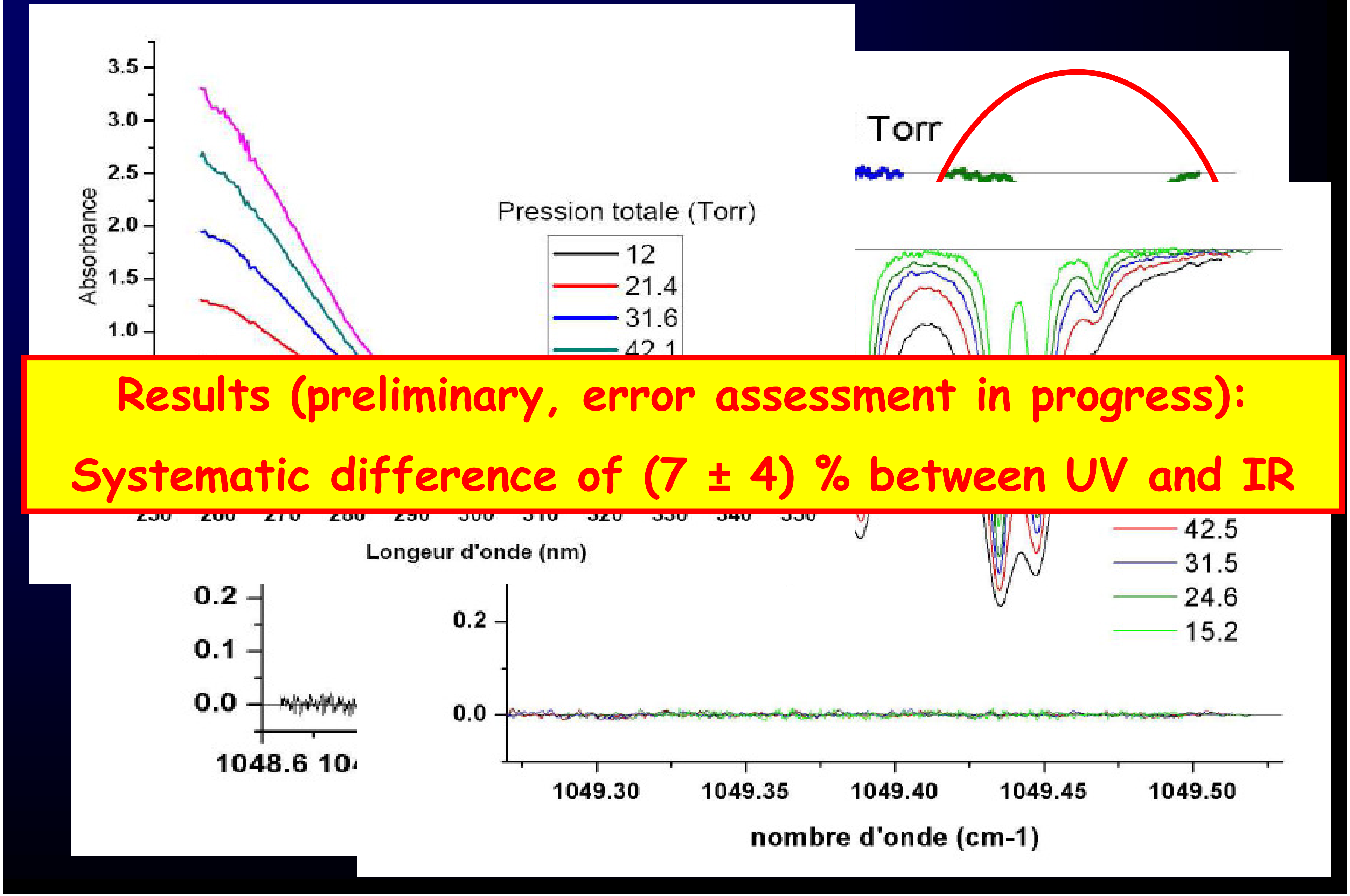
O_3 intercomparison using laser/CCD



O_3 intercomparison using laser/CCD



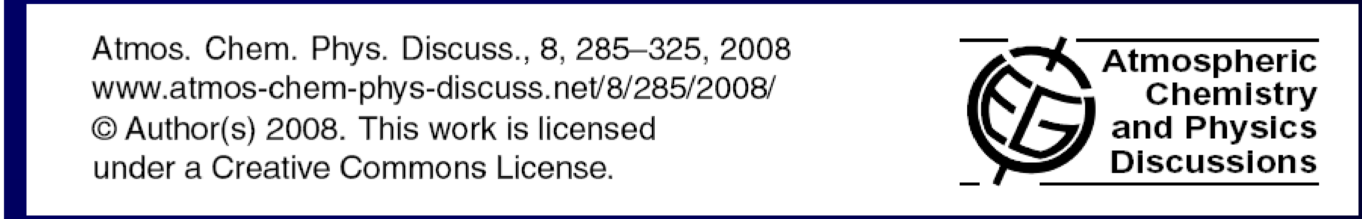
O_3 intercomparison using laser/CCD



Results (preliminary, error assessment in progress):

Systematic difference of (7 ± 4) % between UV and IR

What is seen in atmospheric ozone data?

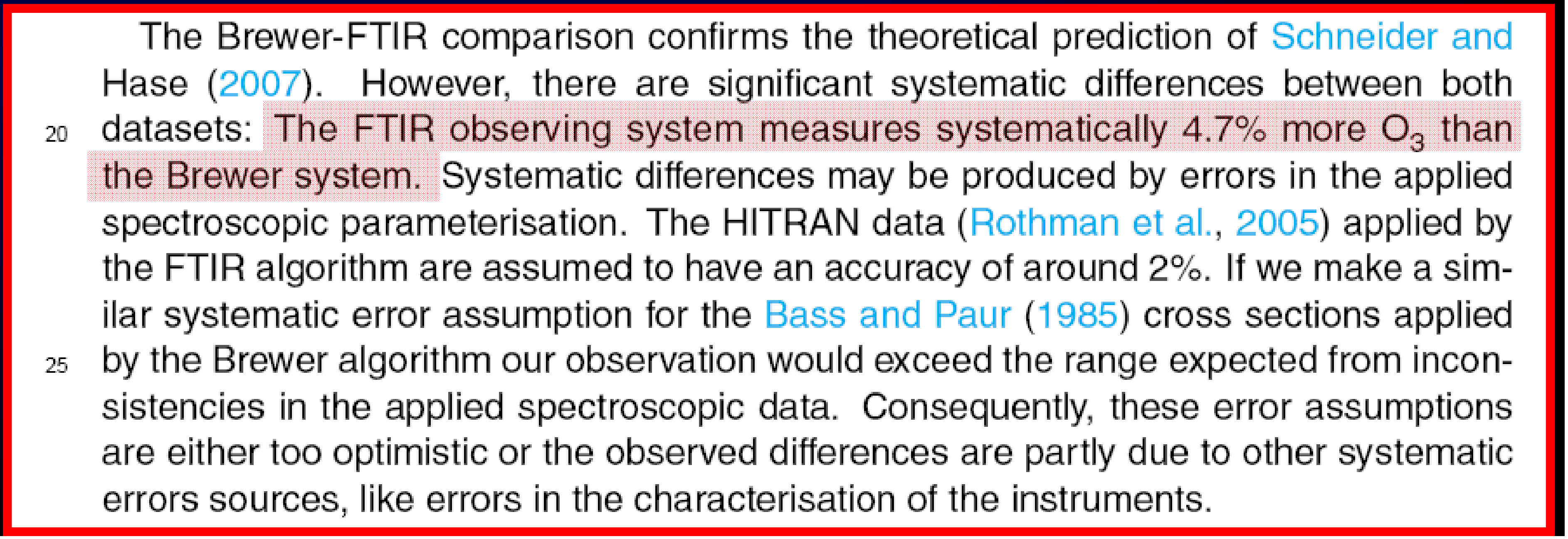

Atmos. Chem. Phys. Discuss., 8, 285–325, 2008
www.atmos-chem-phys-discuss.net/8/285/2008/

Atmospheric
Chemistry
and Physics
Discussions

Comparison of ground-based Brewer and FTIR total O_3 monitoring techniques

M. Schneider[1], A. Redondas[2], F. Hase[1], C. Guirado[2], T. Blumenstock[1], and E. Cuevas[2]

[1]IMK-ASF, Forschungszentrum Karlsruhe, Karlsruhe, Germany
[2]Observatorio Atmosférico de Izaña, Instituto Nacional de Meteorología, Spain



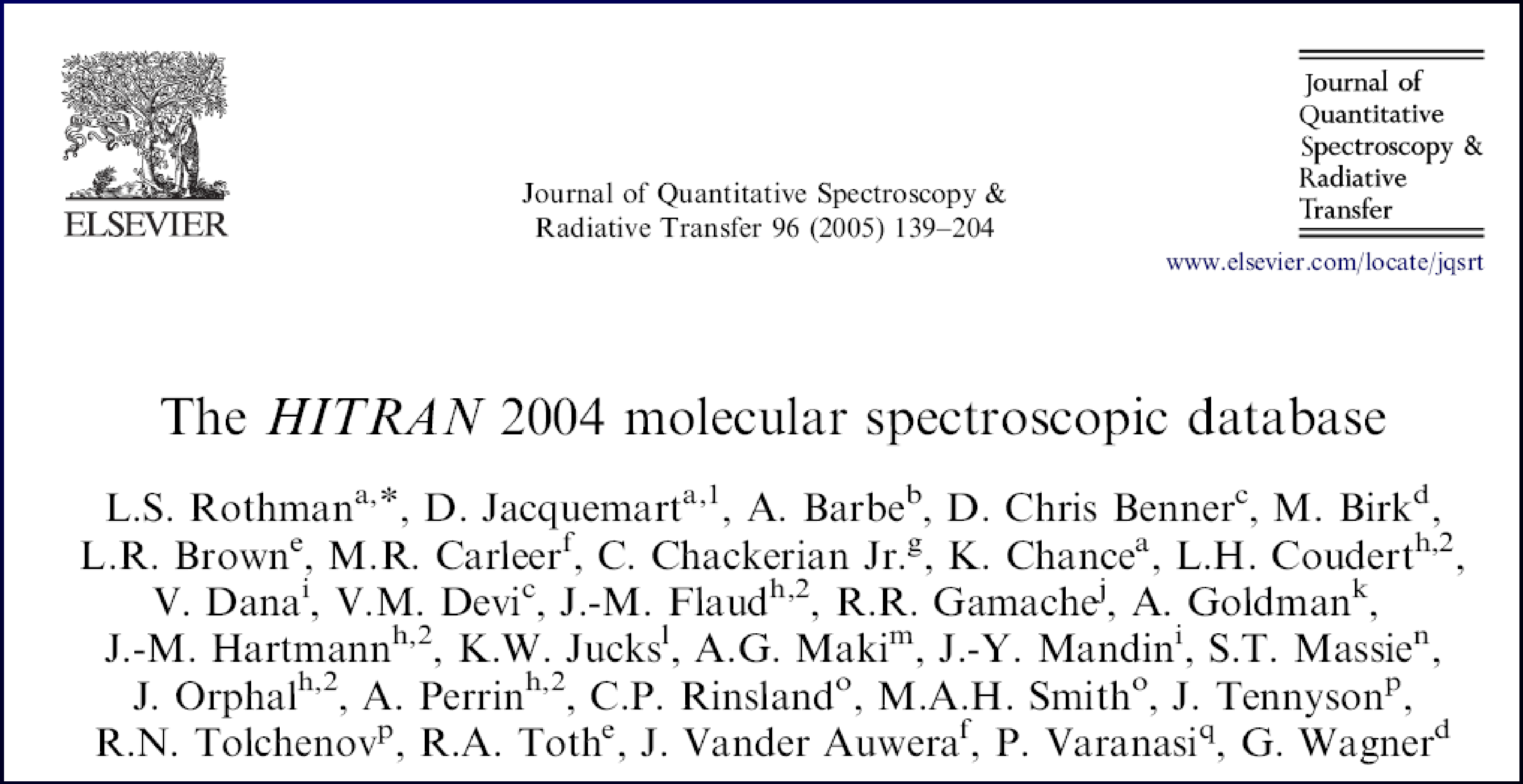
The Brewer-FTIR comparison confirms the theoretical prediction of Schneider and Hase (2007). However, there are significant systematic differences between both datasets: The FTIR observing system measures systematically 4.7% more O_3 than the Brewer system. Systematic differences may be produced by errors in the applied spectroscopic parameterisation. The HITRAN data (Rothman et al., 2005) applied by the FTIR algorithm are assumed to have an accuracy of around 2%. If we make a similar systematic error assumption for the Bass and Paur (1985) cross sections applied by the Brewer algorithm our observation would exceed the range expected from inconsistencies in the applied spectroscopic data. Consequently, these error assumptions are either too optimistic or the observed differences are partly due to other systematic errors sources, like errors in the characterisation of the instruments.

Conclusions from UV/IR intercomparison

- depend on spectral regions
  - Hartley / Huggins / Chappuis for UV-VIS
  - 10 or 5 microns bands for IR
- possible systematic difference of about 5%
- more laboratory studies needed

O_3 cross-sections in spectroscopy databases

HITRAN database (2004)



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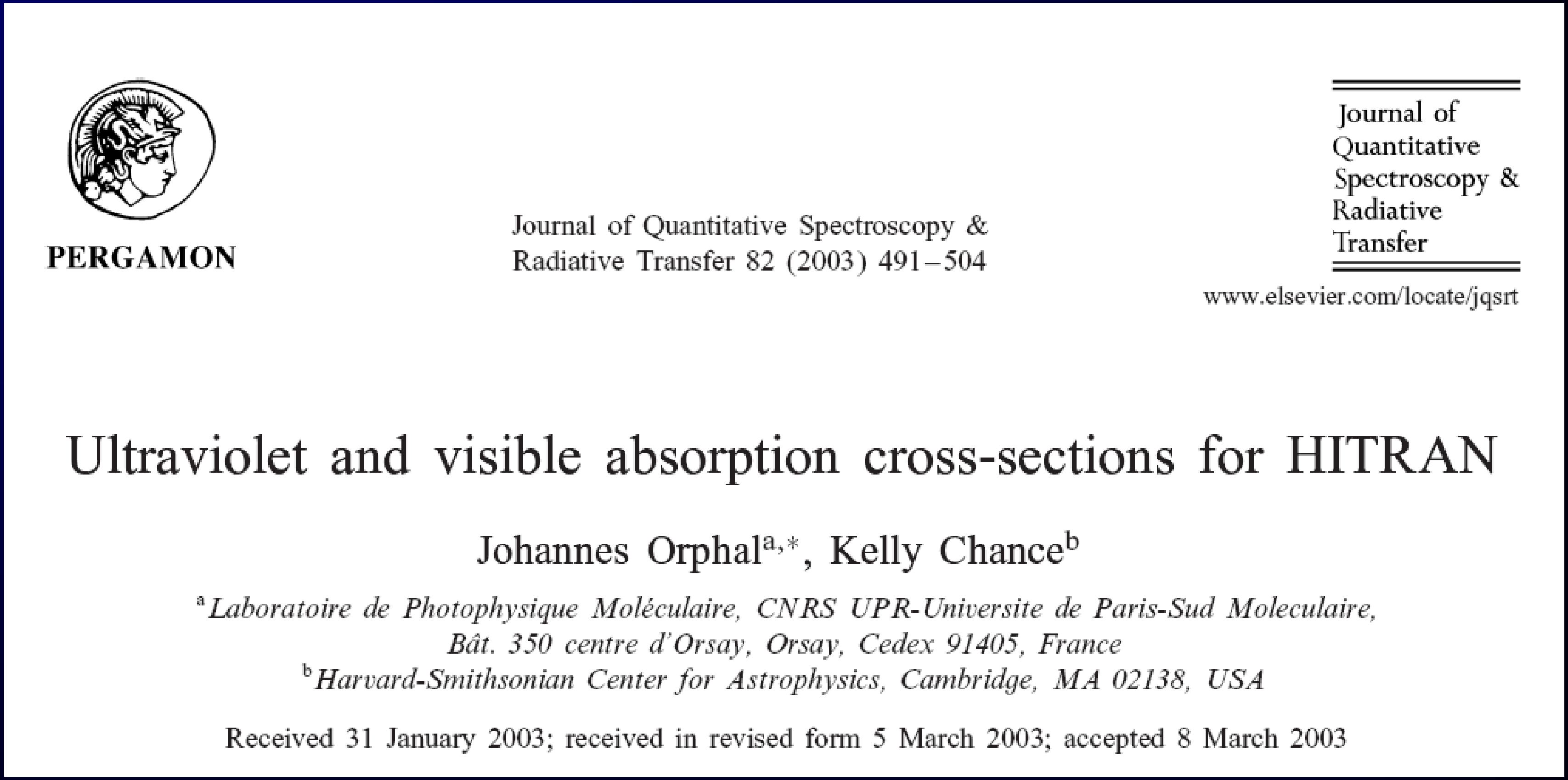
The *HITRAN* 2004 molecular spectroscopic database

L.S. Rothman[a,*], D. Jacquemart[a,1], A. Barbe[b], D. Chris Benner[c], M. Birk[d],
L.R. Brown[e], M.R. Carleer[f], C. Chackerian Jr.[g], K. Chance[a], L.H. Coudert[h,2],
V. Dana[i], V.M. Devi[c], J.-M. Flaud[h,2], R.R. Gamache[j], A. Goldman[k],
J.-M. Hartmann[h,2], K.W. Jucks[l], A.G. Maki[m], J.-Y. Mandin[i], S.T. Massie[n],
J. Orphal[h,2], A. Perrin[h,2], C.P. Rinsland[o], M.A.H. Smith[o], J. Tennyson[p],
R.N. Tolchenov[p], R.A. Toth[e], J. Vander Auwera[f], P. Varanasi[q], G. Wagner[d]

HITRAN database (2004)



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Journal of Quantitative Spectroscopy &
Radiative Transfer 82 (2003) 491–504

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Ultraviolet and visible absorption cross-sections for HITRAN

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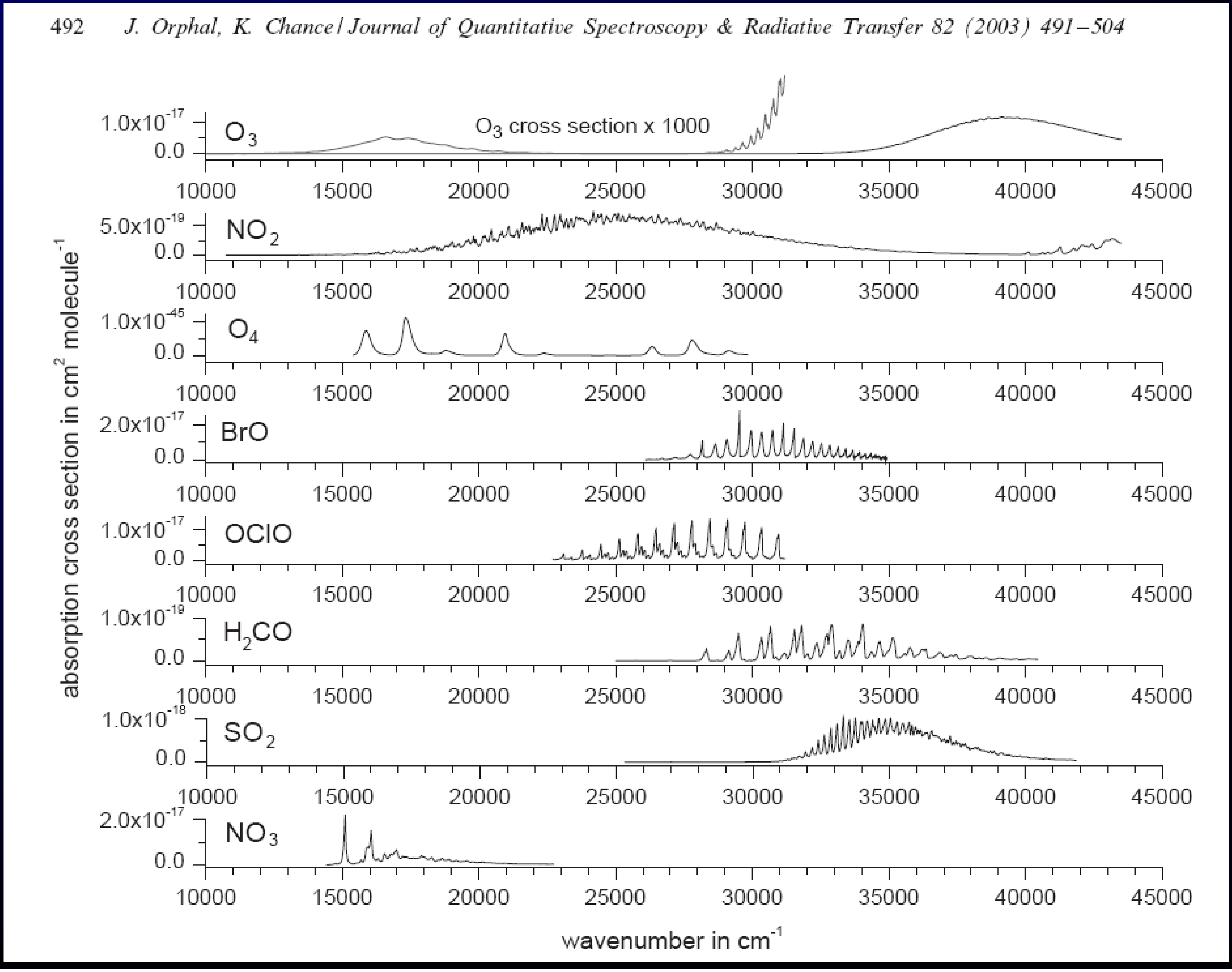
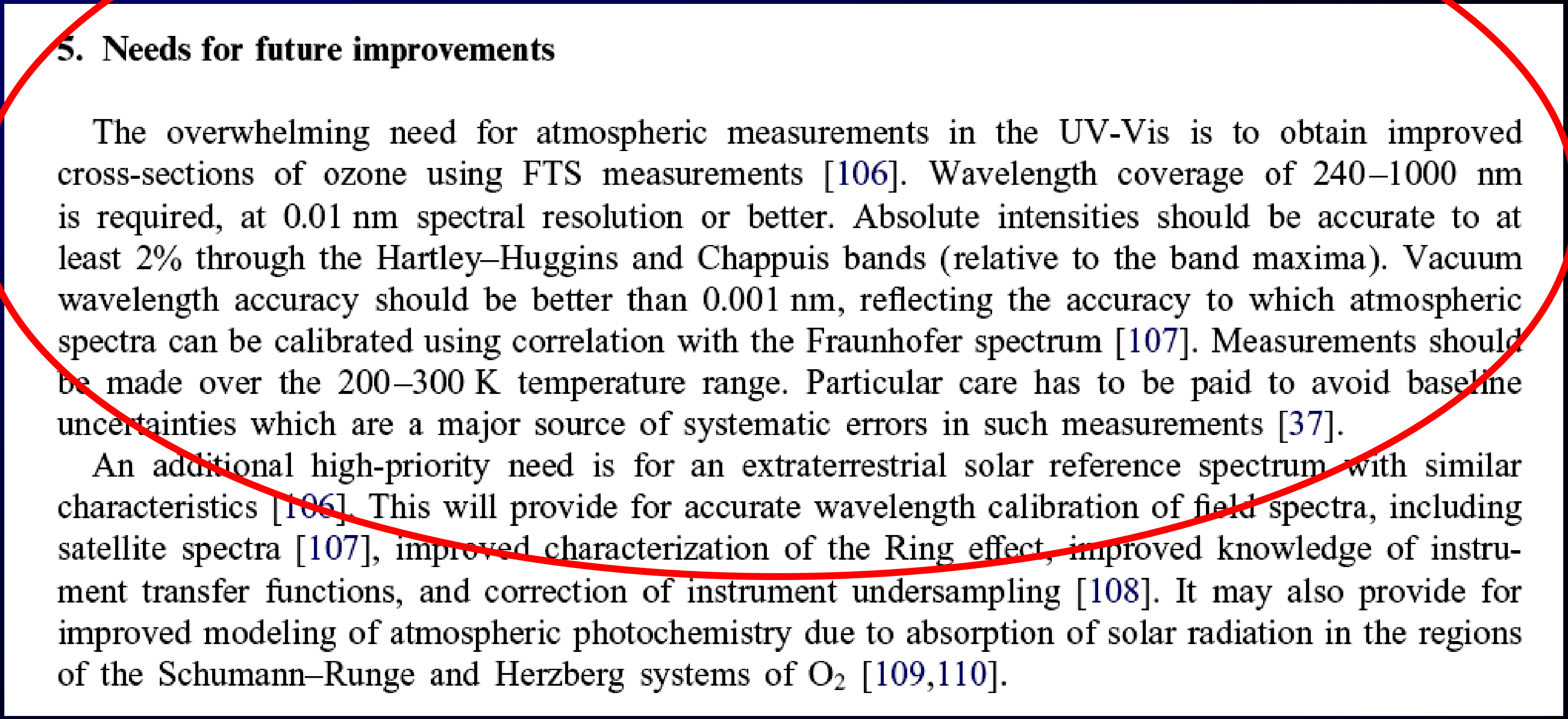
Received 31 January 2003; received in revised form 5 March 2003; accepted 8 March 2003

HITRAN database (2004)



492 J. Orphal, K. Chance / Journal of Quantitative Spectroscopy & Radiative Transfer 82 (2003) 491–504

HITRAN database (2004)

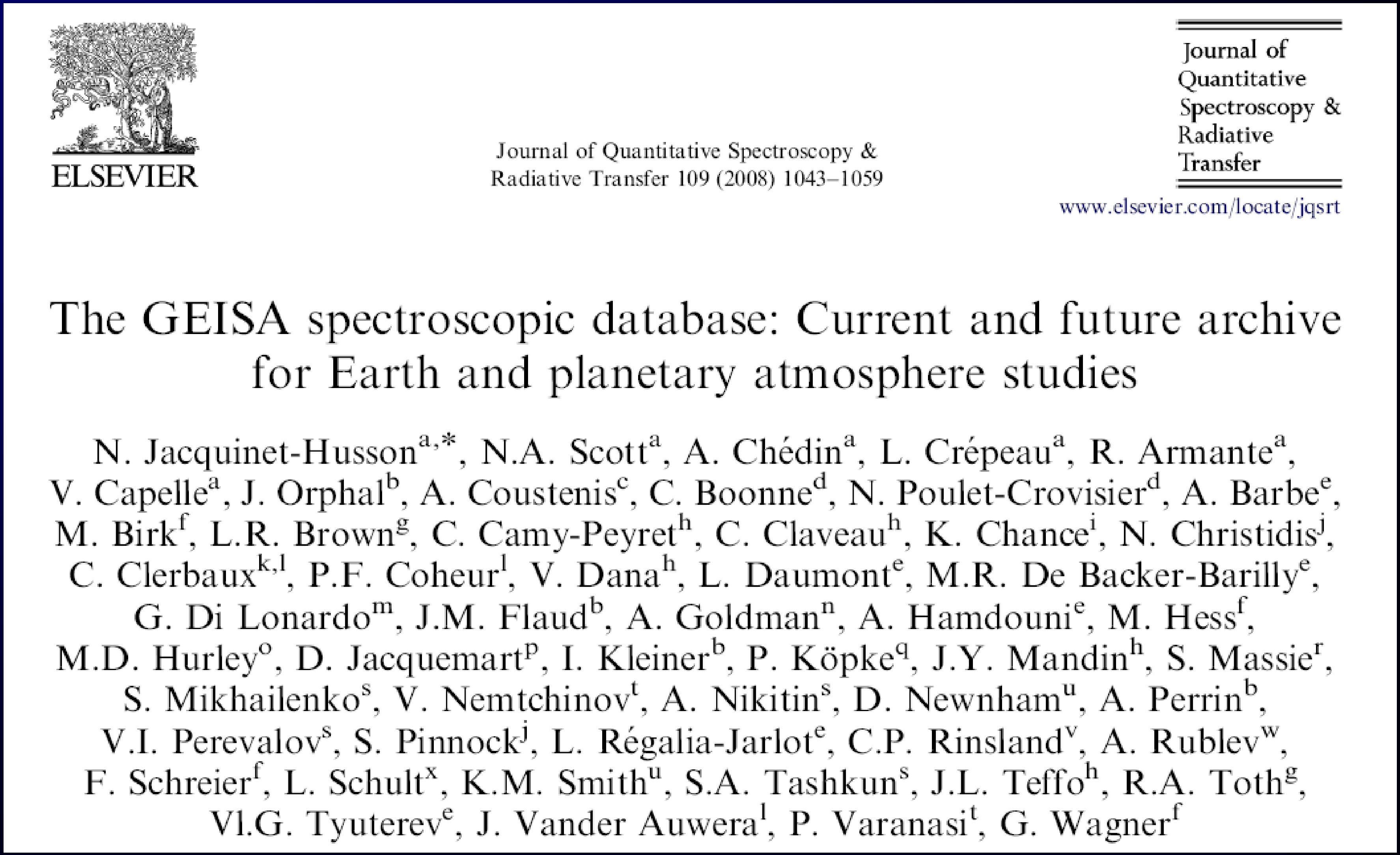


5. Needs for future improvements

The overwhelming need for atmospheric measurements in the UV-Vis is to obtain improved cross-sections of ozone using FTS measurements [106]. Wavelength coverage of 240–1000 nm is required, at 0.01 nm spectral resolution or better. Absolute intensities should be accurate to at least 2% through the Hartley–Huggins and Chappuis bands (relative to the band maxima). Vacuum wavelength accuracy should be better than 0.001 nm, reflecting the accuracy to which atmospheric spectra can be calibrated using correlation with the Fraunhofer spectrum [107]. Measurements should be made over the 200–300 K temperature range. Particular care has to be paid to avoid baseline uncertainties which are a major source of systematic errors in such measurements [37].

An additional high-priority need is for an extraterrestrial solar reference spectrum with similar characteristics [106]. This will provide for accurate wavelength calibration of field spectra, including satellite spectra [107], improved characterization of the Ring effect, improved knowledge of instrument transfer functions, and correction of instrument undersampling [108]. It may also provide for improved modeling of atmospheric photochemistry due to absorption of solar radiation in the regions of the Schumann–Runge and Herzberg systems of O_2 [109,110].

GEISA database (2008)



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The GEISA spectroscopic database: Current and future archive for Earth and planetary atmosphere studies

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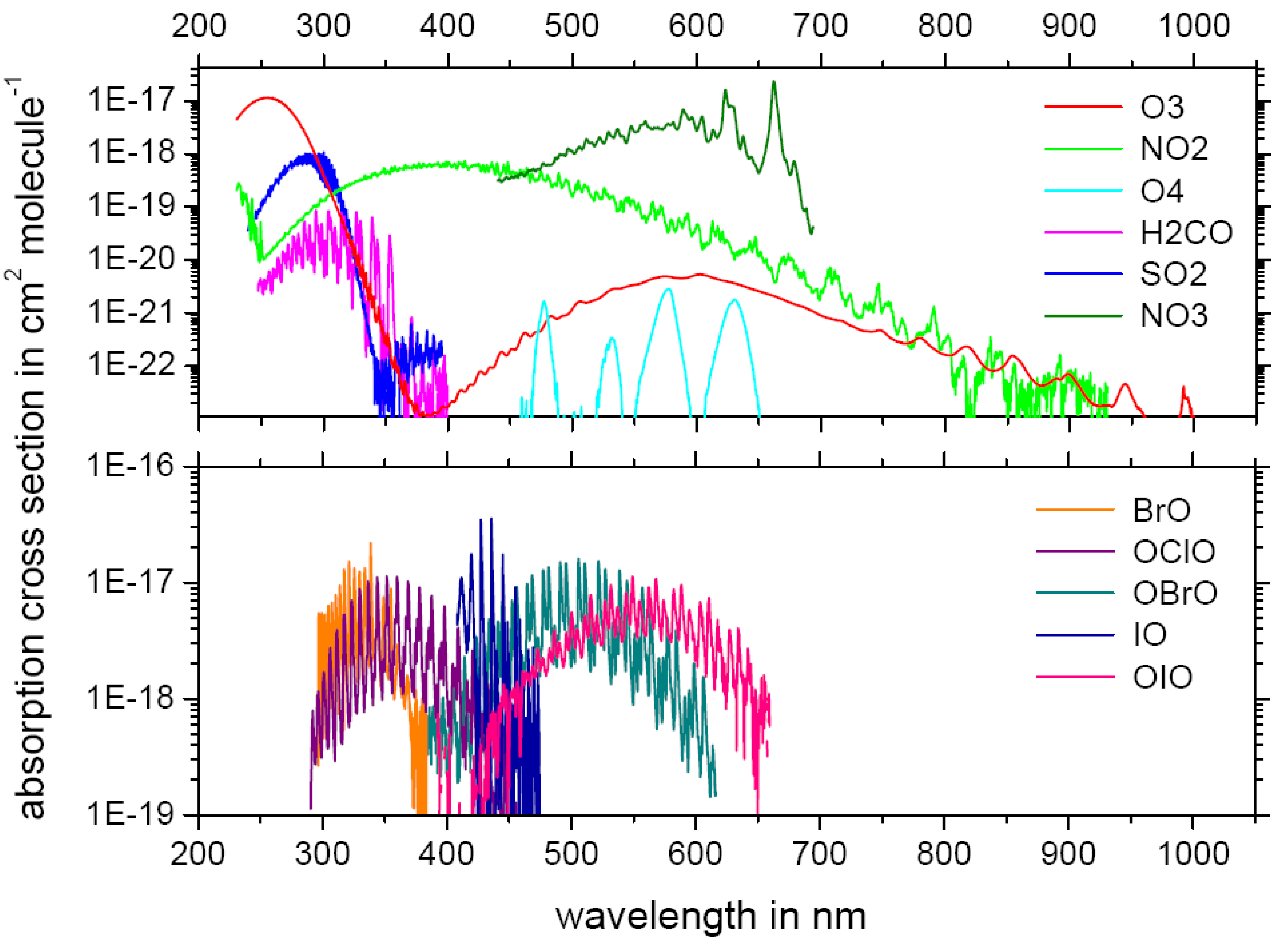
GEISA database (2008)



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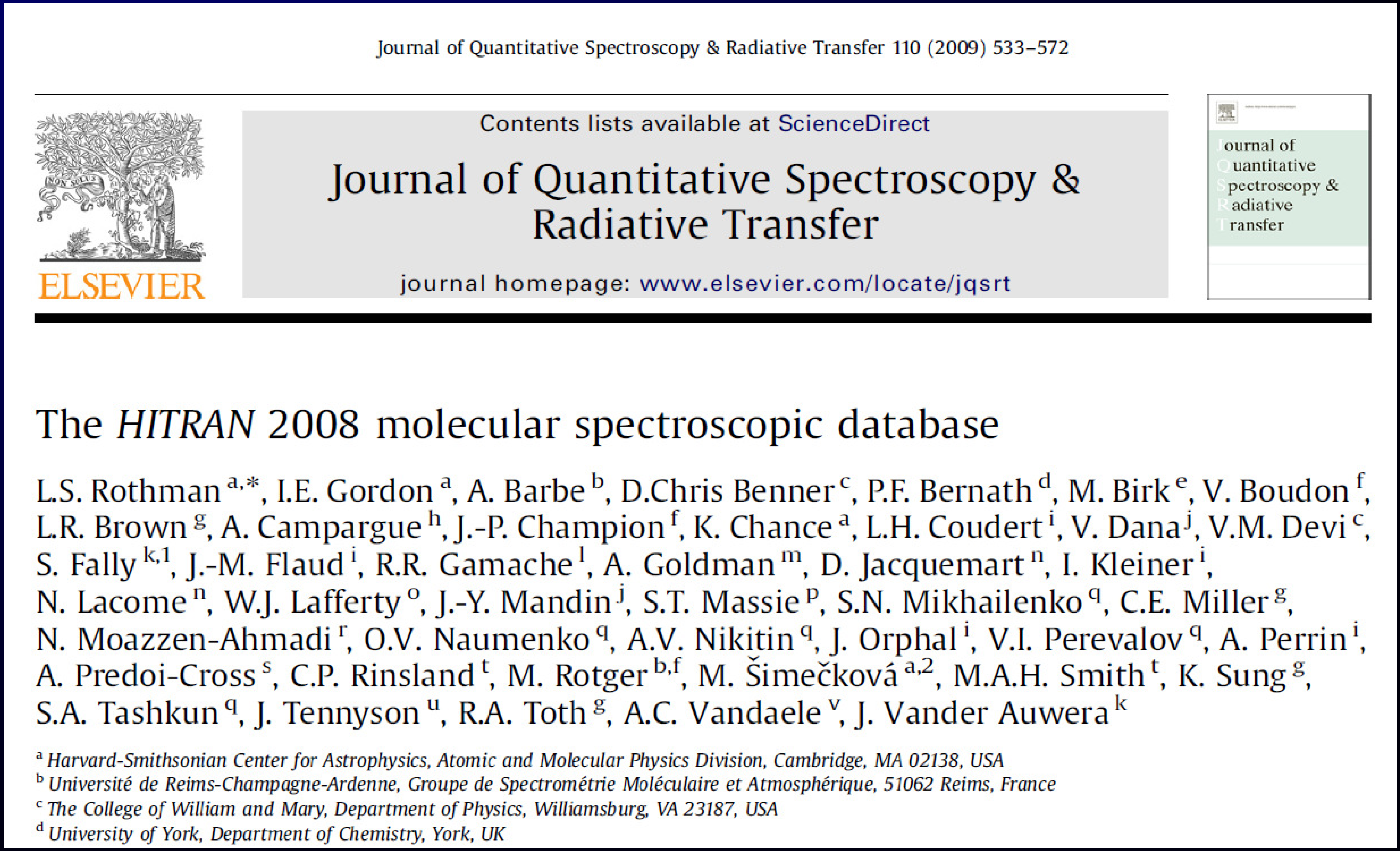

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The *HITRAN* 2008 molecular spectroscopic database

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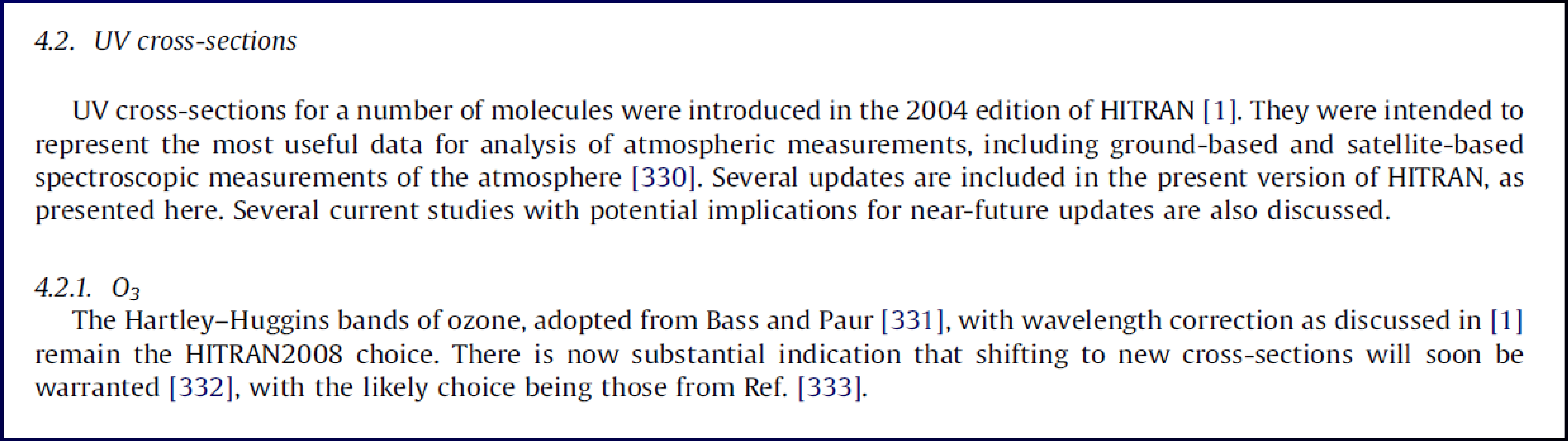
HITRAN database (2008)

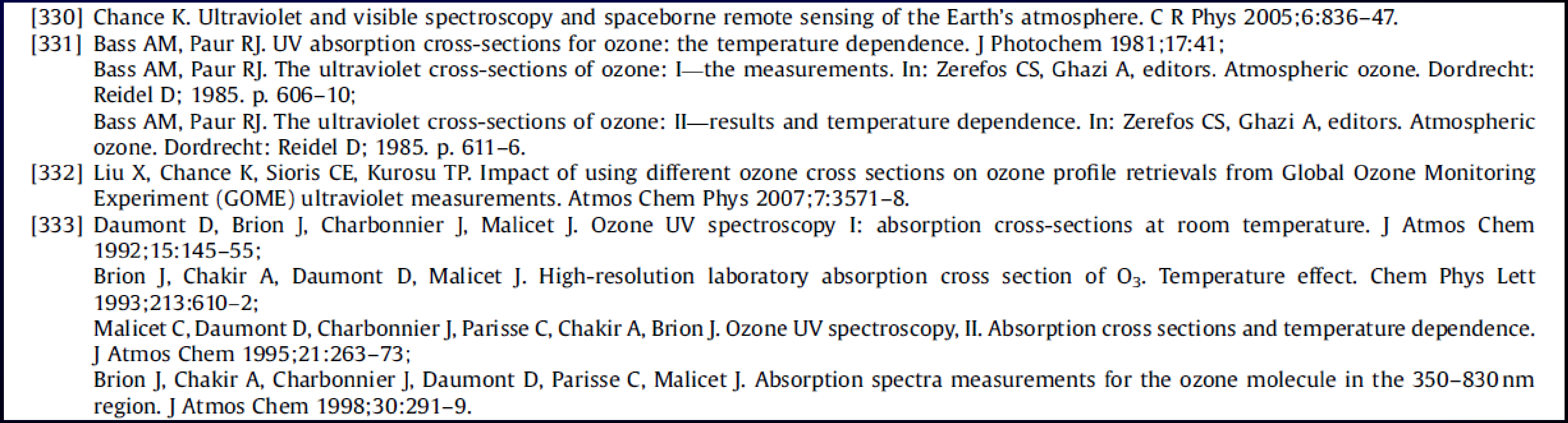


4.2. UV cross-sections

UV cross-sections for a number of molecules were introduced in the 2004 edition of HITRAN [1]. They were intended to represent the most useful data for analysis of atmospheric measurements, including ground-based and satellite-based spectroscopic measurements of the atmosphere [330]. Several updates are included in the present version of HITRAN, as presented here. Several current studies with potential implications for near-future updates are also discussed.

4.2.1. O_3

The Hartley–Huggins bands of ozone, adopted from Bass and Paur [331], with wavelength correction as discussed in [1] remain the HITRAN2008 choice. There is now substantial indication that shifting to new cross-sections will soon be warranted [332], with the likely choice being those from Ref. [333].



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Conclusions

1. "New" O_3 cross-sections since 1999
Progress, but many requirements are not met.

2. "Critical Review" for ESA (2003)
Problems all around. Who defines O_3 "standard" ?

3. Are the O_3 reference data consistent ?
Probably not to the 1-2 % level.

4. Need for peer-reviewed recommendations.