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SPECTROSCOPY AND RADIATIVE TRANSFER IN PLANETARY ATMOSPHERES

Guest Editors:

Laurence S. Rothman, F. Javier Martin-Torres and Jean-Marie Flaud

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

N. Jacquinet-Husson^{a,*}, N.A. Scott^a, A. Chédin^a, L. Crépeau^a, R. Armante^a, V. Capelle^a, J. Orphal^b, A. Coustenis^c, C. Boone^d, N. Poulet-Crovisier^d, A. Barbe^e, M. Birk^f, L.R. Brown^g, C. Camy-Peyret^h, C. Claveau^h, K. Chanceⁱ, N. Christidis^j, C. Clerbaux^{k,1}, P.F. Coheur^l, V. Dana^h, L. Daumont^e, M.R. De Backer-Barilly^e, G. Di Lonardo^m, J.M. Flaud^b, A. Goldmanⁿ, A. Hamdouni^e, M. Hess^f, M.D. Hurley^o, D. Jacquemart^p, I. Kleiner^b, P. Köpke^q, J.Y. Mandin^h, S. Massie^r, S. Mikhailenko^s, V. Nemtchinov^t, A. Nikitin^s, D. Newnham^u, A. Perrin^b, V.I. Perevalov^s, S. Pinnock^j, L. Régalia-Jarlot^e, C.P. Rinsland^v, A. Rublev^w, F. Schreier^f, L. Schult^x, K.M. Smith^u, S.A. Tashkun^s, J.L. Teffo^h, R.A. Toth^g, V.I. Tyuterev^e, J. Vander Auwera^l, P. Varanasi^t, G. Wagner^f

^aLaboratoire de Météorologie Dynamique/Institut Pierre Simon Laplace, Ecole Polytechnique, Route Départementale 36, 91128 Palaiseau, France

^bLaboratoire Inter-Universitaire des Systèmes Atmosphériques, Faculté des Sciences et Technologie, 61 avenue du Général de Gaulle, 94010 Créteil, France

^cLaboratoire d'Etudes Spatiales et d'Instrumentation en Astrophysique, Observatoire de Paris-Meudon, 5 place Jules Janssen, 92195 Meudon, France

^dInstitut Pierre Simon Laplace, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris, France

^eGroupe de Spectrométrie Moléculaire et Atmosphérique, Université de Reims-Champagne-Ardenne, 51062 Reims, France

^fRemote Sensing Technology Institute, German Aerospace Center (DLR), Oberpfaffenhofen, D-82234 Weßling, Germany

^gJet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA

^hLaboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique, Université Pierre et Marie Curie, 3, rue Galilée 94200 Ivry sur Seine, France

ⁱHarvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA

^jDepartment of Meteorology, University of Reading, 2 Earley Gate, Whiteknights, Reading RG6 2AU, UK

^kService d'Aéronomie/ Institut Pierre Simon Laplace, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris, France

^lService de Chimie Quantique et Photophysique, Université Libre de Bruxelles, C.P. 160/09, B-1050 Brussels, Belgium

^mUniversità di Bologna, Dipartimento di Chimica Fisica ed Inorganica, Viale del Risorgimento 4, 40136 Bologna, Italy

ⁿDepartment of Physics, University of Denver, Denver, CO 80208, USA

^oFord Research Laboratory, 2101 Village Road, Dearborn, MI 48124, USA

^pLaboratoire de Dynamique, Interactions et Réactivité, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris, France

^qMeteorologisches Institut der Universität München, München D-80333, Germany

^rNational Center for Atmospheric Research, Boulder CO 80307, USA

^sLaboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 634055 Tomsk, Russian Federation

^tState University of New York at Stony Brook, Stony Brook, NY 11794, USA

*Corresponding author. Tel.: +33 1 69 33 51 62; fax: +33 1 69 33 52 18.

E-mail address: jacquinet@lmd.polytechnique.fr (N. Jacquinet-Husson).

^uRutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK^vNASA Langley Research Center, Science Directorate, Mail Stop 401A, Hampton, VA 23681-2199, USA^wInstitute of Molecular Physics at Russian Research Center Kurchatov Institute, Moscow 123183, Russian Federation^xMax-Planck-Institut für Meteorologie, D-20146 Hamburg, Germany

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Abstract

The development of Gestion et Etude des Informations Spectroscopiques Atmosphériques (GEISA: Management and Study of Spectroscopic Information) was started over three decades at Laboratoire de Météorologie Dynamique (LMD) in France. GEISA is a computer accessible spectroscopic database, designed to facilitate accurate forward radiative transfer calculations using a line-by-line and layer-by-layer approach. More than 350 users have been registered for on-line use of the GEISA facilities. The current 2003 edition of GEISA (GEISA-03) is a system comprising three independent sub-databases devoted respectively to: line transition parameters, infrared and ultraviolet/visible absorption cross-sections, microphysical and optical properties of atmospheric aerosols.

Currently, GEISA is involved in activities related to the assessment of the capabilities of IASI (Infrared Atmospheric Sounding Interferometer on board of the METOP European satellite) through the GEISA/IASI database derived from GEISA.

The GEISA-03 content is presented, placing emphasis on molecular species of interest for Earth and planetary atmosphere studies, with details on the updated 2008 archive underway. A critical assessment on the needs, in terms of molecular parameters archive, related with recent satellite astrophysical missions is made. Detailed information on free on-line GEISA and GEISA/IASI access is given at <http://ara.lmd.polytechnique.fr> and <http://ether.ipsl.jussieu.fr>.

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1. Introduction

Adequate tools are required to perform reliable radiative transfer modelling calculations to meet the needs of communities involved in understanding the atmospheres of the Earth and other planets. Among these tools, compilations of spectroscopic parameters are used for a vast array of applications and especially for planetary atmospheric remote sensing. Consequently, there is an acute need for comprehensive, trustworthy and operational interactive spectroscopic databases to benefit the research in direct and inverse radiative transfer. In this context, since over three decades, the ARA group at LMD has developed GEISA, a computer accessible spectroscopic database system [1–4], designed to facilitate accurate and fast forward, calculations of atmospheric radiative transfer using a line-by-line and (atmospheric) layer-by-layer approach. This effort has proven to be beneficial to the atmospheric scientific community participating in direct and inverse radiative transfer studies.

The role of molecular spectroscopy in modern atmospheric research has entered a new phase with the advent of highly sophisticated spectroscopic instruments and computers. For example, the performance of Earth atmospheric sounders like AIRS (<http://airs.jpl.nasa.gov/>) in the USA, and IASI (<http://earth-sciences.cnes.fr/IASI/>) in Europe, which have a better vertical resolution and accuracy, compared to the previous existing satellite infrared vertical sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases, since these are essential input in the forward models used to simulate recorded radiance spectra. Consequently, a strong demand exists for highly comprehensive, well-validated, efficiently operational, and desirably interactive computer-based spectroscopic databases to benefit the research in direct and inverse radiative transfer. In this purpose, GEISA is currently involved [5] in activities related to the assessment of the capabilities IASI through the GEISA/IASI database, extensively described in Jacquinet-Husson et al. [6]. Since the Metop (<http://www.eumetsat.int>) European polar satellite launch

(October 19, 2006), GEISA/IASI-03 is the reference spectroscopic database for the validation of the level 1 IASI data, using the 4A radiative transfer model [7,8] (4A/LMD <http://ara.lmd.polytechnique.fr>); 4A/OP co-developed by LMD and Noveltis (<http://www.noveltis.fr/>) with support of CNES.

In this paper, the contents of the 2003 edition of GEISA (GEISA-03) [4,9] will be presented including an example of critical assessment, in terms of archived spectroscopic parameter differences, by comparisons with two other current public spectroscopic databases, i.e. HITRAN-04 [10] and MIPAS [11]. Preliminary information on the GEISA 2008 update underway will be given as well, placing emphasis on the needs for molecular species of interest for other than Earth's planetary atmosphere studies.

GEISA is implemented on the CNES/CNRS Ether Products and Services Centre WEB site (<http://ether.ipsl.jussieu.fr>), where all their archived spectroscopic data can be handled freely through general and user-friendly associated management software facilities.

2. GEISA-03 system overview

The GEISA-03 edition of GEISA is a system comprising three independent sub-databases devoted, respectively to: line transition parameters, infrared and ultraviolet/visible absorption cross-sections, microphysical and optical properties of atmospheric aerosols. Detailed description is given in [4,9].

2.1. Line transition parameters sub-database

GEISA-03 sub-database of line transition parameters involves 42 molecules (98 isotopic species) representing 1,668,371 entries, in the spectral range from 10^{-6} to $35,877.031\text{ cm}^{-1}$. The included molecules are of interest for the atmospheres of Earth (major permanent and trace molecules) and of other planets (like Jupiter, Saturn, Uranus, Titan, etc.), i.e. C_2H_4 , GeH_4 , C_3H_8 , C_2N_2 , C_4H_2 , HC_3N , H_2S , HCOOH , and C_3H_4 .

A summary of changes made in GEISA-03 since GEISA-97 is provided in Table 1. The items related to each updated molecular species listed in column 1 are: the updated spectral intervals minimum and maximum wavenumbers (cm^{-1}), and for each spectral interval: the related isotope(s) identified by its (their) GEISA code(s) [3], the corresponding numbers of lines and references describing these updates, in columns 2–6, respectively. The spectroscopic parameters which have mainly been changed are: the vacuum wavenumber, the intensity, the air-broadened half-width, and the lower-state energy. For this edition of GEISA, in the spectral intervals identified through columns 2 and 3, the updates have consisted of a total replacement, by new line lists, of the former existing parameters or of a simple addition, in case of not already available data. Besides the references of column 6, summarized specific information on these updates is given in [6] for the GEISA/IASI selected molecules in the spectral range $599\text{--}3100\text{ cm}^{-1}$.

2.2. Absorption cross-sections sub-database

As described in [3], besides the line transition parameters data catalog itself, GEISA includes, a second catalog, providing, at various temperatures and pressures, the cross-sections (unit: $\text{cm}^2\text{ molecule}^{-1}$) of species exhibiting dense spectra, not suitable for a discrete parameterized format. This catalog is devised in two parts corresponding to two spectral regions:

2.2.1. In the infrared

In the spectral range from 200 to 2000 cm^{-1} , 35 molecular species are archived, i.e.: CFC-13, CFC-113, CFC-114, CFC-115 (non-updated since GEISA-97); CFC11, CFC12, CFC14, HCFC22, HCFC123, HCFC124, HFC125, HFC134a, HCFC141b, HCFC142b, HFC152a, HCFC225ca, HCFC225cb, HFC32, HFC143a, HFC134, N_2O_5 , SF_6 , ClONO_2 (updated in GEISA-03); HFC-143, HCFC-21, CCl_4 , C_2F_6 , C_2H_2 , C_2H_4 , C_2H_6 , C_3H_8 , C_4H_8 , HNO_4 , SF_5CF_3 , HCH-365mfc (new molecular species for GEISA-03). Detailed contents and references of this archive are given in [4,9].

Table 1
Summary of updates in GEISA-03 line transition parameters since GEISA-97

Molecule	Updated spectral interval			# Lines	Refs.
	Minimum wavenumber (cm ⁻¹)	Maximum wavenumber (cm ⁻¹)	Isotope code		
H ₂ O	500.035	2819.848	161, 171, 181, 162, 182, 172	10,755	[12–15]
	9603.750	11,399.414	161, 171, 181	5002	[16]
	13,184.4152	25,232.004	161	9316	[17,18]
CO ₂	436.123	2488.222	626	19,865	[19–22]
	494.472	2395.279	636	7813	
	498.933	2499.966	628	12,046	
	514.430	2442.235	627	7759	
	2491.941	2806.199	627	306	
	2500.024	2826.650	628	733	
O ₃	600.179	1231.881	666, 668, 686	79,374	[23]
	928.198	1272.422	666	14,165	[24]
	1311.101	3391.609	666	73,500	[25–28]
N ₂ O	872.399	1243.755	446	279	[29]
CH ₄	0.010	6184.492	211, 311	175,941	[30,31]
	4800.142	9199.286	211	40,255	
O ₂	7664.726	8064.312	66, 68	341	[32]
	11,483.727	15,927.806	66, 67, 68	665	[33]
NO	1487.366	2188.447	46	9610	[34,35]
	3547.318	3799.155	46	2962	[36,37]
NO ₂	2719.057	3074.366	646	9219	[38,39]
NH ₃	0.058	5294.502	411, 511	29,082	[40,41]
PH ₃	770.877	2478.765	131	11,790	[40,41]
OH	29,808.501	35,877.031	61	1080	[42]
HBr	16.692	396.474	11, 19	308	[43]
	2123.812	2790.533	11, 19	719	
HI	12.842	319.820	17	245	[43]
	1950.689	2403.162	17	390	
C ₂ H ₆	2975.331	2977.926	226	421	[44]
CH ₃ D	7.760	3306.810	212	35,518	[30,31]
C ₂ H ₂	604.774	2254.963	221, 231	2833	[45–47]
	1248.262	1414.802	221	71	[48]
HOCl	1178.673	1320.332	165, 167	3972	[49–51]
CH ₃ Cl	1261.562	1645.899	215, 217	8989	[52,53]
COF ₂	1856.730	2001.348	269	28,884	[54]
HO ₂	0.173	908.168	166	331,288	[55,56]

Spectral range: 0.010–35,877.031 cm⁻¹.

2.2.2. In the ultraviolet/visible regions

Absorption cross-sections in the ultraviolet (UV) and visible regions (200–800 nm) have been newly included in GEISA-03 for the most important atmospheric molecules. The database contains different sets of

cross-sections that correspond to various kinds of applications, i.e. either, at high signal/noise ratio but reduced spectral resolution, recorded with grating spectrometers and diode-array detectors, or, at very high spectral resolution but somewhat smaller signal/noise, recorded with FTS. Note that most of the data presented here was obtained in the last decade since 1998. The involved molecular species are:

2.2.2.1. O_3 . Three different data sets are archived: (1) absorption cross-sections measured with the GOME (<http://earth.esa.int/ers/gome>) instrument [57] in the 231–794 nm spectral range at five temperatures between 202 and 293 K, with a spectral resolution of 0.2 nm below and 0.4 nm above 400 nm; (2) absorption cross-sections measured with an FTS in the 230–830 nm range [58], again at five temperatures between 203 and 293 K, with a spectral resolution that is significantly higher than the O_3 absorption features [59] and with very accurate spectral calibration; (3) absorption cross-sections measured with GOME [60] in the 230–1070 nm spectral range, at five temperatures between 203 and 293 K, with a spectral resolution that is slightly lower than for the first data set. The O_3 absorption cross-sections recorded with the FTS are particularly useful when high spectral resolution and/or calibration is required, while the O_3 cross-sections recorded with GOME and SCIAMACHY (<http://envisat.esa.int/instruments/sciamachy>) are less resolved but show significantly smaller noise, which is important when retrieving very weak absorbers from atmospheric spectra in this region.

2.2.2.2. NO_2 . Several data sets are available that show only small differences concerning the absolute values, however spectral resolution and total pressure are very important experimental parameters [59]; in addition the presence of the dimer N_2O_4 or of impurities like HONO can affect the data. The NO_2 archived cross-sections have been recorded: (1) with the GOME [61] and SCIAMACHY [60] instruments (the latter one including NO_2 cross-sections at a temperature as low as 203 K); (2) with an FTS from two different studies, the first one at two different total pressures (100 and 1000 hPa) and five temperatures between 223 and 293 K covering the 230–830 nm range [62] the second one at a smaller number of temperatures but over a wider spectral range (238–1000 nm) and including a systematic study of pressure effects [63–66].

2.2.2.3. $OCIO$ and SO_2 . Two kinds of cross-section data have been archived: one kind recorded at lower spectral resolution (but at very high signal/noise ratio) with SCIAMACHY [60] and in addition another kind recorded with an FTS. For $OCIO$, there are cross-sections available at five different temperatures in the 213–293 K range for the FTS data [67], while for SO_2 the FTS data were recorded at different pressures but only at room temperature [68]. The SO_2 data recorded with SCIAMACHY [60] cover five temperatures between 203 and 293 K.

2.2.2.4. BrO and $OBrO$. Only cross-sections recorded by an FTS were selected. For BrO these data cover the 300–385 nm spectral range at five temperatures between 203 and 298 K [69], while for $OBrO$ (385–616 nm spectral range) cross-sections are available only at room temperature [70].

2.2.2.5. O_2 and O_4 . Absorption cross-sections are available from different studies related with data for the Schumann-Runge and Herzberg bands of O_2 in the UV [71–74] and for visible regions [75,76], from measurements with an FTS at temperatures between 223 and 294 K.

2.2.2.6. H_2CO . The absorption cross-sections at 293 K covering the 240–400 nm spectral range have been recorded with SCIAMACHY [60].

2.2.2.7. CS_2 . The absorption cross-sections, recorded with an FTS at 294 K covering the 290–350 nm spectral range are from [76].

It has to be noted that in general, the cross-sections recorded by an FTS have a wavelength calibration of better than 0.01 nm [59], which is an important advantage for atmospheric applications, in particular when retrieving several absorbers simultaneously.

2.3. Microphysical and optical properties of atmospheric aerosols sub-database

Besides the molecular species that define the gaseous infrared opacity in the Earth's atmosphere, aerosol particles, also contribute to this opacity. Consequently, a new sub-database, related with aerosols particle properties has been added to the GEISA system in 2003. It gathers the microphysical and optical properties from four published aerosol data catalogs, i.e. [77–80], the overall content of which deals with the archive of complex refractive indices and possibly computed optical-related properties, for selected basic aerosol components. Software for data management and user-selected aerosol mixtures elaboration are available from [78–81]. Details and references are given in Ref. [5].

3. Assessment of GEISA-03 contents

Some comparisons, in terms of spectroscopic parameters contents, of GEISA-03 with two other current public spectroscopic databases, i.e. HITRAN-04 [10] and MIPAS [11] in its PF3.2 version are presented in the following. It has to be noted that the initial emphasis of the three compilations have been different (see related publications).

3.1. Comparison of GEISA-03 and HITRAN-04 contents

The last updates of HITRAN and GEISA have been finalized at nearly the same time (which is not always the case), and include very similar data sources for many molecules. Because of its origin, certain molecules, related with planetary atmospheres (especially those of the Giant Planets) are specific to GEISA, such as GeH₄, C₃H₈, C₄H₂, HC₃N, and C₃H₄. Table 2 summarizes the GEISA contents for these molecules, the list of which is given in column 1 with, for each molecular species: the related isotope identification in column 2, the archived line list minimum and maximum wavenumbers (cm⁻¹) in columns 3 and 4, respectively; for each list of archived lines, the intensity average (cm molecule⁻¹) is in column 5; the associated number of lines is in column 6 and the general reference, i.e. GEISA-97 [3] in column 7. Also, the molecular species: HOBr, CH₃OH, O, NO+, are specific of the HITRAN archive.

As an illustration, a summary of differences for common molecular species cataloged in the line parameter portion of GEISA-03 and HITRAN-04 is given in Table 3. Molecular species formula are listed in column 1 and their identification codes for database management in column 2, where GEISA-03 is referred to as “G” and HITRAN-04 as “H”. For each molecular species, the numbers of bands, isotopes and lines, are given in columns 3, 4, and 5, respectively, for both databases. The minimum and maximum spectral ranges (in cm⁻¹), corresponding to the GEISA and HITRAN archives, are in columns 6 and 7, respectively. The results of a detailed evaluation of spectroscopic parameters differences between HITRAN-04 and GEISA-03, in selected spectral ranges for H₂O, CO₂, O₃, N₂O, and CH₄, have been presented at ISSWG-20 [82]. An illustration of these differences, in the case of H₂O, is given below, in Section 3.2. It has to be noted that, as described in [4,9,10], GEISA and HITRAN do not archive exactly the same kind of line spectroscopic parameters, in addition of the mandatory ones which are common, such as vacuum wavenumber, intensity, air-broadened half-width, lower-state energy. Consequently, the fields of the formats are also different for both databases.

Table 2

Molecules GEISA specific for planetary (other than terrestrial) atmosphere studies

Molecule	Isotope	Minimum wavenumber (cm ⁻¹)	Maximum wavenumber (cm ⁻¹)	Intensity average (cm mol. ⁻¹)	# Lines	Refs
GeH ₄	⁷⁴ GeH ₄	1937.371	2224.570	4.978 × 10 ⁻²⁰	824	[3]
C ₃ H ₈	¹² C ₃ H ₈	700.015	799.930	4.139 × 10 ⁻²³	8983	
C ₂ N ₂	¹² C ₂ ¹⁴ N ₂	203.955	2181.690	2.668 × 10 ⁻²¹	2577	
C ₄ H ₂	¹² C ¹⁴ H ₂	190.588	654.425	3.445 × 10 ⁻²¹	1405	
HC ₃ N	H ¹² C ₃ ¹⁴ N	474.293	690.860	2.693 × 10 ⁻²¹	2027	
C ₃ H ₄	¹² C ₁₃ H ₄	290.274	359.995	4.277 × 10 ⁻²²	3390	

Table 3

Summary of differences for common molecular species cataloged in the line parameter portion of GEISA-03 and HITRAN-04

Mol.	Mol ID		# Bands		# Isot		# Lines		Spectral coverage (cm ⁻¹)			
	G	H	G	H	G	H	G	H	Minimum wavenumber (cm ⁻¹)		Maximum wavenumber (cm ⁻¹)	
									G	H	G	H
H ₂ O	1	1	192	254	6	6	58,726	63,196	0.007	0.007	25,232.004	25,232.004
CO ₂	2	2	741	597	9	8	76,826	62,913	436.123	0.736	9648.007	12,784.060
O ₃	3	3	120	137	5	5	319,248	311,481	0.026	0.026	4060.783	4060.783
N ₂ O	4	4	162	350	5	5	26,681	47,835	0.838	0.838	5131.249	7796.633
CO	5	5	104	47	6	6	13,515	4477	3.414	3.462	8464.883	8464.881
CH ₄	6	6	74	150	2	3 ^a	216,196	251,440	0.010	0.010	9199.284	9199.284
O ₂	7	7	18	19	3	3	6290	6428	0.000	0.000	15,927.806	15,927.806
NO	8	8	293	238	3	3	99,123	102,280	0.000	0.000	9273.213	9273.214
SO ₂	9	9	9	9	2	2	38,853	38,853	0.017	0.017	4092.948	4092.948
NO ₂	10	10	11	11	1	1	104,224	104,223	0.498	0.498	3074.365	3074.152
NH ₃	11	11	79	78	2	2	29,082	29,084	0.058	0.058	5294.501	5294.501
PH ₃	12	28	10	9	1	1	11,740	11,790	17.805	17.805	2445.553	3601.652
HNO ₃	13	12	12	15	1	1	171,504	271,166	0.035	0.035	1769.982	1769.982
OH	14	13	245	220	3	3	42,866	42,273	0.004	0.002	35,877.030	19,267.869
HCl	16	15	17	17	2	2	533	613	20.240	20.240	13,457.841	13,457.841
HBr	17	16	16	16	2	2	1294	1293	16.232	16.232	9758.564	9758.564
OCS	20	19	151	119	6	4	24,922	19,920	0.381	0.380	4118.004	4118.004
C ₂ H ₆	22	27	3	2	2	1	14,981	4749	725.603	725.602	2977.926	2977.926
CH ₃ D ^a	23	^a	13	^a	1 ^a	^a	35,518 ^a	^a	7.760		3146.460	
C ₂ H ₂	24	26	29	34	2	2	3115	3517	604.774	604.774	3374.222	3374.222
HCN	27	23	41	30	3	3	2550	4253	2.870	0.014	18407.973	3423.926
HOCl	32	21	6	8	2	2	17,862	16,276	0.024	1.080	3799.681	3799.681
CH ₃ Cl	34	24	14	16	2	2	18,344	31,119	674.142	674.142	3172.926	3172.926
H ₂ O ₂	35	25	2	19	1	1	100,781	100,781	0.043	0.043	1499.487	1499.487
H ₂ S	36	31	30	30	3	3	20,788	20,788	2.985	2.985	4256.546	4256.546
HCOOH	37	32	1	2	1	1	3388	24,808	1060.962	10.018	1161.251	1234.676
COF ₂	38	29	7	7	1	1	83,750	70,601	725.005	725.005	2001.347	2001.347
SF ₆ ^b	39	30	1	1	1	1	11,520	22,901 ^b	940.424	929.977	952.238	963.972
HO ₂	41	33	4	4	1	1	38,804	22,901	0.172	0.172	3675.818	3675.818
ClONO ₂ ^b	42	35	3	3	2	2	32,199	32,199 ^b	763.641	763.641	797.741	797.741

^aIndividual molecule in GEISA; isotope of CH₄ in HITRAN.^bMolecule included in HITRAN supplemental line list.

Among the GEISA management facilities, is a software program making it possible to convert a database format into the other database one (GEISA to HITRAN format, or HITRAN to GEISA format).

Independent of their line parameter files, HITRAN and GEISA include cross-sections and aerosols sub-databases that present differences in their structure and contents. For example: (1) related with the infrared region cross-sections sub-database, the molecular species: HFC-143, C₂H₂, C₂H₄, C₂H₆, C₄H₈, C₃H₈, and HCH-365mfc are specific of GEISA; (2) in the UV/Visible cross-sections sub-database of HITRAN, a single set of absorption cross-sections is available for each molecule [83] and the data for O₃ are only related with the Hartley and Huggins band (about 200–350 nm).

3.2. Evaluation of the impact of H₂O spectroscopic archive differences on IASI radiative transfer simulations

The purpose of this section is to present an evaluation of the impact of differences in spectroscopic line parameters, made through IASI sounding simulations, in terms of brightness temperatures (K). The LMD 4A fast forward line-by-line radiative transfer model [7,8] has been used, considering, at a first stage, only the H₂O archive differences in three spectroscopic databases, i.e. GEISA, HITRAN, and MIPAS. The chosen

thermodynamic conditions were those of a mean tropical atmospheric profile from the TIGR data set [84–86], in its latest version (TIGR-2000). The spectral resolution was the IASI one for the levels 1C simulation.

In the whole IASI spectral range, $645\text{--}2760\text{ cm}^{-1}$ (X -axis), an illustration of obtained results is presented in Fig. 1. This figure is split in two horizontal parts: (1) the above part displays, using GEISA-03, the IASI-simulated brightness temperature spectrum (in red, with corresponding scale, in K , on the left hand Y -axis), to show where are the major atmospheric absorption bands; (2) the lower part corresponds to plots of the differences in brightness temperature simulations: on one hand, between HITRAN-04 and GEISA-03 (green curve) and on the other hand, between MIPAS PF 3.2 and GEISA-03 (blue curve), with corresponding scale in (K), on the right hand Y -axis. The differences are evaluated as the following: [“simulation with H_2O HITRAN-04 (or MIPAS PF 3.2) data replacement in GEISA-03” – “simulation with GEISA-03”]. The IASI noise (NedT at 280 K) has been added (black curve), to evaluate the importance of the simulation differences compared with the instrument noise.

A “zoom” of Fig. 1 in the H_2O main absorption band (at $6.3\ \mu\text{m}$), in the spectral region $1200\text{--}2100\text{ cm}^{-1}$, is presented Fig. 2a (with similar legend as in Fig. 1). The analysis of the exhibited differences shows that the spectroscopy impact can be higher than the instrument noise, in particular for spikes appearing in comparisons with HITRAN-04.

Figs. 2b and c aim at the identification (in term of spectroscopic parameter individually) of the origin of displayed differences. Comparisons with HITRAN were selected. In this purpose, 4A simulations were processed, replacing, in GEISA-03, only one kind of spectroscopic parameter at a time. For comparisons with HITRAN-04, Fig. 2b (green curve) shows the individual impact of intensity; similarly, Fig. 2c shows the individual impact of air-broadened half-width. These two figures show that mainly responsible spectroscopic parameter for the simulation differences is the air-broadened half-width. It has to be noted that only the intensity and the air-broadened half-width have been considered for difference impact evaluations in Fig. 2a and b. Other spectroscopic parameters (such as the lower-state energy, the temperature dependence exponent for air-broadened half-width, etc.) have a non-negligible impact in radiative transfer simulations. Consequently, this explains why certain important spikes visible in Figs. 2b and 2c are missing in Fig. 2a, due to compensation of these other spectroscopic parameter impacts.

For finalizing this study, comparisons have been made with the last H_2O HITRAN update made in 2006 (referred to as HITRAN-06), as described in [87]. The results are displayed on the pink curves of Figs. 2b and c.

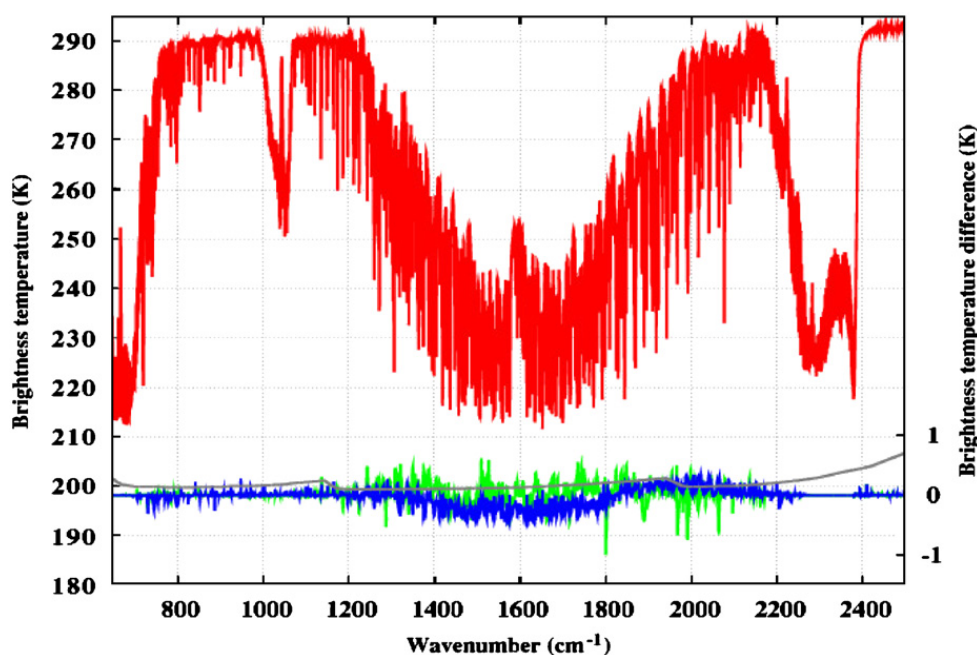


Fig. 1. IASI brightness temperature (K) simulation with GEISA-03 (upper curve); impact of replacement of HITRAN-04 or MIPAS PF3.2 H_2O data in GEISA-03 (differences (K) in lower curves), with associated *standard IASI noise* at $T = 280\text{ K}$.

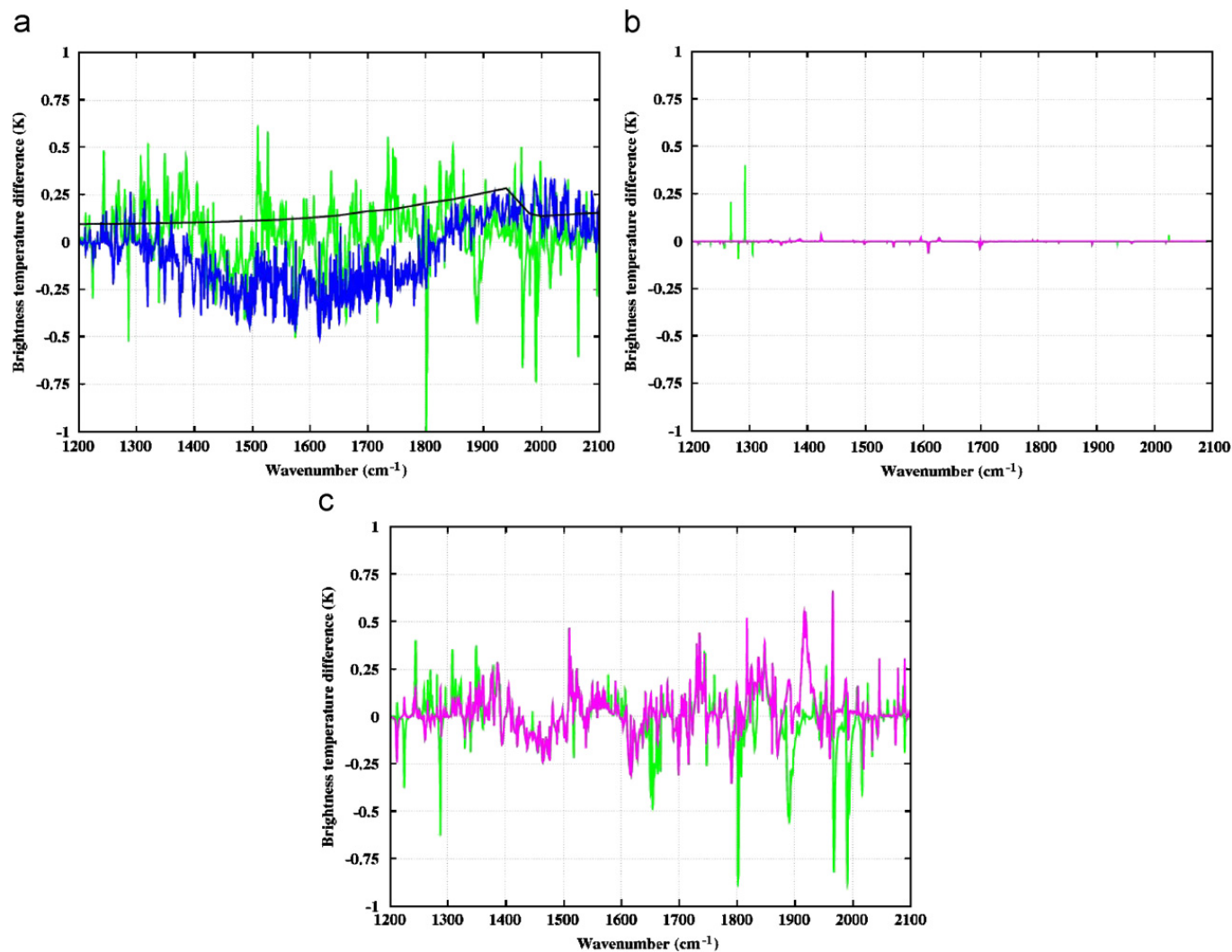


Fig. 2. (a) IASI brightness temperature simulation differences (K). Impact of replacement of HITRAN-04 or MIPAS PF3.2 H₂O data in GEISA-03 with associated *standard IASI noise* at $T = 280$ K. (b) IASI brightness temperature simulation differences (K). Intensity individual impact evaluation: (1) Impact of replacement of HITRAN-04 H₂O intensities in GEISA-03. (2) Impact of replacement of HITRAN-06 H₂O intensities in GEISA-03. (c) IASI brightness temperature simulation differences (K). Air broadened half-widths individual impact evaluation: (1) Impact of replacement of HITRAN-04 H₂O air broadened half-widths in GEISA-03. (2) Impact of replacement of HITRAN-06 H₂O air broadened half-widths in GEISA-03.

The intensity spikes seem to have totally disappeared and those from air broadened half-width are very significantly reduced, but with still some of them potentially not negligible in comparison of the instrument noise. It is not possible to go further in these first conclusions without making comparisons with real observations, a task which has just started.

4. Ether products and services centre for GEISA interactive distribution

GEISA is maintained by the ARA group at LMD (<http://ara.lmd.polytechnique.fr>) for its scientific part and by the Ether Products and Services Centre for its technical part.

The main goal of the Ether Centre is to promote and help research in the field of Atmospheric Chemistry. The objective is to progressively develop operational products and services oriented towards end-users. Ether activities include data management produce by space borne, ground based or balloon borne instruments and

also the development of satellite scientific products and the development of tools to help data use and data analysis.

Through a website (<http://ether.ipsl.jussieu.fr>) Ether provides information on French scientific activities. It forms part of the Ether Products and Services Centre, which uses this site as a forum for publishing: measurement data from French laboratories, as well as from many international centres; forecasts such as potential vorticity; modelling results; downloadable procedures; browse images, on-line processing software (which can be activated through the Ether interface).

In this context, GEISA and GEISA/IASI databases have been implemented on the Ether Products and Services Centre since January 2007. Ether provides users with free and easy access (with tools and WEB interfaces) to products from these two databases. The facilities associated with GEISA and GEISA/IASI distribution are the same for both databases, i.e.:

- Interactive access to individual lines with tools to have a look and to download any information on the database, i.e. contents (total or in user's selected spectral range), histogram (on various parameters values), transition analysis, etc.
- FTP access to individual molecular species to download data easily.
- On-line access to IR and UV/Vis cross-sections and aerosols.
- Information about the data.

Users have to click on the GEISA logo on the first page of the Ether WEB site (<http://ether.ipsl.jussieu.fr>) to access freely to GEISA and GEISA/IASI data and information.

5. GEISA spectroscopy enhancement needed: towards GEISA-08

The regularly updated and evolving spectroscopic databases, such as GEISA, still have their limitations and faults, which have to be corrected or improved upon, in order to meet the requirements of a diverse group of users.

5.1. Earth's atmosphere studies evaluation and requirements

A detailed (but not exhaustive) list of major improvements needed has been given in paragraph 6 of Ref. [3] and is still relevant today, such as the following important remaining spectroscopy-related problems:

- The water vapor spectroscopic parameters: still need to be validated.
- The water vapor continuum: more tuning to be done when more validation data (especially with high water vapor content) become available.
- The bands of freons 850 and 920 cm^{-1} : temperature dependence to be refined.

Table 4

Update requirement index for selected molecules and spectroscopic parameters in major public spectroscopic databases

Molecules	Line position	Line intensities	Line broadening	Line mixing	Continuum	Cross-sections
H ₂ O	1	1	1		1	
CO ₂	Y	Y	1	1		
O ₃	3	1?	1			
CH ₄	2	2	1	1		
CO	Y	Y	Y			
N ₂ O	?	?	2	2		
HNO ₃	1	1	3			
O ₂ and N ₂ collision-induced spectrum					Y	
CFCs, HCFCs, N ₂ O ₅						Y

“1” parameters that need to be improved; “2” and “3” second and third priority for improvement; “Y” no problem clearly identified; “?” the databases have to be checked. A blank corresponds to non-applicable information.

- O₃ in the 9.6 μm region: the spectroscopic parameters still need to be validated.
- Some CO₂-Q branches: further improvement/tuning of the line mixing.

More details are given in Table 4, in terms of individual spectroscopic parameter quality improvement required, in the major spectroscopic data public databases, for individual molecules, i.e. H₂O, CO₂, O₃, CH₄, CO, N₂O, and HNO₃ with some additional information on continuum and IR cross-sections evaluation given as well. The molecule names are in column 1; the 4 other columns, 2–5, correspond respectively to the following spectroscopic parameters, i.e. line position, line intensity, line broadening, and line mixing; the two remaining columns, 6 and 7, are for continuum and IR cross-sections, respectively. For each molecule listed in column 1, coded index of quality have been given (from conclusions of IASI/ISSWG working group [6]) for the spectroscopic parameters of columns 2–7, if applicable, as the following: “1” parameters that need to be improved; “2” and “3” second and third priority for improvement; “Y” no problem clearly identified; and “?” the databases have to be checked. A blank corresponds to non-applicable information.

5.2. Space studies of outer planets and Titan requirements

The GEISA database has been extensively used in the modelling of Titan's atmosphere and in the comparison with observations performed by Voyager (<http://voyager.jpl.nasa.gov/>), ground-based telescopes and more recently by the instruments on board the Cassini-Huygens mission (<http://www.esa.int/SPECIALS/Cassini-Huygens/index.html>).

In the past, large uncertainties and lacks existed on the spectroscopic data for several of the compounds found on Titan. Consequently, complementary data (to those already archived in GEISA) have been used, i.e. for benzene (C₆H₆), data provided by Dang-Nhu [88]; for the ν₈ band and the hot bands ν₈ + ν₉ – ν₉ of C₄H₂, generated line lists from Arié and Johns [89] and band intensities from Koops et al. [90]; Graner [91] had provided the propyne (CH₃CCH for C₃H₄) ν₉ band data; C₂H₄ spectroscopic data were from Blass et al [92] and Rotger [93]. In addition, the ethane (C₂H₆) band between 1400 and 1500 cm⁻¹ (observed on Jupiter and Titan), all the propane (C₃H₈) bands other than the one at 748 cm⁻¹, the C₄H₂ band at 628 cm⁻¹, the C₂N₂ band at 735 cm⁻¹, the allene (C₃H₄) band near 350 cm⁻¹, etc. were partially analyzed. This was also the case for heavier molecules predicted on Titan, such as C₆H₂, C₄N₂, and HC₅N, for which very little spectroscopic data existed.

In the past year, spectroscopic parameters on several of the aforementioned molecules have become available and thus enhanced the analysis of Titan observations. Thus, the monochromatic radiance of the satellite is now calculated based on spectroscopic parameters as described in Coustenis et al. [94], mainly from GEISA-03 [4,9] and from recent additions to be implemented in the 2008 update of the database (see the next paragraph). Data on some of the molecules of interest to the planetary community can be also found in international databases such as the NIST atomic and molecular physics databases (<http://www.nist.gov/srd/atomic.htm>), the JPL spectral line catalog [95] (<http://spec.jpl.nasa.doc>), and the CDMS database [96,97] (<http://www.ph1.uni-koeln.de/vorhersagen/>).

Some of the data that remain to be obtained and implemented in GEISA can be listed as follows:

(a) Hydrocarbons

- CH₄: in the near-infrared region (from 0.8 to 5 μm) both from theory and laboratory measurements.
- C₆H₂: the band at 642 cm⁻¹ which is studied by the LISA group.
- C₂H₆: a complete analysis of the 1400–1500 cm⁻¹ band to be made, following the new spectroscopic parameters by Vander Auwera et al. [98].
- C₃H₈: needs in all bands beyond 800 cm⁻¹.
- C₃H₄ (propyne and allene): the data of the CDMS archive to be considered.
- C₆H₆: a re-analysis of the Dang-Nhu [88] data is required.

(b) Nitriles

- C₂N₂: presently no data on the combination band at 735 cm⁻¹ (which interferes with C₂H₂ and C₃H₈).
- CH₃CN: acetonitrile has been observed in the millimeter range, but also has bands in the mid and far IR.
- Other heavier nitriles such as propionitrile, etc.

(c) For Titan's atmosphere

- A global analysis to identify the hot bands and retrieve the intensities of the present molecular species is urgently needed.
- Furthermore, numerous isotopes now identified in Titan's spectrum (e.g. [99–101]) cannot be properly analyzed in the absence of adequate spectroscopic data. Updates in the available spectroscopic databases are essential to the study of the outer planets and their satellites with atmospheres.

5.3. Line transition parameters sub-database updates for the 2008 edition of GEISA (GEISA-08)

A systematic evaluation of the spectroscopy works underway for possible update in GEISA-08 has been made. A preliminary list, of the currently molecular species to be considered for the line transition sub-database, has been established and is summarized in Table 5a. In the first column are given the 16 selected molecular species, i.e. H₂O, CO₂, N₂O, CH₄, PH₃, HNO₃, H₂CO, C₂H₆, CH₃D, C₂H₂, C₂H₄, HCN, C₂N₂, C₄H₂, C₃H₄, and HC₃N (related with HCN, the whole GEISA-03 contents will be replaced). It has to be noted

Table 5a

Molecular species currently selected for GEISA-08 edition update (preliminary non-exhaustive list)

Molecule	Spectral range or Bande ID	Origin
H ₂ O	500–8000 cm ⁻¹	JPL
CO ₂	2200–7000 cm ⁻¹ 4000–9000 cm ⁻¹	JPL
N ₂ O	1900–6800 cm ⁻¹	JPL
CH ₄	750–1350 cm ⁻¹ 2850–3150 cm ⁻¹ 4800–9200 cm ⁻¹	ICB, JPL, LISA, LPMAA
PH ₃	770–3601 cm ⁻¹	JPL, LISA
HNO ₃	Submillimeter ν ₅ –ν ₉ (421 cm ⁻¹) 2ν ₉ –ν ₉ (438 cm ⁻¹) 11.2 μm (ν ₅ and 2ν ₉) 8.3 μm (ν ₈ + ν ₉) and (ν ₆ + ν ₇)	JPL, LISA, SAO Wright State, South Alabama, Ohio State Universities
H ₂ CO	1.573 μm 5–10 μm (ν ₂ , ν ₃ , ν ₄ , ν ₆)	Anhui Institute of Optics LISA, LADIR
C ₂ H ₆	12 μm region	LISA, ULB
CH ₃ D	3250–3700 cm ⁻¹	ICB, JPL, LTS
C ₂ H ₂	2.5 and 3.8 μm 1.5 μm region 0.83 μm region	LADIR LPMAA ULB
C ₂ H ₄	850–1500 cm ⁻¹	ICB, ULB, Univ. LOUVAIN
HCN	0.006–17,943 cm ⁻¹	University College London A. Maki
C ₂ N ₂	203–266 cm ⁻¹	LISA/GPCOS, LESIA
C ₄ H ₂	199–244 cm ⁻¹ ; 605–651 cm ⁻¹	LISA/GPCOS, LESIA
C ₃ H ₄	290–360 cm ⁻¹ 593–673 cm ⁻¹	LESIA
HC ₃ N	16 μm (ν ₅) 20 μm (ν ₆)	LISA/GPCOS

Table 5b
New molecular species for GEISA-08 edition (preliminary non exhaustive list)

Molecule	Spectral range	Origin
CH ₃ Br	7–10 μm	LADIR, LISA
CH ₃ CN	305–415 cm ⁻¹	JPL, LISA, PNNL
CH ₃ OH	0.02–33 cm ⁻¹ 10 μm region	JPL, University of New Brunswick
C ₂ HD	451–580 cm ⁻¹ 600–760 cm ⁻¹	LISA/GPCOS
C ₆ H ₆	642–705 cm ⁻¹	LESIA

that this list is neither final nor exhaustive. In columns 2 and 3 are respectively the updated spectral range (in cm⁻¹, μm, or as band identification) and the institution of origin of the work. Details on author participations and nature of the updates will be given at the time of GEISA-08 final issue description. In Table 5b (same organization as Table 5a), are listed new molecular species to be archived in GEISA-08, i.e. CH₃Br, CH₃CN, CH₃OH, C₂HD, and C₆H₆.

For the GEISA-08 edition, special emphasis will be laid on updates of molecular species of planetary atmospheres interest, considering recent spectroscopy results having already proven their impact on Cassini-Huygens mission instrument soundings analysis. As examples should be quoted the works of:

- Bénilan et al. [102] and Jolly et al. [103] who began at LISA an important work of band analysis for C₄H₂, HC₃N, HC₅N, C₂HD, and C₂N₂ which: (1) allowed for an improved match of the Cassini/CIRS data among other; (2) made it possible [94] to identify C₂HD for the first time, to improve on the abundances retrieved for C₃H₄, HC₃N, and C₄H₂ (with a re-analysis of the Arié and Johns [89] and Graner et al. [91] data as described in [94] and rule out some speculations about HC₅N. For HC₃N the new line lists for the two bands visible in the CIRS spectra at 499 and 663 cm⁻¹ with new infrared integrated intensities [103] have proven their positive impact.
- Auwera et al. [98] who generated a new database for the ethane band in the 12 μm region.

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Appendix A

List of acronyms

4A	Atlas Automatisé des Absorptions Atmosphériques
AIRS	Advanced InfraRed Sounder
ARA	Atmospheric Radiation Analysis
CDMS	The Cologne Database for Molecular Spectroscopy
CIRS	Composite InfraRed Spectrometer
CNRS	Centre National de la Recherche Scientifique (France)
CNES	Centre National d'Etudes Spatiales (France)
EPS	European Polar System
FTS	Fourier Transform Spectrometer
GEISA	Gestion et Etude des Informations Spectroscopiques Atmosphériques ; Management and study of Atmospheric Spectroscopic Information

GOME	Global Ozone Monitoring Experiment
HITRAN	HIgh-resolution TRANsmision molecular absorption data base
IASI	Infrared Atmospheric Sounder Interferometer
ICB	Institut Carnot de Bourgogne
INSU	Institut National des Sciences de l'Univers (France)
IR	Infrared
ISSWG	IASI Sounding Science Working Group
LISA/GPCOS	Laboratoire Inter-Universitaire des Systèmes Atmosphériques/ Groupe de Physico-Chimie Organique Spatiale
JPL	Jet Propulsion Laboratory
LADIR	Laboratoire de Dynamique, Interaction et réactivité
LESIA	Laboratoire d'Etudes Spatiales et d'Instrumentation en Astrophysique
LISA	Laboratoire Inter-Universitaire des Systèmes Atmosphériques
LMD	Laboratoire de Météorologie Dynamique
LPMAA	Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique
LTS	Laboratory of Theoretical Spectroscopy
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
METOP	Meteorological Operational Satellite
NASA	National Aeronautics and Space Administration (USA)
NEdT	Noise Equivalent Temperature difference
NIST	National Institute of Standards and Technology
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
TIGR	Thermodynamic Initial Guess Retrieval
ULB	Université Libre de Bruxelles
UV	Ultra Violet
VIS	Visible

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