

THE 2003 EDITION OF GEISA: A SPECTROSCOPIC DATABASE SYSTEM FOR THE SECOND GENERATION VERTICAL SOUNDERS RADIANCE SIMULATION

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Introduction

The performances of the second generation vertical sounders, like AIRS (Atmospheric Infrared Sounder: <http://www-airs.jpl.nasa.gov/>) in the USA, and IASI (Infrared Atmospheric Sounding Interferometer: <http://earth-sciences.cnes.fr/IASI/>) in Europe, will be highly dependent on the present-day knowledge of the accuracy of the spectroscopic parameters of the optically active atmospheric gases, since they are essential input in the forward models used to simulate recorded radiance spectra. 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 1974 the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie

Dynamique, France) has developed GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information), a computer accessible database system (Chédin et al (1982); Husson et al. (1992;1994). Currently, GEISA is involved in activities related to the assessment of the capabilities of IASI, as described in Jacquinet-Husson et al. (1998).

The GEISA database in its 2003 Edition: an overview

Since its 1997 edition (GEISA-97), the GEISA database, extensively described in Jacquinet-Husson et al. (1999), has been updated twice: partially in 2001 (Jacquinet-Husson et al. 2003) and extensively in 2003 (GEISA-03).

The GEISA-03 system comprises three sub-databases, i.e.:

- **The GEISA-03 sub-database on line transition parameters:**

GEISA-03 sub-database of line transition parameters involves 42 molecules (98 isotopic species) and contains 1,668,371 entries (321,905 supplementary entries since GEISA-97), in the spectral range from 10^{-6} to $22,656\text{ cm}^{-1}$.

The included molecules are constituents of the atmospheres of Earth (major permanent and trace molecules) and of other Planet (such as: C_2H_4 , GeH_4 , C_3H_8 , C_2N_2 , C_4H_2 , HC_3N , H_2S , HCOOH and C_3H_4 , for the Giant Planets). Among the spectroscopic parameters archived in GEISA, the most important for atmospheric radiative transfer modelling are: the wavenumber (cm^{-1}) of the line associated with a vibro-rotational transition, the intensity of the line (cm molecule^{-1} at 296K), the Lorentzian collision halfwidth ($\text{cm}^{-1}\text{ atm}^{-1}$ at 296 K), the energy of the lower level of the transition (cm^{-1}), the transition quantum identifications for the lower and upper levels of the transition, the temperature dependence coefficient of the halfwidth, the database management identification codes for isotopes and for molecules.

Details for updates

Twenty molecules have been updated in GEISA-03, i.e.:

H₂O: Three spectral regions have been re-investigated. In the 500 to 2850 cm^{-1} region, the line parameters were replaced with a compilation of 10755 water transitions obtained by Toth (1998, 1999, 2000) and Toth et al. (1998). In the 9650-11400 cm^{-1} region, the update comes from of empirical line parameters of H_2^{16}O obtained by Brown et al. (2002). In the 13000-26000 cm^{-1} region the new line parameters are from Carleer et al. (1999), Coheur et al. (2002) and Fally et al. (2003).

CO₂: The previous line parameters of the transitions belonging to the four most abundant isotopomers $^{12}\text{C}^{16}\text{O}_2$, $^{13}\text{C}^{16}\text{O}_2$, $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ and $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ in the 442-2797 cm^{-1} spectral region, have been replaced with 48627 new ones covering the 436-2826 cm^{-1} spectral range, issued of the results described in Tashkun et al. (1998, 2001) and Teffo et al. (2002, 2003).

O₃: Updates occur in four spectral regions: In the 600-1232 cm^{-1} spectral region, new and more accurate line parameters for the ν_1 and ν_3 bands of $^{16}\text{O}_3$ were derived by Wagner et al. (2002) and Flaud et al. (2003). A complete new study of the 1300-1500 cm^{-1} spectral range, related with the $2\nu_2$, $3\nu_2-\nu_2$, $\nu_1+\nu_3+\nu_3-\nu_2$ and $2\nu_3-\nu_2$ bands of $^{16}\text{O}_3$, has been made by Barbe et al. (1998). The 1820-2260 cm^{-1} ($2\nu_3$, $\nu_1+\nu_3$ and $2\nu_1+\nu_3$ interactive bands of $^{16}\text{O}^{18}\text{O}^{16}\text{O}$) and the 2600-2900 cm^{-1} (triad: $\nu_2+2\nu_3$, $\nu_1+\nu_2+\nu_3$ with $2\nu_1+\nu_2$) regions, have been reinvestigated by De Backer-Barilly et al. (2003) and by Mikhailenko et al. (2002), respectively.

N₂O: 279 lines in the spectral region 870-1240 cm⁻¹, recently revisited by Daumont et al. (2002), have been substituted in two bands, $\nu_3-\nu_1$ and $\nu_3-2\nu_2$, the intensities of which were doubtful. In addition, a technical update has removed 118 duplicated lines in the spectral interval 564 cm⁻¹ - 629 cm⁻¹.

CH₄ and CH₃D: The CH₄ and CH₃D contents of GEISA have been extensively updated. The spectral range has been extended from 6184.492cm⁻¹ to 9199.2846 cm⁻¹, and the number of entries increased from 66883 to 216196 (weaker transitions of ¹²CH₄ and new bands of ¹³CH₄ and CH₃D included). Full details about the revision in the spectral interval from 0.01 to 6184.492 cm⁻¹ can be found in a review paper by Brown et al. (2003). The new CH₄ near infrared data from 4800-5500 cm⁻¹ and 6180-10000cm⁻¹ are from an empirical list obtained by Brown (2003), from a few selected FTS laboratory spectra.

O₂: The two spectral regions, 7664.726-8064.311 cm⁻¹ and 11483.727-15927.806 cm⁻¹, have been updated thanks to new results by Goldman et al. (2003) and by Brown and Plymate (2000), respectively.

NO: A new line list has been produced (Goldman 2003) in the first overtone region of the main isotopic species ¹⁴N¹⁶O, i.e. between 3547.318 and 3799.155 cm⁻¹. This calculation has been issued from experimental data from Mandin et al. (1997,1998) and theoretical results from Gillis and Goldman (1982).

NO₂: A new linelist was set up in the spectral region of the $\nu_1+\nu_3$, $\nu_1+2\nu_2$ and $\nu_1+\nu_2+\nu_3-\nu_2$ bands of the ¹⁴N¹⁶O₂ main isotopic species. New line parameters come from the works of Mandin et al. (1997), Dana et al. (1997), Devi et al. (1982), May and Webster (1990).

NH₃: The line parameters of the interval 0.058-5294.502 cm⁻¹ have been totally replaced by those issued by Kleiner and Brown (2003) and described in Kleiner et al. (2003).

PH₃: New data from Brown and Kleiner (2003), described in Kleiner et al. (2003), have replaced the whole content of the region from 770.877 to 2478.765 cm⁻¹.

OH: Line parameters in the ultraviolet region from 29808.500 to 35877.030 cm⁻¹, from Gillis et al. (2001) have been added to the GEISA archive.

HBR: New line parameters of H⁷⁹Br and H⁸¹Br, for the spectral regions of the pure rotation band X¹Σ⁺ (0-0) (16.692-396.474 cm⁻¹) and of the fundamental band (1-0) (2123.812-2790.533 cm⁻¹), have been derived for spectroscopic databases update, as described in Goldman et al. (2003).

HI: The description of the updates in the spectral regions of the X¹Σ⁺ (0-0) (12.842-319.820 cm⁻¹) and of the (0-1) (1950.689-2403.162 cm⁻¹) bands, is given in Goldman et al. (2003).

C₂H₆: In the spectral region 2975.331-2977.926 cm⁻¹, a modified list by Rinsland et al. (1998), for the ^pQ₃ sub-branch in the ν_7 band, has replaced the previously archived line parameters.

C₂H₂: The updates of the database has concerned three spectral regions: the 13.6- and 5- μ m regions, from work performed by Mandin et al. (2000), Jacquemart et al. (2001, 2002), and the 7.5 - μ m region, from results by Vander Auwera (2000).

HOCl: A new line list has been created in the spectral interval 1178.673-1320.332 cm⁻¹, corresponding to the ν_2 region, on the basis of the works of Flaud et al. (1998), Flaud (2002) and Vander Auwera et al. (2000).

CH₃Cl: In the spectral region from 1261.562 to 1645.899 cm⁻¹, a list of 8989 transitions of the [ν_2 , ν_5 , $2\nu_3$] -vibrational-band triad, prepared by Brown (2002) and based upon the work of Chackerian et al. (1998), has been newly archived, for CH₃³⁵Cl and CH₃³⁷Cl.

COF₂: An update of the 1856.730-2001.348 cm⁻¹ region has been made thanks to a list generated by Brown (2001), based on an unpublished analysis of the line positions.

HO₂: Spectroscopic parameters for the ground state have replaced by those generated upon the basis of the work of Chance (1997, 2003)).

A summary of GEISA-03 line transition parameters sub-database content, in terms of number of entries, is given in Table 1. The molecular species formulas are listed in column 1 with, in column 2, their associated identification codes. In columns 3 and 4 are given the number of entries, for each molecular species, in GEISA-97 and in GEISA-03, respectively, with, in column 5, the differences between the numbers of entries in these two editions of the database. Updated molecular species have been coloured in red, if the number of entries has been increased, or in blue, on the contrary. Light green background corresponds to GEISA/IASI-03 specific archive (see related section in the following). It has to be noticed that, in this new edition of GEISA, particular attention has been paid to remove duplicated lines and to harmonize default values for unknown spectroscopic parameters.

- **The GEISA-03 sub-database on absorption cross-sections**

As described in Jacquinet-Husson et al. (1999), besides the line transition parameters data catalog itself, GEISA includes, a second catalog, providing, at various temperatures and pressures, the cross-sections (unit: cm² molecule⁻¹) of species exhibiting dense spectra, not suitable for a discrete parameterized format. The GEISA-03 archive has been significantly enriched since the GEISA-97 issue. The spectral range has been extended: from 200 cm⁻¹ to 2000 cm⁻¹ (from 556 cm⁻¹ to 1763 cm⁻¹, previously) and the number of molecules has increased, as well, from 23 to 35. The updated already archived species are: CFC11, CFC12, CFC14, HCFC22, HCFC123, HCFC124, HFC125, HFC134a, HCFC141b, HCFC142b, HFC152a, HCFC225ca, HCFC225cb, HFC32, HFC143a, HFC134, N₂O₅, SF₆, ClONO₂. No update has occurred for CFC-13, CFC-113, CFC-114, CFC-115. Eleven molecular species are new for GEISA-03 archive, these are: HFC-143, HCFC-21, C₂F₆, C₂H₂, C₂H₄, C₂H₆, C₃H₈, C₄H₈, HNO₄, SF₅CF₃, HCH-365mfc.

A summary of the GEISA-03 sub-database on absorption cross-sections is given in Table 2. The molecular species names, with their associated identification codes, are listed in columns 1 and 2, respectively. In the three following columns are the experimental conditions associated with the data files, i.e.: the spectral coverage (cm⁻¹), in column 3; the overall temperature range (K), in column 4; the total pressure range (Pa), in column 5. For each file, the number of associated temperature-pressure sets is in column 7 and the related references, in column 8. Reference “GEISA-97” corresponds to non updated molecules. New archived molecular species have been coloured in red. Light green background corresponds to the GEISA/IASI-03 specific archive (see related section in the following).

- **The GEISA-03 sub-database on microphysical and optical properties of atmospheric aerosols**

A common GEISA and GEISA/IASI aerosol sub-database has been recently issued for GEISA/IASI-01 (see Jacquinet-Husson et al. (2003) for details). It gathers the micro-physical and optical properties from published aerosol data catalogs, the overall content of which deals with the archive of complex refractive indices and possibly computed optical related properties, for selected basic aerosol components. Softwares for data management and user-selected aerosol mixtures elaboration are available from the archive. No update of this sub-database has occurred for GEISA-03.

The GEISA/IASI database: 2003 Edition

The GEISA/IASI database derives from GEISA as described in Jacquinet-Husson et al.(1998, 2003). GEISA/IASI is being elaborated with the purpose of assessing the IASI measurements capabilities, within the ISSWG (IASI Sounding Science Working Group), in the frame of CNES (Centre National d'Etudes Spatiales, France)/EUMETSAT (EUropean organization for the exploitation of METeorological SATellites) European Polar System (EPS), by simulating high resolution radiance spectra and/or experimental data. To benefit as soon as possible from improvements in the knowledge of spectroscopic parameters and to ensure the continuous upgrade and maintenance of GEISA/IASI during the fifteen years of life of the IASI instrument, EUMETSAT and CNES have created a GEISA/IASI Database Scientific Committee (GIDSC). EUMETSAT is planning to implement GEISA/IASI into the EPS ground segment.

The GEISA/IASI database, in its 2003 edition (GEISA/IASI-03), is an extraction of GEISA-03 within the IASI or AIRS spectral range ($599- 3001 \text{ cm}^{-1}$) with a similar structure, including the three independent sub-databases described above.

GEISA/IASI-03 line transition sub-database contains spectroscopic line parameters stored following the GEISA-03 standard with extended line parameter information (including associated error estimations), for 14 molecules (53 isotopic species) representing 702,550 entries. The GIDSC selected molecules are: H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, HNO₃, OCS, C₂H₂, N₂.

It has to be noticed that in GEISA/IASI, CH₃D is considered as an isotope of CH₄. It is considered as an independent molecule in GEISA. Related with the H₂O archive in the 10 μm region, alternative line parameters, from Stewart (2003), have been issued as a support study for IASI, and archived in GEISA/IASI-03.

In the GEISA/IASI-03 sub-database on Absorption cross-sections, six molecular species, among the 35 present in GEISA-03, have been selected. These are : CFC-11, CFC-12, CFC-14, CCl₄, N₂O₅ and HCFC-22.

GEISA/IASI-03 is detailed extensively in a paper in preparation, to be submitted at JQSRT.

Table 1: GEISA-03 individual lines sub-database summarized updates and contents
Spectral Range: 10^{-6} – 25232.004100 cm^{-1}

Molécule	ID.	GEISA 97	GEISA 2003	2003 - 1997
H ₂ O	1	50217	58726	8509
CO ₂	2	62816	76826	14010
O ₃	3	281607	319248	37641
N ₂ O	4	26771	26681	-90
CO	5	13515	13515	0
CH ₄	6	66883	216196	149313
O ₂	7	6292	6290	-2
NO	8	94738	99123	4385
SO ₂	9	38853	38853	0
NO ₂	10	100680	104224	3544
NH ₃	11	11152	29082	17930
PH ₃	12	4635	11740	7105
HNO ₃	13	171504	171504	0
OH	14	41786	42866	1080
HF	15	107	107	0
HCl	16	533	533	0
HBr	17	576	1294	718
HI	18	237	806	569
ClO	19	7230	7230	0
OCS	20	24922	24922	0
H ₂ CO	21	2702	2701	-1
C ₂ H ₆	22	14981	14981	0
CH ₃ D	23	11524	35518	23994
C ₂ H ₂	24	1668	3115	1447
C ₂ H ₄	25	12978	12978	0
GeH ₄	26	824	824	0
HCN	27	2775	2550	-225
C ₃ H ₈	28	9019	8983	-36
C ₂ N ₂	29	2577	2577	0
C ₄ H ₂	30	1405	1405	0
HC ₃ N	31	2027	2027	0
HOCl	32	15565	17862	2297
N ₂	33	117	120	3
CH ₃ Cl	34	9355	18344	8989
H ₂ O ₂	35	100781	100781	0
H ₂ S	36	20788	20788	0
HCOOH	37	3388	3388	0
COF ₂	38	54866	83750	28884
SF ₆	39	11520	11520	0
C ₃ H ₄	40	3390	3390	0
HO ₂	41	26963	38804	11841
ClONO ₂	42	32199	32199	0
Total lines :		1,346,466	1,668,371	+321,905

Table 2: GEISA-03 Cross-Sections Sub-Database

Molecule	Mol ID	Spectral coverage (cm ⁻¹)	Temperature range (K)	Pressure range (Pa)	Number of TP sets	References
CFC-11	1	210 - 2000	296	93325	1	Hurley(2003); Christidis(1997)
		500 - 1600	297	0	1	MSF/ RAL (2003)
		810 - 1120	190 - 296	1000 - 101325	55	Li & Varanasi (1994) ; Varanasi (2000)
CFC-12	2	850 - 1190	253 - 287	0	3	Clerbaux (1993)
		210 - 2000	296	93325	1	Hurley(2003)
		800 - 1200	190 - 296	1000 - 101392	57	Varanasi & Nemtchinov (1994); Varanasi (2000)
CFC-13	3	765 - 1235	203 - 293	0	3	GEISA97
CFC-14	4	220 - 2000	296	93325	1	Hurley (2003)
		1250 - 1290	180 - 296	1005 - 101458	55	Nemtchinov & Varanasi (2003a)
CFC-113	5	780 - 1232	203 -293	0	6	GEISA97
CFC-114	6	815 - 1285	203 -293	0	6	GEISA97
CFC-115	7	955 - 1260	203 -293	0	6	GEISA97
HFC-32	8	204 - 2000	296	93325	1	Hurley (2003); Pinnock (1995)
		995 - 1475	203 - 297	0 - 100000	17	MSF/ RAL (2003)
		700 - 1465	287	0	1	Clerbaux (1993)
HFC-125	9	495 - 1504	203 -293	0 - 80000	16	Di Lonardo (2000)
		208 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
		210 - 2000	296	93325	1	Hurley(2003); Christidis(1997)
HFC-134	10	600 - 1700	203 - 297	0 - 100000	9	MSF/ RAL (2003)
		815 - 1485	253 - 287	0	3	Clerbaux (1993)
		203 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HFC-134a	11	600 - 1600	203 - 296	0 - 100000	15	MSF/ RAL (2003)
		1035 - 1340	190 - 296	2666 - 101376	33	Nemtchinov & Varanasi (2004)
		204 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HFC-143	12	204 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HFC-143a	13	694 - 1504	203 - 293	0 - 800000	19	Di Lonardo (2000)
		200 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
		580 - 1500	203 - 297	0 - 100000	9	MSF/ RAL (2003)
HFC-152a	14	700 - 1600	203 - 293	0 - 80000	16	Vander Auwera (2000)
		840 - 1490	253 - 287	0	3	Clerbaux (1993)
		200 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HCFC-21	15	785 - 840	296	133	1	Massie et al. (1985)

Molecule	Mol. ID	Spectral coverage (cm-1)	Temperature range (K)	Pressure range (Pa)	Number of TP sets	References
HCFC-22	16	700 - 1500	203 - 293	0 - 80000	8	Vander Auwera (2003)
		765 - 1380	253 - 287	0	3	Clerbaux (1993)
		208 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
		760 - 1195	181 - 297	2666 - 101936	51	Varanasi (2001)
HCFC-123	17	740 - 1450	253 - 287	0	3	Clerbaux (1993)
		204 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HCFC-124	18	675 - 1425	287	0	1	Clerbaux (1993)
		208 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HCFC-141b	19	209 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
		710 - 1470	253 - 287	0	3	Clerbaux (1993)
HCFC-142b	20	650 - 1475	253-287	0	3	Clerbaux (1993)
		200 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HCFC-225ca	21	695 - 1420	253 - 287	0	3	Clerbaux (1993)
		600 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
HCFC-225cb	22	715 - 1375	253 - 287	0	3	Clerbaux (1993)
		600 - 2000	296	93325	1	Pinnock (1995); Hurley (2003)
N2O5	23	540 - 1380	205 - 293	0	5	Wagner & Birk (2003)
SF6	24	650 - 2000	296	93325	1	Hurley (2003)
		925 - 955	180 - 295	2693 - 101350	29	Varanasi (2001)
ClONO2	25	500 - 1330	190 - 297	0 - 15580	25	Wagner & Birk (2003)
		1265 - 1325	201 - 222	0	3	GEISA97
CCl4	26	750 - 812	208 - 297	1070 - 101272	32	Nemtchinov & Varanasi (2003b)
C2F6	27	1061 - 1285	180 - 296	3320 - 101363	43	Zou & al. (2004)
		210 - 2000	296	93325	1	Highwood (1999);Hurley (2003)
		600 - 2750	203 - 293	0 - 80000	15	MSF/ RAL (2003)
C2H2	28	450 - 2000	296	93325	1	Highwood (1999);Hurley (2003)
C2H4	29	220 - 2000	296	93325	1	Highwood (1999);Hurley (2003)
C2H6	30	220 - 2000	296	93325	1	Highwood (1999);Hurley (2003)
C3H8	31	220 - 2000	296	93325	1	Highwood (1999);Hurley (2003)
C4F8	32	500 - 1600	203 - 297	0 - 65000	19	MSF/ RAL (2003)
HNO4	33	770 - 830	268	93	1	Massie et al. (1985)
SF5CF3	34	600 - 2000	296	93325	1	Hurley (2003)
HCH-365mfc	35	665 - 1480	287	0	1	Clerbaux (1993)

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