

# The GEISA spectroscopic database system updated for IASI (direct radiative transfer modeling)

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The performances of the second generation vertical sounders like AIRS (Atmospheric Infrared Sounder) in the USA, and IASI (Infrared Atmospheric Sounding Interferometer) in Europe, are highly dependent on the accuracy of spectroscopic parameters of the optically active atmospheric gases. In this context, since 1974, the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie Dynamique, France) has developed the GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information) computer accessible database system to perform reliable radiative transfer calculations. The 2001 version of GEISA (further GEISA-01) and GEISA/IASI (GEISA version dedicated to the IASI experiment) are described. GEISA-01 database involves information on line transition parameters for 42 molecules (96 isotopic species) and contains 1 361 667 entries, between 0 and 22 656  $\text{cm}^{-1}$ .

## Introduction

New instruments of high resolution for sensing vertical atmosphere, like AIRS (Atmospheric Infrared Sounder: <http://www-airs.jpl.nasa.gov/>) in the USA, and IASI (Infrared Atmospheric Sounding Interferometer: <http://www-projet.cst.cnes.fr:8060/IASI/index.html>) in Europe, which have a better vertical resolution and accuracy compared to the presently available, are mainly meant for operational meteorology associated with Numerical Weather Prediction, as well as for provision of an improved knowledge of the vertical atmospheric structure and surface properties.

The performances of these sounders will be highly dependent on the present-day knowledge of accuracy of the spectroscopic parameters of the optically active atmospheric gases, since they are an essential input in the forward models used to simulate the recorded radiance spectra. Consequently, there is an acute need for comprehensive, trustworthy, and operational interactive spectroscopic databases. In this context, since 1974 the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie Dynamique, France) has developed GEISA, the computer accessible database system<sup>1-3</sup> intended to reliably calculate the radiative transfer in the atmosphere using the "line-by-line and layer-by-layer" approach. This benefits the researchers in direct and inverse radiative transfer studies. Currently, GEISA is actively used in assessment of capabilities of improved atmospheric sounders.<sup>4</sup>

## GEISA spectroscopic database overview

The 1997 GEISA database,<sup>5</sup> has been partially updated in 2001 (GEISA-01). The GEISA-01 system comprises three sub-databases.

### The GEISA-01 sub-database of line transition parameters:

GEISA-01 sub-database of line transition parameters involves 42 molecules (96 isotopic species) and contains 1 361 667 entries (15 401 supplementary entries since GEISA-97), between 0 and 22 656  $\text{cm}^{-1}$ .

The included molecules are of interest for the Earth and other planet atmospheres ( $\text{C}_2\text{H}_4$ ,  $\text{GeH}_4$ ,  $\text{C}_3\text{H}_8$ ,  $\text{C}_2\text{N}_2$ ,  $\text{C}_4\text{H}_2$ ,  $\text{HC}_3\text{N}$ ,  $\text{H}_2\text{S}$ ,  $\text{HCOOH}$ , and  $\text{C}_3\text{H}_4$ ). Among spectroscopic parameters archived in GEISA, the most important for the atmospheric radiative transfer modelling are: the line wavenumber ( $\text{cm}^{-1}$ ) associated with a vibro-rotational transition, the line intensity ( $\text{cm}\cdot\text{molecule}^{-1}$  at 296 K), the Lorentzian collision halfwidth ( $\text{cm}^{-1}\text{atm}^{-1}$  at 296 K), the energy of the transition lower level ( $\text{cm}^{-1}$ ), 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 molecules. These parameters are stored following the GEISA standard as described in Ref. 5.

Three molecules have been updated in GEISA-01, i.e.,

H<sub>2</sub>O: 10 755 transitions<sup>6–12</sup> in the spectral range 500–2900 cm<sup>-1</sup>,

CO<sub>2</sub>: 48 000 new transitions<sup>13–16</sup> in the spectral range 430–2820 cm<sup>-1</sup>,

N<sub>2</sub>O: 118 replicate lines were removed from the spectral range 564 – 629 cm<sup>-1</sup>.

### The GEISA-01 sub-database on absorption cross sections:

Besides the catalog of line transition parameters, in the spectral range 556.380–1763.642 cm<sup>-1</sup> GEISA includes one more catalog, referred to as GEISA\_CROSS, providing, at various temperatures and pressures, the cross sections of species exhibiting dense spectra, not suitable for a discrete parameterized format. It represents 4 716 743 entries related to 23 molecules, i.e.: CFC11, CFC12, CFC13, CFC14, CFC113, CFC114, CFC115, HCFC22, HCFC123, HCFC124, HFC125, HFC134a, HCFC141b, HCFC142b, HFC152a, HCFC225ca, HCFC225cb, HFC32, HFC143a, HFC134, N<sub>2</sub>O<sub>5</sub>, SF<sub>6</sub>, and ClONO<sub>2</sub>.

The absorption cross sections are determined through the following expression:

$$\sigma(\omega) = \frac{\ln[I_0(\omega)/I(\omega)]}{nl}$$

where  $\omega$  is the wavenumber (cm<sup>-1</sup>);  $\sigma(\omega)$  is the absorption cross section (cm<sup>2</sup>·molecule<sup>-1</sup>);  $I_0(\omega)$  and  $I(\omega)$  are the intensities of the incident and transmitted radiation, respectively, at the frequency  $\omega$ ;  $n$  is the concentration of molecules (molecule cm<sup>-3</sup>) and  $l$  is the optical path length (cm). It is just the  $\sigma(\omega)$  value, derived from high-resolution experimental data, that is cataloged in the GEISA cross section file. A management program, supplied with GEISA\_CROSS, has been designed to use and manage this sub-database. No update occurred since the GEISA-97 edition.

### The GEISA-01 sub-database on microphysical and optical properties of atmospheric aerosols

The new edition of GEISA-01 sub-database on microphysical and optical properties of atmospheric aerosols is described in the next section (GEISA/IASI database).

User-friendly management softwares<sup>3,17</sup> are associated with each of these three GEISA-01 sub-database catalogs. The current edition of the GEISA system, with associated softwares, are accessible freely via the ARA/LMD group workstations Web site, upon prior request for password at: nicole.jacquinet@lmd.polytechnique.fr.

## GEISA/IASI database description

### General context of the GEISA/IASI-01 database

The GEISA/IASI database derives from GEISA as described in Refs. 4 and 18. GEISA/IASI is designed to assess the IASI measurement 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 the improved spectroscopic parameters and to ensure the continuous upgrade and maintenance of GEISA/IASI during fifteen-year 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 2001 edition of the GEISA/IASI database, (GEISA/IASI-01), is both an extraction from IASI or AIRS within the spectral range 600–3000 cm<sup>-1</sup> and a partial update of GEISA-97 and GEISA-01, with a similar structure, including the above three independent sub-databases.

### GEISA/IASI-01 sub-database on line transition parameters

GEISA/IASI-01 line transition sub-database contains spectroscopic line parameters stored following the GEISA standard with extended information on line parameters (including associated error estimates) for 14 molecules (53 isotopic species) representing 650 274 entries. The GIDSC selected molecules are: H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CO, CH<sub>4</sub>, O<sub>2</sub>, NO, SO<sub>2</sub>, NO<sub>2</sub>, HNO<sub>3</sub>, OCS, C<sub>2</sub>H<sub>2</sub>, and N<sub>2</sub>.

It has to be noticed that CH<sub>3</sub>D is considered as an isotope of CH<sub>4</sub> in GEISA/IASI, although in GEISA-97 and in GEISA-01 it is considered as an independent molecule. The GEISA/IASI-01 content is given in Table 2.

Along with GEISA-97 and GEISA-01, updates were made in GEISA/IASI-2001 for spectroscopic line parameters of molecules:

**H<sub>2</sub>O**: update is similar to that made in GEISA-01;

**CO<sub>2</sub>**: update insignificantly differs from that made in GEISA-01;

**O<sub>3</sub>**: by Refs. 19 and 20;

**CH<sub>4</sub>**: by Refs. 21–28;

**HNO<sub>3</sub>**: by Ref. 29;

**C<sub>2</sub>H<sub>2</sub>**: by Ref. 30.

All the archived data can be handled through the database associated general GEISA user-friendly software.

Table 1. Detailed content of GEISA/IASI-01 I line transition parameters sub-database

Mol.	MolID	Lines	Intensity average, $\text{cm}\cdot\text{mol}^{-1}$	$\alpha$ , $\text{cm}^{-1}$	Iso. ID	Lines	$F_{\text{min}}$ , $\text{cm}^{-1}$	$F_{\text{max}}$ , $\text{cm}^{-1}$	Int., $\text{cm}\cdot\text{mol}^{-1}$	
									min	max
H <sub>2</sub> O	1	13279	8.112E-22	0.0655	161	5218	600.104	2999.854	9.010E-28	2.989E-19
					162	4584	604.366	2999.340	1.000E-27	2.505E-23
					171	1203	599.702	2999.532	1.490E-27	1.210E-22
					181	1661	604.933	3001.175	2.025E-27	6.051E-22
					182	438	1173.772	1684.226	2.033E-27	5.083E-26
					172	175	1234.235	1598.766	2.033E-27	9.319E-27
CO <sub>2</sub>	2	50375	2.185E-21	0.0711	626	18614	599.222	2488.222	3.440E-39	3.530E-18
					636	7517	599.026	2395.279	1.820E-39	3.750E-20
					628	11912	599.007	2826.650	1.390E-36	6.850E-21
					627	7575	599.183	2806.198	1.000E-27	1.250E-21
					638	1833	599.165	2605.481	3.704E-27	7.227E-23
					637	1346	599.008	2314.307	3.708E-27	1.361E-23
					828	994	615.974	2350.898	1.760E-40	1.309E-23
					728	288	626.438	2358.226	3.866E-27	2.495E-24
					838	296	2115.685	2276.481	4.870E-42	1.760E-25
O <sub>3</sub>	3	151775	1.141E-22	0.0701	666	124863	600.179	3000.984	1.010E-26	4.090E-20
					668	13728	640.037	1177.493	9.680E-26	7.760E-23
					686	4858	640.141	1145.690	9.620E-26	7.560E-23
					667	5515	599.123	820.380	3.561E-27	5.570E-25
					676	2811	599.382	822.795	3.527E-27	6.057E-25
					446	13273	599.027	2836.125	8.260E-27	1.003E-18
N <sub>2</sub> O	4	18938	3.634E-21	0.0744	447	791	599.420	2560.588	6.180E-26	4.154E-22
					448	1596	599.321	2543.215	1.226E-25	2.045E-21
					456	1623	599.826	2595.681	1.218E-25	3.666E-21
					546	1655	599.129	2585.207	1.214E-25	3.601E-21
					26	1499	1523.979	2316.048	6.840E-70	4.461E-19
CO	5	3674	2.749E-21	0.0467	27	229	1831.283	2278.721	1.248E-36	1.602E-22
					28	240	1797.966	2254.309	1.253E-36	8.317E-22
					36	1263	1544.497	2259.947	1.880E-65	4.685E-21
					38	226	1779.750	2196.287	1.503E-36	8.698E-24
					37	217	1807.871	2221.114	1.030E-36	1.679E-24
					211	68777	922.651	3000.999	1.000E-27	1.202E-19
CH <sub>4</sub>	6	121282	6.890E-23	0.0498	311	22688	998.884	3000.999	9.488E-28	1.344E-21
					212	29817	855.753	3000.997	6.158E-29	3.658E-23
					66	435	1366.105	1717.235	1.100E-35	1.490E-28
O <sub>2</sub>	7	435	2.191E-29	0.0466	46	24705	599.089	3000.718	1.401E-85	6.211E-20
					48	679	1601.909	2038.846	4.190E-28	1.390E-22
					56	699	1609.585	2060.462	4.430E-28	2.550E-22
SO <sub>2</sub>	9	22301	1.566E-21	0.1132	626	22014	599.173	2787.861	5.000E-26	6.094E-20
					646	287	2463.470	2496.088	9.736E-24	3.428E-23
NO <sub>2</sub>	10	68252	9.087E-22	0.0666	646	68252	599.083	2938.381	9.470E-26	1.302E-19
HNO <sub>3</sub>	13	152586	6.928E-22	0.1101	146	152586	599.003	1769.982	1.051E-25	3.020E-20
OCS	20	19768	5.288E-21	0.0898	822	11005	814.581	2962.986	1.010E-23	1.077E-18
					623	3810	813.860	2926.274	1.010E-23	4.719E-20
					634	2048	825.716	2880.701	1.008E-23	1.198E-20
					822	955	818.098	2875.829	1.008E-23	2.089E-21
					623	1593	825.659	2930.386	1.016E-23	8.430E-21
					634	357	1972.188	2032.039	1.010E-23	5.240E-22
C <sub>2</sub> H <sub>2</sub>	24	1409	2.294E-20	0.0609	221	1307	604.774	1469.865	1.371E-27	1.187E-18
					231	150	613.536	843.872	3.820E-26	1.577E-20
N <sub>2</sub>	33	117	5.729E-29	0.0469	44	117	2001.711	2619.230	2.330E-34	3.410E-28

Notes. 1) Total number of lines in GEISA/IASI-2001 is 650 274. 2) Value 8.112E-22 should be read 8.112·10<sup>-22</sup>, the same for others.

### GEISA/IASI-01 sub-database on absorption cross-sections

In this file, referred to as GEISA\_CROSS/IASI-01, six molecular species other than those 23 presented in GEISA-97 and GEISA-01, have been selected. They are: CFC-11, CFC-12 (Refs. 31, 32), CFC-14 (Ref. 33), CCl<sub>4</sub> (Ref. 34), N<sub>2</sub>O<sub>5</sub> (Ref. 35), and HCFC-22 (Refs. 36 and 37). The format of the database entries is similar to formats of GEISA-97 and GEISA-01.

Table 2. Content of GEISA\_CROSS / IASI-01 sub-database

Molecule	Spectral range, cm <sup>-1</sup>	The number of temperature modes (T,K)	Ref.
CFC-11	810–880	55 (190–296)	31
CCl <sub>3</sub> F	1050–1120		
CFC-12	800–950	52 (190–296)	32
CCl <sub>2</sub> F <sub>2</sub>	1050–1200		
CFC-14	1250–1290	55 (180–296)	33
CF <sub>4</sub>			
CCl <sub>4</sub>	750–812	32 (208–296)	34
N <sub>2</sub> O <sub>5</sub>	557–1763	4 (233–293)	35
HCFC-22	750–870	8 (216–294)	36
	765–1380		37

A program, supplied with GEISA\_CROSS/IASI, has been designed to use and to manage the data on CFC-11, CFC-12, CFC-14, CCl<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>, and HCFC-22 absorption cross sections. It is similar to those of GEISA-CROSS-97 and GEISA-01.

### GEISA/IASI-01 sub-database on microphysical and optical properties of atmospheric aerosols

Besides the molecular species which define the gaseous infrared opacity in the Earth's atmosphere, the aerosol particles also contribute to this opacity. Consequently, a common GEISA and GEISA/IASI aerosol sub-database, referred to as GEISA\_AEROS, has been recently elaborated. It includes microphysical and optical properties from four published aerosol data catalogs (see Refs. 38–41), the overall content of which deals with the archive of complex refractive indices and data for computation of optical properties of basic aerosol components. Data processing software is available in Refs. 39–41.

### The GEISA\_AEROS database structure

1) *The database on refractive indices of 10 varieties of basic aerosol components.* This database (originally Ref. 38) was updated by Massie in 2000. It comprises an extensive archive of complex refractive indices, determined both *in situ* and in the

laboratory from spectral transmission and reflection measurements (more than 40 references) of various aerosol components.

2) *The database of microphysical and optical properties of atmospheric aerosols (Ref. 39).* The first part of the archive consists of complex indices of refraction for seven basic aerosol components from Ref. 42, i.e., dust-like, water-soluble, soot, and oceanic salt particles, sulfuric acid solution droplets, volcanic ash and water. They have been used in Ref. 39 for computation of integrated optical properties of aerosol, i.e., the extinction coefficient, single scattering albedo, and asymmetry factor.

In the second part, the so-called AERCOMP (FORTRAN code) software package, allowing the determination of optical properties for user-defined aerosol mixtures (including scattering phase functions), has been archived with associated basic optical properties of the aerosol constituent.

3) *The database and associated software package OPAC (Optical Properties of Aerosols and Clouds) (Ref. 40).* The first part of this archive is a data set of microphysical and optical properties of:

- ten basic aerosol components: insoluble, soot, water soluble, two sea salt modes, i.e., various kinds of salt contained in seawater, three mineral modes, i.e., mixture of quartz and clay minerals, transported minerals, sulfate droplets;

- six types of water clouds: stratus (continental and maritime), cumulus (continental clean and polluted, as well as maritime), fog, and three kinds of cirrus ice clouds, both in the solar and terrestrial spectral ranges.

The second part is a FORTRAN program making it possible to extract data from the above archive and allowing the calculation of any user-defined mixtures of these components. A set of computed typical mixtures is archived as well.

4) *The Global Aerosol Data Set GADS (Ref. 41).* Using the OPAC aerosol archive, GADS provides the data on the global aerosol distribution as climatologically averaged values both for the winter (December to February) and summer (June to August) seasons on a global grid with a resolution of 5° by 5° (longitude and latitude) for the components selected in OPAC. A GADS-associated FORTRAN program makes it possible to calculate the global distributions of the user-selected aerosol optical or microphysical properties.

The above GEISA/IASI spectroscopic database system, including data files and management software, is available at:

ftp://ara01.lmd.polytechnique.fr/pub/geisa/iasi2001.

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