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

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Abstract : The **GEISA** (**G**estion et **E**tude des **I**nformations **S**pectroscopiques **A**tmosphériques: Management and Study of Atmospheric Spectroscopic Information) computer accessible spectroscopic database system, in its 2003 version comprises three sub-databases with their associated management softwares, i.e: a database of spectroscopic parameters required to describe adequately the individual spectral lines belonging to 42 molecules, 96 isotopic species and located in a spectral range from the microwave to the limit of the visible (1,668,371 entries). The featured molecules are of interest in studies of the terrestrial as well as the other planetary atmospheres, especially those of the Giant Planets; a database of absorption cross-sections of molecules such as chlorofluorocarbons which exhibit unresolvable spectra; a database of refractive indices of basic atmospheric aerosol components. The so-called GEISA/IASI sub-database (spectral interval 500-3001 cm^{-1}) system has been elaborated from GEISA, in the purpose of assessing the IASI instrument (Infrared Atmospheric Sounding Interferometer; http://smsc.cnes.fr/IASI/index.htm) atmospheric sounding capabilities performances, from direct and inverse radiative transfer modeling, using high quality spectroscopic parameters of the optically active gases. All the archived data can be handled through general and user friendly associated management software facilities, which are interfaced on the ARA (Atmospheric Radiation Analysis)/LMD (Laboratoire de Météorologie Dynamique) group web site at: http://ara.lmd.polytechnique.fr.

Key-Words : GEISA; GEISA/IASI; Spectroscopic database; Atmospheric absorption; CFC's cross-sections; Atmospheric aerosols.

1 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, is highly dependent on the 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. [1]; Husson et al. [2][3]). Currently, GEISA is involved in activities related to the assessment of the capabilities of IASI, as described in Jacquinet-Husson et al. [4].

2 The GEISA database in its 2003 Edition: an overview

Since its 1997 edition (GEISA-97), the GEISA database, extensively described in [5], has been updated twice: partially in 2001 [6] and extensively in 2003 (GEISA-03).

The GEISA-03 system comprises three independent sub-databases devoted respectively to:

- individual line transition spectroscopic parameters ,
- infrared absorption cross-sections,
- micro-physical and optical properties of atmospheric aerosols.

All the archived data can be handled through general and user friendly *GEISA* associated management softwares.

2.1 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 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 (cm^{-1} 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.:

H_2O: Three spectral regions have been re-investigated. In the 500 to 2850 cm^{-1} region, the line parameters were replaced with a compilation of 10,755 water transitions obtained by Toth [7-9] and Toth et al. [10]. In the 9,650-11,400 cm^{-1} region, the update comes from of empirical line parameters of $H_2{}^{16}O$ obtained by Brown et al. [11]. In the 13000-26000 cm^{-1} region the new line parameters are from Carleer et al. [12], Coheur et al. [13] and Fally et al. [14].

CO_2: The previous line parameters of the transitions belonging to the four most abundant isotopomers $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C\,^{18}O$ and $^{16}O^{12}C\,^{17}O$ in the 442-2797 cm^{-1} spectral region, have been replaced with 48627 new ones covering the 436-2,826 cm^{-1} spectral range, issued of the results described in Tashkun et al. [15] [16] and Teffo et al. [17] [18] .

O_3: 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 $^{16}O_3$ were derived by Wagner et al. [19] and Flaud et al. [20]. A complete new study of the 1300-1500 cm^{-1} spectral range, related with the $2\nu_2$, $3\nu_2$-ν_2, $\nu_1+\nu_3+\nu_3-\nu_2$ and $2\nu_3-\nu_2$ bands of $^{16}O_3$, has been made by Barbe et al. [21]. The 1,820-2,260 cm^{-1} ($2\nu_3$, $\nu_1+\nu_3$ and $2\nu_1+\nu_3$ interactive bands of $^{16}O^{18}O^{16}O$) 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. [22] and by Mikhaïlenko et al. [23], respectively.

N_2O: 279 lines in the spectral region 870-1240 cm^{-1}, recently revisited by Daumont et al. [24], have been substituted in two bands, ν_3-ν_1 and ν_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 - 629 cm^{-1}.

CH_4 and CH_3D: The CH_4 and CH_3D contents of GEISA have been extensively updated. The spectral range has been extended from 6184.492cm^{-1} to 9199.285 cm^{-1}, and the number of entries increased from 66,883 to 216,196 (weaker transitions of $^{12}CH_4$ and new bands of $^{13}CH_4$ and CH_3D included). Full details about the revision in the spectral interval from 0.01 to 6,184.492 cm^{-1} can be found in a review paper by Brown et al. [25]. The new CH_4 near infrared data from 4,800-5,500 cm^{-1} and 6,180-10,000cm^{-1} are from an empirical list obtained by Brown [26], from a few selected FTS laboratory spectra.

O_2: The two spectral regions, 7,664.726-8,064.311 cm^{-1} and 11,483.727-15,927.806 cm^{-1}, have been updated thanks to new results by Goldman et al. [27] and by Brown and Plymate [28], respectively.

NO: A new line list has been produced [29] in the first overtone region of the main isotopic species $^{14}N^{16}O$, i.e. between 3,547.318 and 3,799.155 cm^{-1}. This calculation has been issued from experimental data from Mandin et al. [30] [31] and theoretical results from Gillis and Goldman [32].

NO_2: 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 $^{14}N^{16}O_2$ main isotopic species. New line parameters come from the works of Mandin et al. [33], Dana et al. [34], Devi et al. [35], May and Webster [36].

NH_3: The line parameters of the interval 0.058-5,294.502 cm^{-1} have been totally replaced by those issued by Kleiner and Brown [37] and described in Kleiner et al. [38].

PH_3: New data from Kleiner and Brown [37], described in Kleiner et al. [38], have replaced the whole content of the region from 770.877 to 2,478.765 cm^{-1}.

OH: Line parameters in the ultraviolet region from 29,808.500 to 35,877.030 cm^{-1}, from Gillis et al. [39] have been added to the GEISA archive.

HBR: New line parameters of $H^{79}Br$ and $H^{81}Br$, for the spectral regions of the pure rotation band $X^1\Sigma^+$ (0-0) (16.692-396.474 cm^{-1}) and of the fundamental band (1-0) (2,123.812-2,790.533 cm^{-1}), have been derived for spectroscopic databases update, as described in Goldman et al. [40].

HI: The description of the updates in the spectral regions of the $X^1\Sigma^+$ (0-0) (12.842-319.820 cm^{-1}) and of the (0-1) (1,950.689-2,403.162 cm^{-1}) bands is given in Goldman et al. [40].

C_2H_6: In the spectral region 2,975.331-2,977.926 cm^{-1}, a modified list by Rinsland et al. [41], for the $^pQ_3$ sub-branch in the ν_7 band, has replaced the previously archived line parameters.
C_2H_2: The updates of the database has concerned three spectral regions: the 13.6- and 5-μm regions, from work performed by Mandin et al. [42], Jacquemart et al. [43] [44], and the 7.5 -μm region, from results by Vander Auwera [45].
HOCl: A new line list has been created in the spectral interval 1,178.673-1,320.332 cm^{-1}, corresponding to the ν_2 region, on the basis of the works of Flaud et al. [46], Flaud [47] and Vander Auwera et al. [48].
CH_3Cl: In the spectral region from 1,261.562 to 1,645.899 cm^{-1} , a list of 8,989 transitions of the [ν2, ν5, 2ν3] -vibrational-band triad, prepared by Brown [26] and based upon the work of Chackerian et al. [49], has been newly archived, for $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$.
COF_2: An update of the 1,856.730-2,001.348 cm^{-1} region has been made thanks to a list generated by Brown [26], based on an unpublished analysis of the line positions.
HO_2: Spectroscopic parameters for the ground state have replaced by those generated upon the basis of the work of Chance [50][51].

A summary of the GEISA-03 line transition parameters sub-database content is given in Table 1. The molecular species formulas are given in column 1 with, in column 2 the list of their related isotopes. In columns 3 and 4 are given the minimum and maximum frequencies of the archived transitions, with the minimum and maximum values of the intensities in columns 5 and 6. The total number of entries, for each molecular species of column 1 is given in column 7.

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

As described in Jacquinet-Husson et al. [5], besides the line transition parameters data catalog itself, GEISA includes, a second catalog, providing, at various temperatures and pressures, the cross-sections (unit: cm^2 $molecule^{-1}$) of species exhibiting dense spectra, not suitable for a discrete parameterized format. The GEISA-03 archived has been significantly enriched since the GEISA-97 issue. The spectral range has been extended: from 200 cm^{-1} to 2,000 cm^{-1} (from 556 cm^{-1} to 1,763 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, N_2O_5, SF_6, $ClONO_2$. 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, 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.

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.

2.3 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 Refs. [6] 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.

3. The GEISA/IASI database: 2003 Edition

The GEISA/IASI database derives from GEISA as described in Refs. [4] [6]. 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 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: H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NO, SO_2, NO_2, HNO_3, OCS, C_2H_2, N_2.

It has to be noticed that in GEISA/IASI, CH_3D is considered as an isotope of CH_4. It is considered as an independent molecule in GEISA. Related with the H2O archive in the 10 μm region, alternative line parameters, from Stewart [52], have been issued has 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, CCl_4, N_2O_5 and HCFC-22.

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

4. GEISA and GEISA/IASI management software and availability

Management softwares and user's friendly facilities are associated with the *GEISA/IASI* system.

- The individual line parameters sub-database management software package has been updated and enriched of new functions, since the former editions of GEISA and GEISA/IASI. The user has the choice of:
  - To make data extractions by molecule, isotope and quantum identification, between two given wavenumbers.
  - To analyse selected sampled spectral intervals, in terms of line intensities and/or energy of the lower transitions, thanks to the plots of related histograms.
  - To obtain a complete description of the line parameters content for each molecular species, i.e.: for each existing transition is provided, the number of lines, the wavenumber interval and the intensity minimum and maximum values.

Finally, it is possible to mix, in an intelligent way, two different files for an accurate update, avoiding duplicated information, especially in the database update process.

- *The cross-sections sub-database* management software allows:
  - To make extraction of data, by temperature, pressure and T, P set.
  - To list the available *T, P* sets for each molecule.
  - To obtain a detailed description of the information available for each molecular species, i.e.: for each available *T, P* set, the number of records, the wavenumber interval and the intensity minimum and maximum values are given.

These management software facilities are interfaced on the ARA/LMD group web site at: http://ara.lmd.polytechnique.fr. They are also accessible at the GEISA restricted free access ftp site http://ara.lmd.polytechnique.fr/ftpgeisa. Previously, the potential user has to get a login and a password, at the ARA/LMD web site.

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Table 1: GEISA-03 individual lines sub-database summarized updates and contents
Spectral Range: 10^{-6} – 32,677 cm^{-1}

Molecule	**Isotopes**	**Minimum Frequency cm^{-1}**	**Maximum Frequency cm^{-1}**	**Minimum Intensity cm $molec^{-1}$**	**Maximum Intensity cm $molec^{-1}$**	**# lines**
H_2O	$H^{16}OH$, $H^{18}OH$, $H^{17}OH$, $H^{16}OD$, $H^{18}OD$, $H^{17}OD$	0.007	25232.004	1.01×10^{-32}	2.67×10^{-18}	58,726
CO_2	$^{16}O^{12}C^{16}O$, $^{16}O^{13}C^{16}O$, $^{16}O^{12}C^{18}O$, $^{16}O^{12}C^{17}O$, $^{16}O^{13}C^{18}O$, $^{16}O^{13}C^{17}O$, $^{18}O^{12}C^{18}O$, $^{17}O^{12}C^{18}O$, $^{18}O^{13}C^{18}O$	436.123	9648.007	4.87×10^{-42}	3.53×10^{-18}	76,826
O_3	$^{16}O^{16}O^{16}O$, $^{16}O^{16}O^{18}O$, $^{16}O^{18}O^{16}O$, $^{16}O^{16}O^{17}O$, $^{16}O^{17}O^{16}O$	0.026	4060.783	1.43×10^{-31}	4.06×10^{-20}	319,248
N_2O	$^{14}N^{14}N^{16}O$, $^{14}N^{15}N^{16}O$, $^{15}N^{14}N^{16}O$, $^{14}N^{14}N^{18}O$, $^{14}N^{14}N^{17}O$	0.838	5131.249	1.28×10^{-28}	1.00×10^{-18}	26,681
CO	$^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{17}O$, $^{12}C^{18}O$, $^{13}C^{17}O$, $^{13}C^{18}O$	3.414	8464.882	7.88×10^{-78}	4.46×10^{-19}	13,515
CH_4	$^{12}CH_4$, $^{13}CH_4$	0.010	9199.285	4.06×10^{-34}	2.10×10^{-19}	216,196
O_2	$^{16}O^{16}O$, $^{16}O^{17}O$, $^{16}O^{18}O$	1×10^{-6}	15927.806	8.53×10^{-51}	8.83×10^{-24}	6,290
NO	$^{14}N^{16}O$, $^{14}N^{18}O$, $^{15}N^{16}O$	3×10^{-5}	9273.214	1.51×10^{-85}	2.32×10^{-20}	99,123
SO_2	$^{32}S^{16}O_2$, $^{34}S^{16}O_2$	0.017	4092.948	1.02×10^{-28}	6.09×10^{-20}	38,853
NO_2	$^{14}N^{16}O_2$	0.498	3074.366	4.24×10^{-28}	1.30×10^{-19}	104,224
NH_3	$^{14}NH_3$, $^{15}NH_3$	0.058	5294.502	8.09×10^{-39}	5.67×10^{-19}	29,082
PH_3	$^{31}PH_3$	17.805	2478.765	1.85×10^{-28}	2.52×10^{-19}	11,740
HNO_3	$H^{14}N^{16}O$	0.035	1769.982	3.49×10^{-27}	3.02×10^{-20}	171,504
OH	^{16}OH , ^{16}OD , ^{18}OH	0.005	35877.031	1.50×10^{-85}	6.45×10^{-17}	42,866
HF	$H^{19}F$	41.111	11535.570	1.11×10^{-26}	1.44×10^{-17}	107
HCl	$H^{35}Cl$, $H^{37}Cl$	20.240	13457.841	1.01×10^{-26}	5.03×10^{-19}	533
HBr	$H^{81}Br$, $H^{79}Br$	16.232	9758.565	9.45×10^{-33}	1.21×10^{-19}	1,294
HI	$H^{127}I$	12.509	8487.305	1.64×10^{-30}	3.42×10^{-20}	806

Table 1: following

Molecule	**Isotopes**	**Minimum Frequency cm^{-1}**	**Maximum Frequency cm^{-1}**	**Minimum Intensity cm $molec^{-1}$**	**Maximum Intensity cm $molec^{-1}$**	**# lines**
ClO	$^{35}Cl^{16}O$, $^{37}Cl^{16}O$	0.015	1207.639	5.09×10^{-30}	3.24×10^{-21}	7,230
OCS	$^{16}O^{12}C^{32}S$, $^{16}O^{12}C^{34}S$, $^{16}O^{13}C^{32}S$, $^{16}O^{12}C^{33}S$, $^{16}O^{13}C^{34}S$	0.381	4118.004	2.62×10^{-28}	1.22×10^{-18}	24,922
H_2CO	$H_2{}^{12}C^{16}O$, $H_2{}^{12}C^{18}O$, $H_2{}^{13}C^{16}O$	3×10^{-6}	2998.527	1.02×10^{-38}	7.50×10^{-20}	2,701
C_2H_6	$^{12}C_2H_6$, $^{12}C^{13}CH_6$	725.603	2977.926	1.32×10^{-28}	6.64×10^{-21}	14,981
CH_3D	$^{12}CH3D$	7.760	3306.810	5.57×10^{-30}	5.71×10^{-23}	35,518
C_2H_2	$^{12}C_2H_2$, $^{12}C^{13}CH_2$	604.774	3374.223	9.49×10^{-27}	1.19×10^{-18}	3,115
C_2H_4	$^{12}C_2H_4$, $^{12}C^{13}CH_4$	701.203	3242.172	6.94×10^{-26}	8.41×10^{-20}	12,978
HCN	$H^{12}C^{14}N$, $H^{13}C^{15}N$, $H^{13}C^{14}N$	2.870	18407.973	1.78×10^{-28}	7.10×10^{-19}	2,550
C_3H_8	$^{12}C_3H_8$	700.015	799.930	3.77×10^{-24}	4.31×10^{-22}	8,983
C_2N_2	$^{12}C_2{}^{14}N_2$	203.955	2181.690	6.59×10^{-24}	2.58×10^{-20}	2,577
C_4H_2	$^{12}C^{14}H_2$	190.588	654.425	2.65×10^{-24}	6.93×10^{-20}	1,405
HC_3N	$H^{12}C_3{}^{14}N$	474.293	690.860	6.36×10^{-24}	4.42×10^{-20}	2,027
HOCl	$H^{16}O^{35}Cl$, $H^{16}O^{37}Cl$	0.024	3799.682	$7{,}22\times10^{-28}$	$3{,}59\times10^{-20}$	17,862
N_2	$^{14}N^{14}N$	1992.628	2625.497	2.19×10^{-34}	3.42×10^{-28}	120
CH_3Cl	$^{12}CH_3{}^{35}Cl$, $^{12}CH_3{}^{37}Cl$	674.143	3172.927	$9{,}05\times10^{-32}$	$1{,}13\times10^{-20}$	18,344
H_2O_2	$H_2{}^{16}O^{16}O$	0.043	1499.487	5.09×10^{-29}	5.61×10^{-20}	100,781
H_2S	$H_2{}^{32}S$, $H_2{}^{33}S$, $H_2{}^{34}S$	2.985	4256.547	1.45×10^{-26}	1.36×10^{-19}	20,788
HCOOH	$H^{12}C^{16}O^{16}OH$	1060.962	1161.251	2.14×10^{-22}	2.84×10^{-20}	3,388
COF_2	$^{12}C^{16}O^{19}F_2$	725.006	2001.348	4.74×10^{-24}	3.94×10^{-20}	83,750
SF_6	$^{32}S^{19}F_6$	940.425	952.238	2.16×10^{-22}	1.50×10^{-20}	11,520
C_3H_4	$^{12}C_3H_6$	290.274	359.995	2.02×10^{-23}	3.18×10^{-21}	3,390
$ClONO_2$	$^{15}Cl^{16}O^{14}N^{16}O_2$, $^{17}Cl^{16}O^{14}N^{16}O_2$	763.641	797.741	6.34×10^{-25}	3.85×10^{-22}	32,199

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

Molecule	Spectral coverage (cm^{-1})	Temperature range (K)	Pressure range (Pa)	Number of T,P sets	References
CFC-11	210 - 2000	296	93325	1	Hurley [53]; Christidis [54]
	500 - 1600	297	0	1	MSF/RAL [55]
	810 - 1120	190 - 296	1000 - 101325	55	Li & Varanasi [56]; Varanasi [57]
CFC-12	850 - 1190	253 - 287	0	3	Clerbaux [58]
	210 - 2000	296	93325	1	Hurley [53];
	800 - 1200	190 - 296	1000 - 101392	57	Varanasi & Nemtchinov[59]; Varanasi [57]
CFC-13	765 - 1235	203 - 293	0	3	GEISA97 [5]
CFC-14	220 - 2000	296	93325	1	Hurley [53]
	1250 - 1290	180 - 296	1005 - 101458	55	Nemtchinov & Varanasi [60]
CFC-113	780 - 1232	203 -293	0	6	GEISA97 [5]
CFC-114	815 - 1285	203 -293	0	6	GEISA97 [5]
CFC-115	955 - 1260	203 -293	0	6	GEISA97 [5]
HFC-32	204 - 2000	296	93325	1	Hurley [53]; Pinnock [61]
	995 - 1475	203 - 297	0 - 100000	17	MSF/RAL [55]
HFC-125	700 - 1465	287	0	1	Clerbaux [58]
	495 - 1504	203 -293	0 - 80000	16	Di Lonardo [62]
	208 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HFC-134	210 - 2000	296	93325	1	Hurley [53]; Christidis [54]
	600 - 1700	203 - 297	0 - 100000	9	MSF/RAL [55]
HFC-134a	815 - 1485	253 - 287	0	3	Clerbaux [58]
	203 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
	600 - 1600	203 - 296	0 - 100000	15	MSF/RAL [55]
	1035 - 1340	190 - 296	2666 - 101376	33	Nemtchinov & Varanasi [63]
HFC-143	204 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HFC-143a	694 - 1504	203 - 293	0 - 800000	19	Di Lonardo [62]
	200 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
	580 - 1500	203 - 297	0 - 100000	9	MSF/RAL [55]
HFC-152a	700 - 1600	203 - 293	0 - 80000	16	Vander Auwera [64]
	840 - 1490	253 - 287	0	3	Clerbaux [58]
	200 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HCFC-21	785 - 840	296	133	1	Massie et al. [65]

Table 2: following

Molecule	Spectral coverage (cm^{-1})	Temperature range (K)	Pressure range (Pa)	Number of T,P sets	References
HCFC-22	700 - 1500	203 - 293	0 - 80000	8	Vander Auwera [66]
	765 - 1380	253 - 287	0	3	Clerbaux [58]
	208 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
	760 - 1195	181 - 297	2666 - 101936	51	Varanasi [67]
HCFC-123	740 - 1450	253 - 287	0	3	Clerbaux [58]
	204 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HCFC-124	675 - 1425	287	0	1	Clerbaux [58]
	208 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HCFC-141b	209 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
	710 - 1470	253 - 287	0	3	Clerbaux [58]
HCFC-142b	650 - 1475	253-287	0	3	Clerbaux [58]
	200 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HCFC-225ca	695 - 1420	253 - 287	0	3	Clerbaux [58]
	600 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
HCFC-225cb	715 - 1375	253 - 287	0	3	Clerbaux [58]
	600 - 2000	296	93325	1	Pinnock [61]; Hurley [53]
N2O5	540 - 1380	205 - 293	0	5	Wagner & Birk [68]
SF6	650 - 2000	296	93325	1	Hurley [53]
	925 - 955	180 - 295	2693 - 101350	29	Varanasi [67]
ClONO2	500 - 1330	190 - 297	0 - 15580	25	Wagner & Birk [68]
	1265 - 1325	201 - 222	0	3	GEISA97 [5]
CCl4	750 - 812	208 - 297	1070 - 101272	32	Nemtchinov & Varanasi [69]
C2F6	1061 - 1285	180 - 296	3320 - 101363	43	Zou & al. [70]
	210 - 2000	296	93325	1	Highwood [71]; Hurley [53]
	600 - 2750	203 - 293	0 - 80000	15	MSF/RAL [55]
C2H2	450 - 2000	296	93325	1	Highwood [71]; Hurley [53]
C2H4	220 - 2000	296	93325	1	Highwood [71]; Hurley [53]
C2H6	220 - 2000	296	93325	1	Highwood [71]; Hurley [53]
C3H8	220 - 2000	296	93325	1	Highwood [71]; Hurley [53]
C4F8	500 - 1600	203 - 297	0 - 65000	19	MSF/RAL [55]
HNO4	770 - 830	268	93	1	Massie et al. [65]
SF5CF3	600 - 2000	296	93325	1	Hurley [53]
HCH-365mfc	665 - 1480	287	0	1	Clerbaux [58]

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