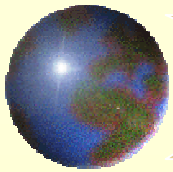


**THE 2003 EDITION OF GEISA:
A SPECTROSCOPIC DATABASE SYSTEM FOR
THE SECOND GENERATION VERTICAL SOUNDERS
RADIANCE SIMULATION**

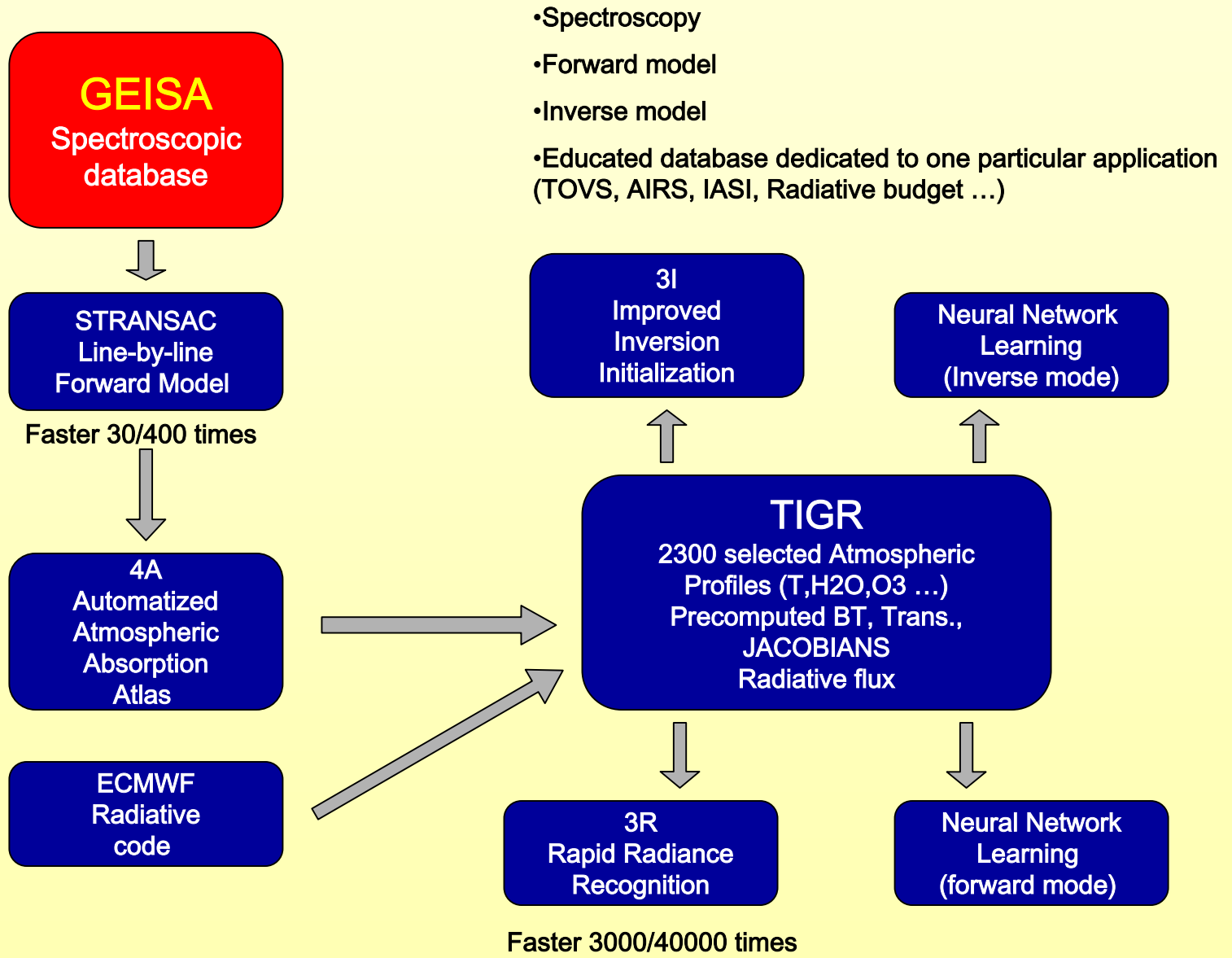
**N. Jacquinet-Husson, N.A. Scott,
A. Chédin, K. Garceran, R. Armante**

<http://ara.lmd.polytechnique.fr>

Laboratoire de **M**étéorologie **D**ynamique
Atmospheric **R**adiation **A**nalysis Group
Ecole Polytechnique
91128, Palaiseau, France



The GEISA spectroscopic database in the ARA/LMD tools





The 1997 spectroscopic GEISA databank

N. Jacquinet-Husson^{a,*}, E. Arié^b, J. Ballard^c, A. Barbe^d, G. Bjoraker^e, B. Bonnet^a,
L. R. Brown^f, C. Camy-Peyret^g, J.P. Champion^h, A. Chédin^a, A. Chursinⁱ,
C. Clerbaux^{j-1}, G. Duxbury^k, J.-M. Flaud^l, N. Fourrié^a, A. Fayt^m, G. Graner^b,
R. Gamacheⁿ, A. Goldman^o, Vl. Golovko^l, G. Guelachvili^b, J.M. Hartmann^b,
J.C. Hilico^h, J. Hillman^f, G. Lefèvre^a, E. Lellouch^p, S.N. Mikhailenkoⁱ,
O.V. Naumenkoⁱ, V. Nemtchinov^q, D.A. Newnham^c, A. Nikitinⁱ, J. Orphal^r,
A. Perrin^l, D.C. Reuter^f, C.P. Rinsland^s, L. Rosenmann^t, L.S. Rothman^u,
N.A. Scott^a, J. Selby^v, L.N. Sinitzaⁱ, J.M. Sirota^f, A.M. Smith^w, K.M. Smith^c,
Vl. G. Tyuterev^d, R.H. Tipping^x, S. Urban^y, P. Varanasi^q, M. Weber^f

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^bLaboratoire de Physique Moléculaire et Applications, CNRS, Bât.350, Université Paris-Sud, Campus d'Orsay, France

^cRutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK

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^eLaboratory for Extraterrestrial Physics, NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA

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

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ⁱInstitute of Atmospheric Optics, Tomsk, Russia

^jLaboratoire de Chimie Physique Moléculaire, Université Libre de Bruxelles, Bruxelles, Belgium

^kDepartment of Physics and Applied Physics, University of Strathclyde, Glasgow, G4 0NG, UK

^lLaboratoire de Photophysique Moléculaire, CNRS, Bât.210, Université Paris Sud, Campus d'Orsay, France

^mLaboratoire de Spectroscopie Moléculaire, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

ⁿDepartment of Environmental, Earth and Atmospheric Sciences, University of Massachusetts Lowell, Lowell, MA 01854, USA

^oDepartment of Physics, University of Denver, Denver, CO 80208, USA

^pDESPA, Observatoire de Paris (Section de Meudon), Meudon, France

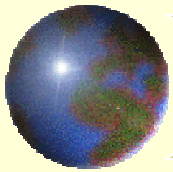
^qInstitute for Terrestrial and Planetary Atmospheres, Marine Sciences Research Center, State University of New York at Stony Brook, Stony Brook, NY 11794-5000, USA

^rInstitute of Environmental Physics/Institute of Remote Sensing, University of Bremen, D-28334 Bremen, Germany

^sNASA Langley Research Center, Atmospheric Sciences Division, Hampton, VA 23665, USA

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¹ Now at Service d'Aéronomie du CNRS, Université Pierre et Marie Curie, Paris, France.



Molecular species in the GEISA individual spectral lines sub-database

- Major Permanent constituents of EARTH's atmosphere :

$O_2, H_2O, CO_2 \dots$

- Minor permanent constituents of the EARTH's atmosphere :

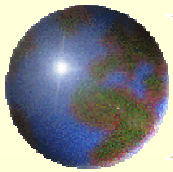
$O_3, CH_4, N_2O, CO \dots$

- Trace molecules in the EARTH's atmosphere :

$NO, SO_2, NO_2, NH_3, HNO_3, OH, HF, HCl, HBr, HI, ClO, OCS, H_2CO, PH_3 \dots$

- Molecules present in the atmospheres of JUPITER, SATURN, URANUS, TITAN etc. :

$C_2H_6, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_8, C_3H_4 \dots$



The GEISA-2003 system

Gestion et **E**tude des **I**nformations **S**pectroscopiques **A**tmosphériques
Management and Study of Atmospheric Spectroscopic Information

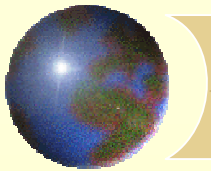
Three SUB-DATABASES

- Individual spectral lines spectroscopic parameters database
42 molecules (96 isotopic species) between 0 and 25,232 cm^{-1}
1,361,667 entries between 0 and 25,232 cm^{-1} .
- Absorption cross-sections database (mainly CFC's)
32 molecular species
- Refractive Indices of Basic Atmospheric aerosol components database
About 20 components

ASSOCIATED MANAGEMENT SOFTWARES

(For each database)

GEISA-03 OVERVIEW

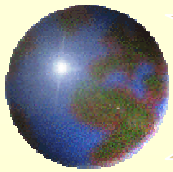


Fields of the format for line transitions in GEISA

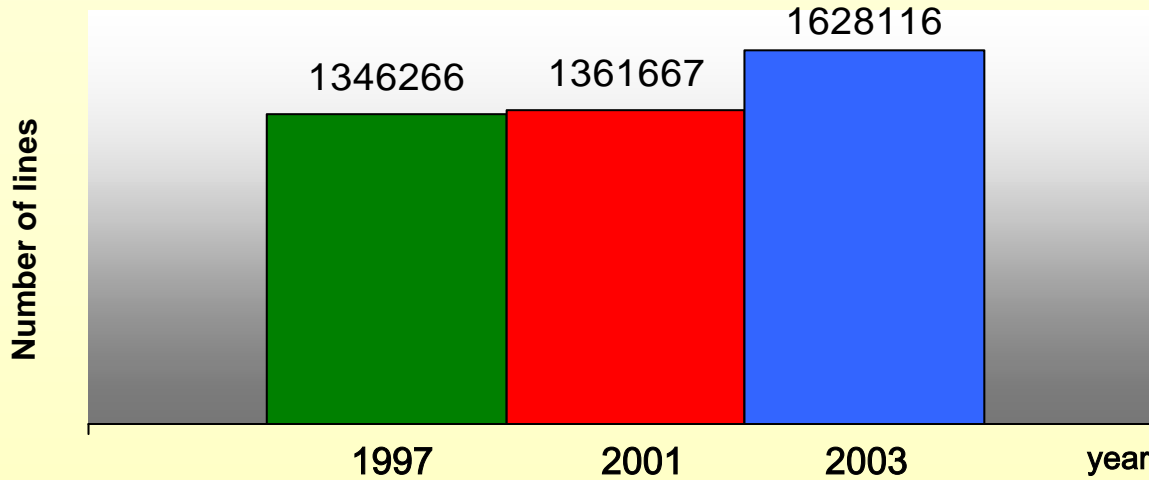
A-J fields used in the GEISA management software

Fortran format descriptor	F12.6	D11.4	F6.4	F10.4	A36	F4.2	I3	I3	A1	I2	I1	E10.3	F5.4	F8.6	I3	I6
Field name	A	B	C	D	E	F	G	I	J	K	L	M	N	O	P	Q

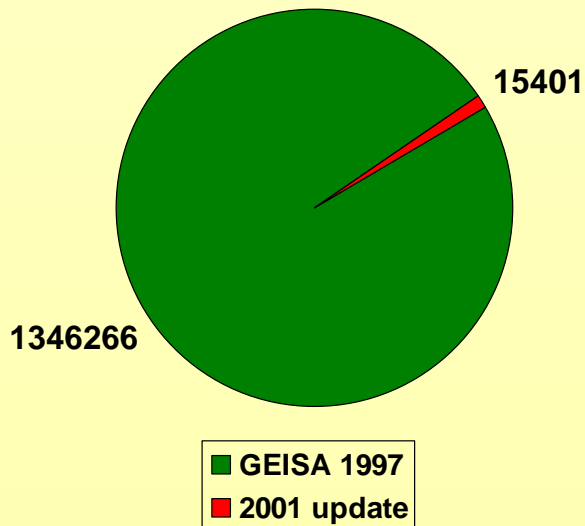
- (A) Wavenumber (cm^{-1}) of the line associated with the vibro-rotational transition.
- (B) Intensity of the line (cm molecule^{-1} at 296K).
- (C) Lorentzian collision halfwidth ($\text{cm}^{-1} \text{atm}^{-1}$ at 296K).
- (D) Energy of the lower transition level (cm^{-1}).
- (E) Transition quantum identifications for the lower and upper levels of the transition, as he following:
TRS1 upper state vibrational identification,
TRS2 lower state vibrational identification,
RN1 upper state rotational identification,
RN2 lower state rotational identification.
Blank fields (spaces) at this place match missing information.
- (F) Temperature dependence coefficient n of the halfwidth (value set to 0.75 if n not available)
- (G) Identification code for isotope.
- (I) Identification code for molecule.
- (J) Internal GEISA code for data identification.



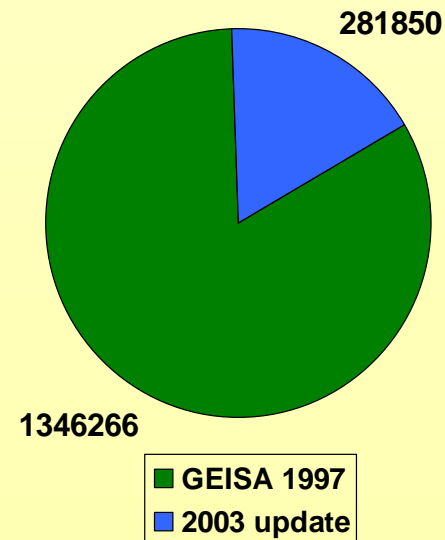
GEISA individual lines sub-database updates since 1997

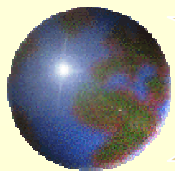


GEISA 2001



GEISA 2003





GEISA-03 individual lines sub-database

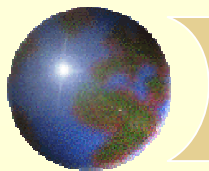
General contents

Molecule	Code	Isotopes	# Transitions
<u>H2O</u>	1	161-162-171-181-182	58726
<u>CO2</u>	2	626-627-628-636-637-638-728-828-838	76826
<u>O3</u>	3	666-668-686-667-676	319248
<u>N2O</u>	4	446-447-448-456-546	26681
CO	5	26- 36- 28- 27- 38- 37	13515
<u>CH4</u>	6	211-311	175941
<u>O2</u>	7	66- 67- 68	6290
<u>NO</u>	8	46- 48- 56	99123
SO2	9	626-646	38853
<u>NO2</u>	10	646	104224
<u>NH3</u>	11	411-511	29082
<u>PH3</u>	12	131	11740
HNO3	13	146	171504
<u>OH</u>	14	61- 62- 81	42866
HF	15	19	107
HCl	16	15-17	533
<u>HBr</u>	17	11-19	1294
<u>HI</u>	18	17	806
ClO	19	56-76	7230
OCS	20	622-624-632-623-822-634-722	24922
H2CO	21	126-128-136	2701

2003 update

line ↑

line =



GEISA-03 individual lines sub-database

General contents (following)

<u>C2H6</u>	22	226-236	14981
<u>CH3D</u>	23	212	35518
<u>C2H2</u>	24	221-231	3115
C2H4	25	211-311	12978
GeH4	26	411	824
HCN	27	124-125-134	2550
C3H8	28	221	8983
C2N2	29	224	2577
C4H2	30	211	1405
hc3n	31	124	2027
<u>HOCl</u>	32	165-167	17862
N2	33	44	120
<u>CH3Cl</u>	34	215-217	18344
H2O2	35	166	100781
H2S	36	121-141-131	20788
hcooh	37	261	3388
<u>COF2</u>	38	269	83750
SF6	39	29	11520
C3H4	40	341	3390
<u>HO2</u>	41	166	38804
CLONO2	42	564-764	32199

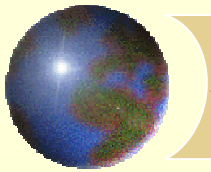
Spectral range: 0.0 – 25232.004100 cm-1

Total : 1,628,116

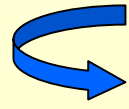
2003 update

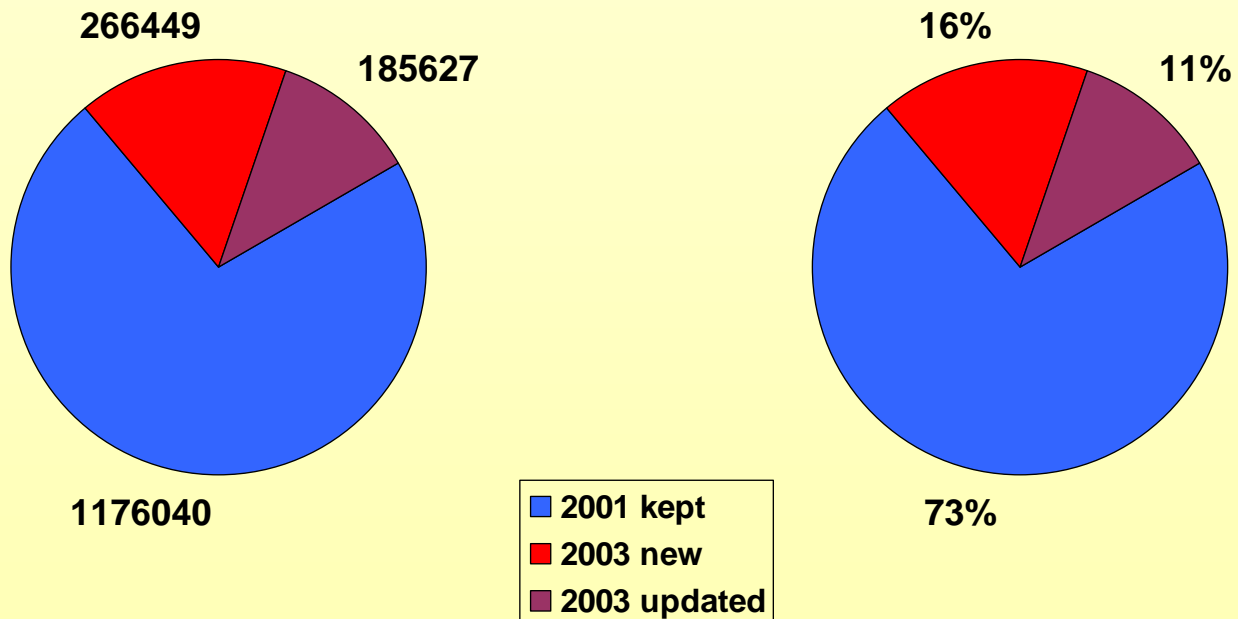
line ↑

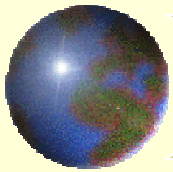
line =



GEISA-03 individual lines sub-database

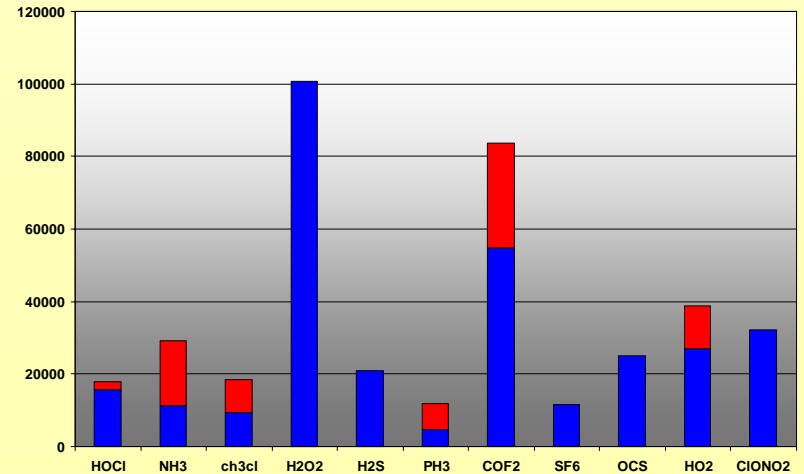
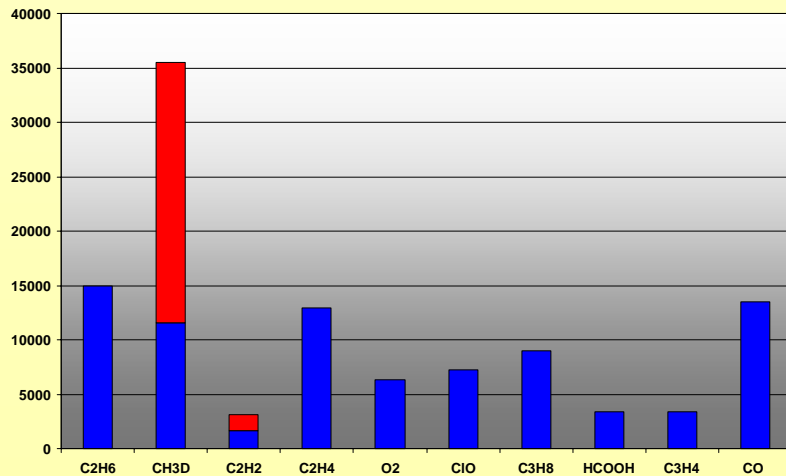
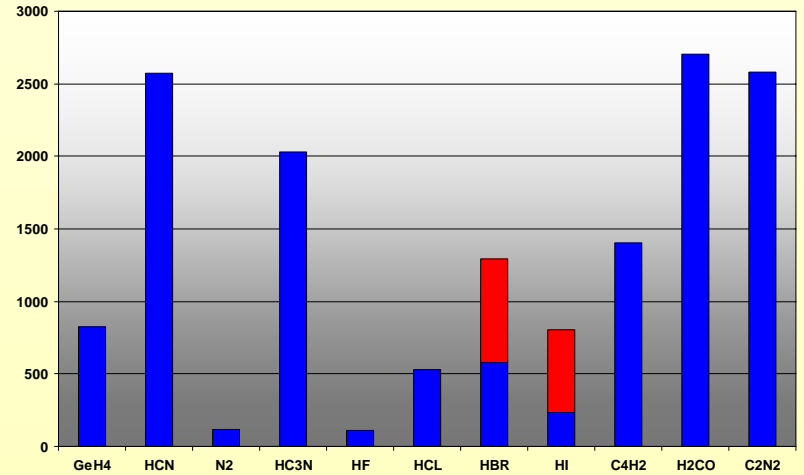
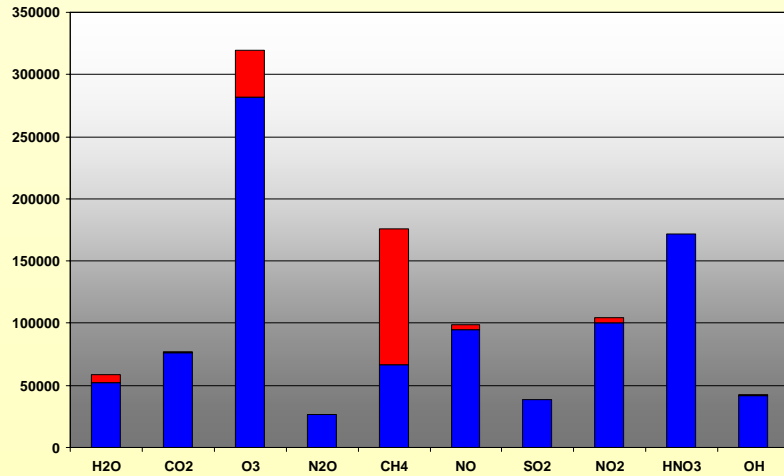
 1,628,116 lines

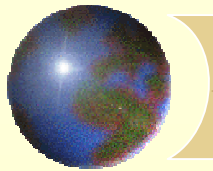




GEISA individual lines sub-database updates since 1997

GEISA 1997 – 2003 NEW





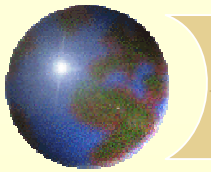
GEISA-03 cross-sections sub-database

23 MOLECULAR SPECIES ALREADY ARCHIVED IN GEISA

CFC-11, CFC-12, CFC-13, CFC-14, HCFC-22, HFC-32,
CFC-113, CFC-114, CFC-115, HCFC-123, HCFC-124, HFC-125,
HFC-134, HFC-134a, HCFC-141b, HCFC-142b,
HFC-143a, HFC-152a, HCFC-225ca, HCFC-225cb,
N₂O₅, SF₆, CLONO₂

9 MOLECULAR SPECIES NEWLY ARCHIVED IN GEISA-03

C₂F₆ Perfluoroethane
C₃H₈ Propane
C₂H₆ ethane
C₂H₂ acetylene
C₂H₄ ethene
SF₅CF₃ trifluoromethyl sulfur pentafluoride
CHF₂CH₂F (HFC-143)
1,2 Dichloroethane



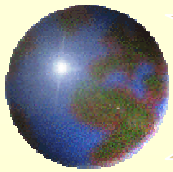
GEISA-03 aerosols sub-database

Data on microphysical and optical properties of basic aerosol components.

4 sub-databases included:

- **A database on refractive indices of basic atmospheric aerosol components:**
 - Acids
 - Water ice
 - Water droplets
 - Water soluble components
 - Thin films
 - Solid Substances
- **A Database on atmospheric aerosols from LITMS (Rublev, 1994)**
- **The software package and database OPAC (Optical Properties of Aerosols and Clouds) (Hess et al., 1998)**
- **The Global Aerosol Data Set: GADS (Koepke et al., 1997)**

GEISA/IASI-03 OVERVIEW



GEISA/IASI-03 database general context

- The GEISA/IASI-03 database is both an extraction (spectral range 599 3001 cm^{-1}) and a partial update of the GEISA-03 Spectroscopic database
- It is maintained and developed with the purpose of assessing the IASI measurements capabilities, within the ISSWG, in the frame of the CNES/EUMETSAT Polar System EPS preparation, by simulating high resolution radiances and/or using experimental data.

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

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**Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk, Russia

Received January 8, 2003

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 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^{1,3} 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.⁴

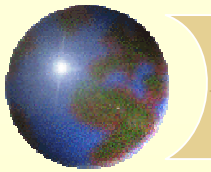
GEISA spectroscopic database overview

The 1997 GEISA database,⁵ 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 cm^{-1} .

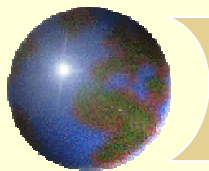
The included molecules are of interest for the Earth and other planet atmospheres (C_2H_4 , GeH_4 , C_3H_8 , C_2N_2 , C_4H_2 , HC_3N , H_2S , HCOOH , and C_2H_4). Among spectroscopic parameters archived in GEISA, the most important for the atmospheric radiative transfer modelling are: the line wavenumber (cm^{-1}) associated with a vibro-rotational transition, the line intensity ($\text{cm}^{-1}\text{molecule}^{-1}$ at 296 K), the Lorentzian collision halfwidth ($\text{cm}^{-1}\text{atm}^{-1}$ at 296 K), the energy of the transition lower level (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.



GEISA/IASI-03 database overall contents

Spectral range: 599-3001 cm⁻¹

- A Sub-database on individual lines of 14 molecules (53 isotopic species) :
H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, HNO₃, OCS, C₂H₂, N₂
- A Sub-database on absorption Cross- Sections of 6 molecules :
CFC-11, CFC-12, CFC-14, CCl₄, N₂O₅, HCFC-22
- A Sub-database on micro-physical and optical properties of atmospheric aerosols



GEISA/IASI-03 individual lines sub-database

General contents

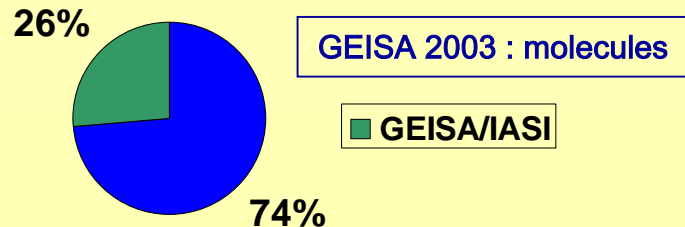
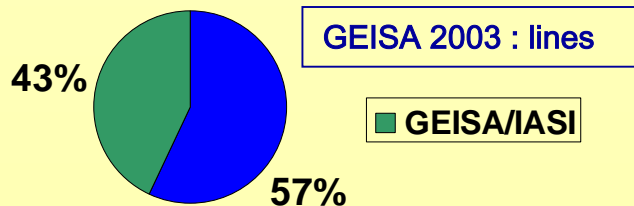
2003 update

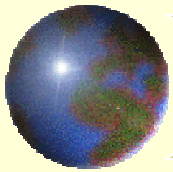
line ↑

line =

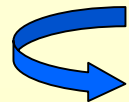
Molecule	Code	Isotopes	# Transitions
<u>h2o</u>	1	161-162-171-181-182	13278
<u>co2</u>	2	626-627-628-636-637-638-728-828-838	50840
<u>o3</u>	3	666-668-686-667-676	195102
<u>n2o</u>	4	446-447-448-456-546	18966
co	5	26- 36- 28- 27- 38- 37	3674
<u>ch4</u>	6	211-311 +CH3D	121281
o2	7	66- 67- 68	435
<u>no</u>	8	46- 48- 56	29608
so2	9	626-646	22301
<u>no2</u>	10	646	71687
hno3	13	146	152586
ocs	20	622-624-632-623-822-634-722	19768
<u>c2h2</u>	24	221-231	2904
n2	33	44	120

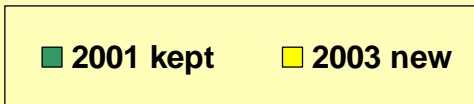
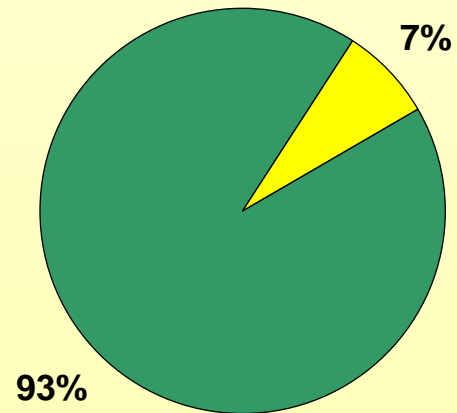
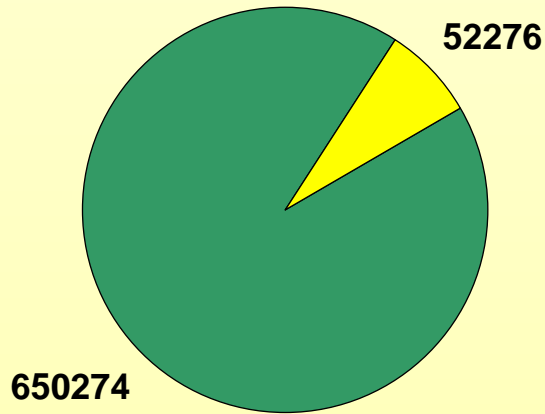
Spectral range: **599 – 3001 cm⁻¹** Total : **702,550**

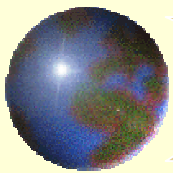




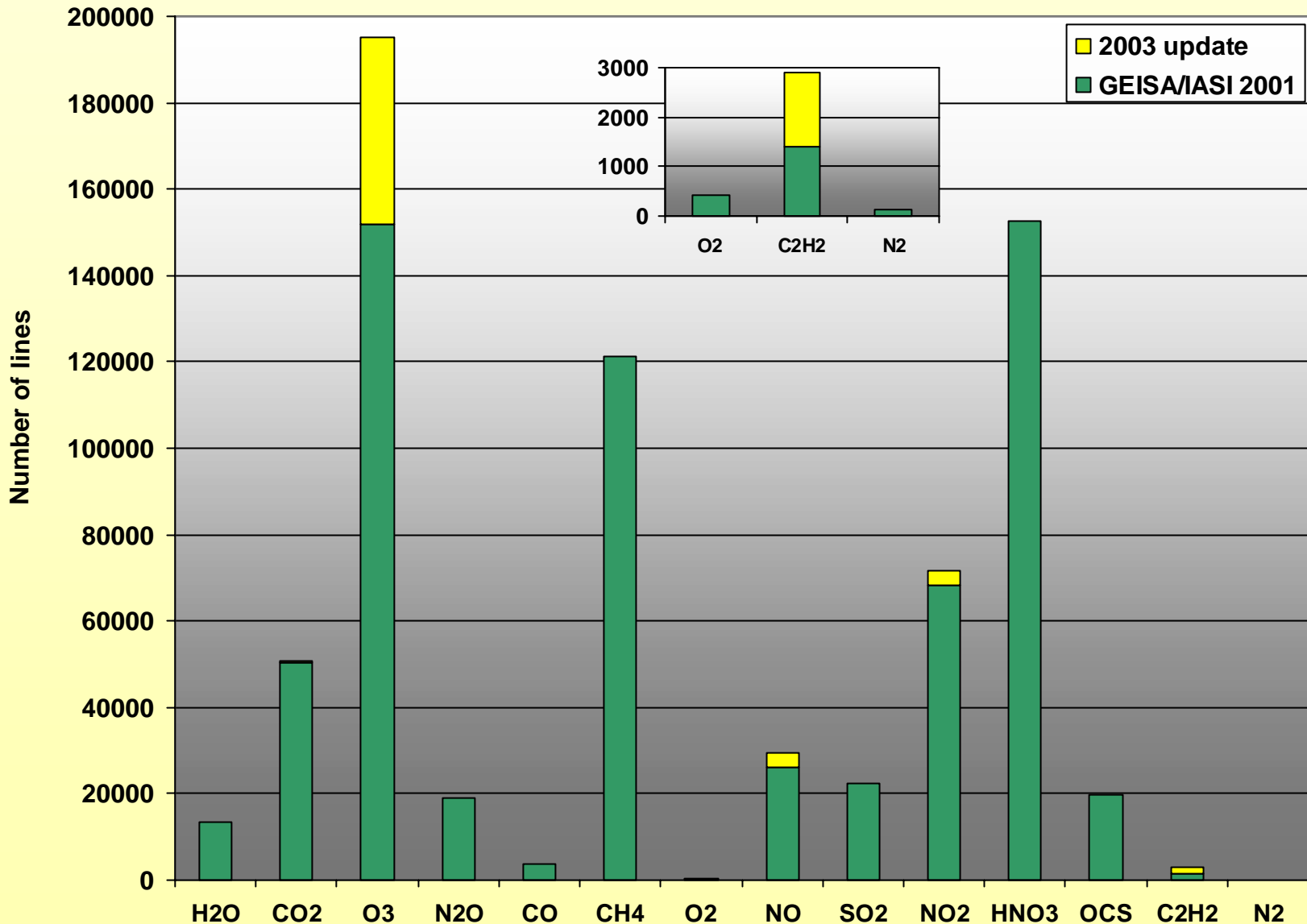
GEISA/IASI 2003 individual lines sub-database updates

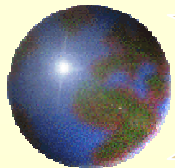
 702,550 lines





GEISA/IASI 2003 individual lines sub-database updates



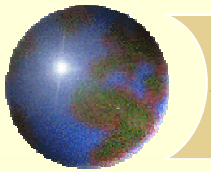


GEISA/IASI-03 cross-sections sub-database

GEISA/IASI-01 – 2003 NEW

Molecule ID. Formula	Spectral coverage (cm ⁻¹)	Temperature Range (K)	Pressure Range (Torr)	Number of T,P sets
CFC11 CCl ₃ F	810 - 880	190 - 296	8 - 760	55
	1050 - 1120	190 - 296	8 - 760	55
	500 - 1601	297	0	1
	599 - 2000	296	700	1
CFC12 CCl ₂ F ₂	850 - 950	190 - 296	8 - 760	52
	1050 - 1120	190 - 296	8 - 760	52
	850 - 1190	253 - 287	0	3
	599 - 2000	296	700	1
CFC-14 CF ₄	1250 - 1290	180 - 296	8 - 760	55
	599 - 2000	296	700	1
HCFC-22 CHClF ₂	750 - 870	216 - 294	0 - 760	9
	765 - 1380	181 - 297	20 - 765	51
	765 - 1380	253 - 287	0	3
	599 - 2000	296	700	1
	700 - 1500	203 - 293	0 - 600	8
CCl ₄	750 - 812	208 - 296	8 - 760	32
N ₂ O ₅	540 - 1380	205 - 293	0	5

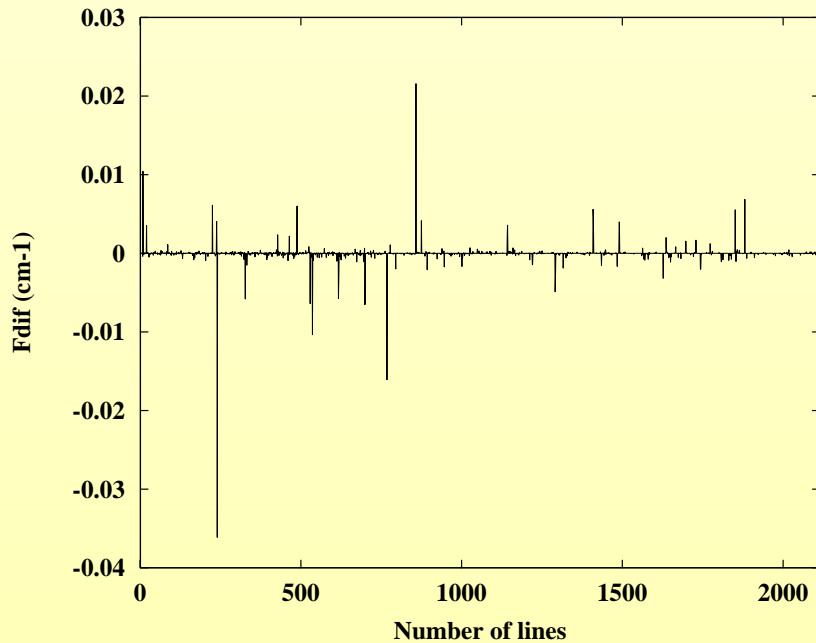
2003 UPDATE ILLUSTRATIONS



H₂O update in GEISA/IASI-03: TOTH VS RAL

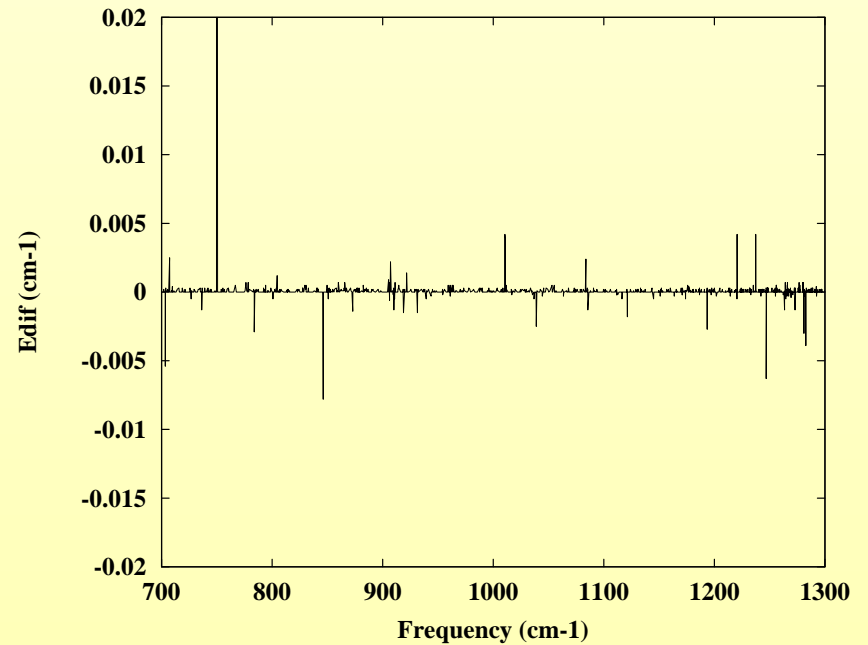
Frequency (cm⁻¹)

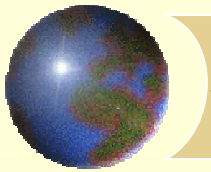
H₂O RAL / geisa+toth Frequency differences :
Fdif = [F(RAL) - F(GS+TOT)] in cm-1



Ground Level Energy (cm⁻¹)

H₂O RAL / geisa+toth Ground Level Energy differences :
Edif = [E(RAL) - E(GS+TOT)] in cm-1

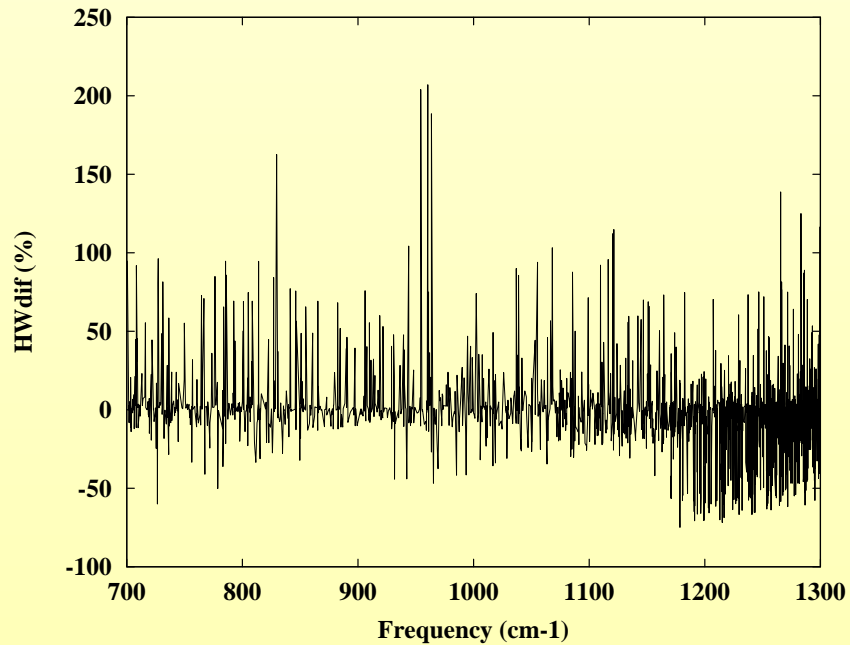




H₂O update in GEISA/IASI-03: TOTTH VS RAL

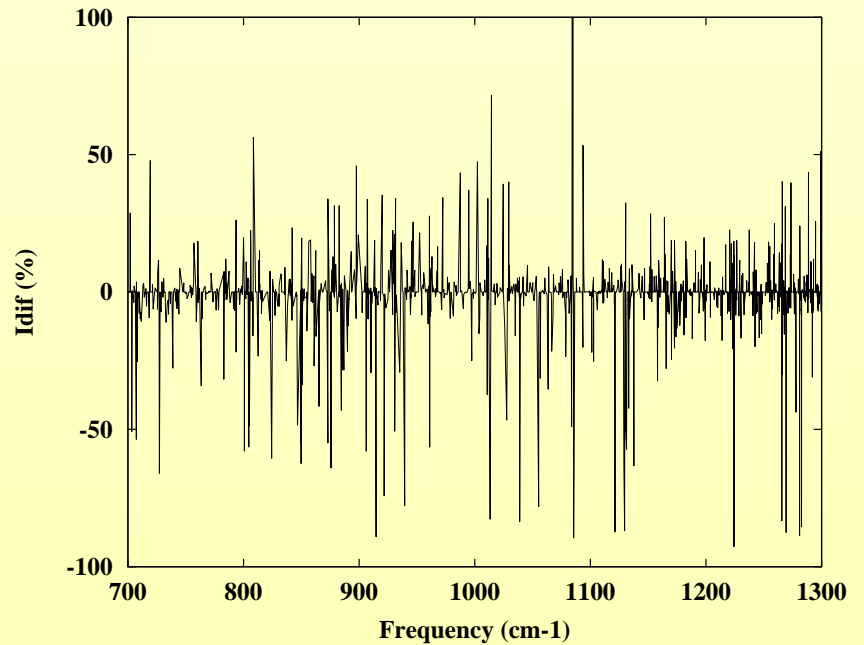
Halfwidths (%)

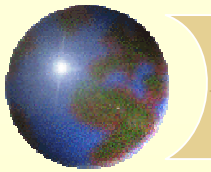
H₂O RAL / geisa+toth air broadened halfwidth differences :
HWdif = [HW(RAL) - HW(GS+TOT)] in percent



Intensity (%)

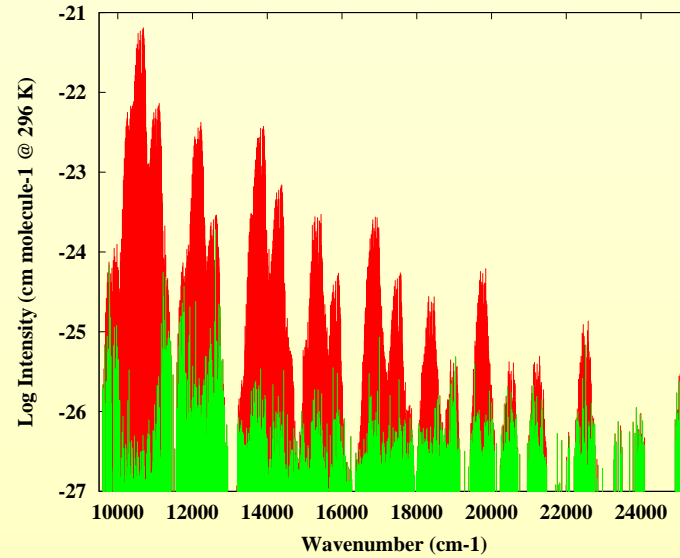
H₂O RAL / geisa+toth Intensity differences :
Idif = [I(RAL) - I(GS+TOT)] in percent



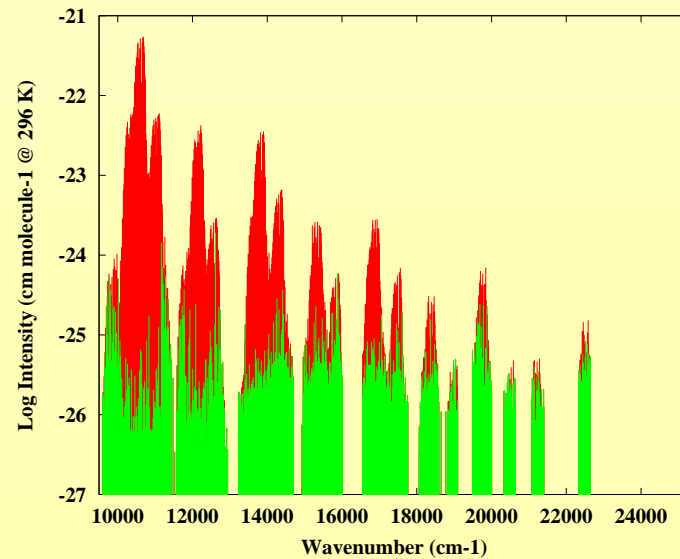


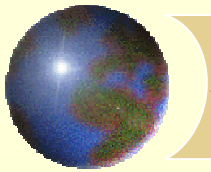
H₂O update in GEISA-03 (NIR – VISIBLE)

GEISA 2003 for H₂O



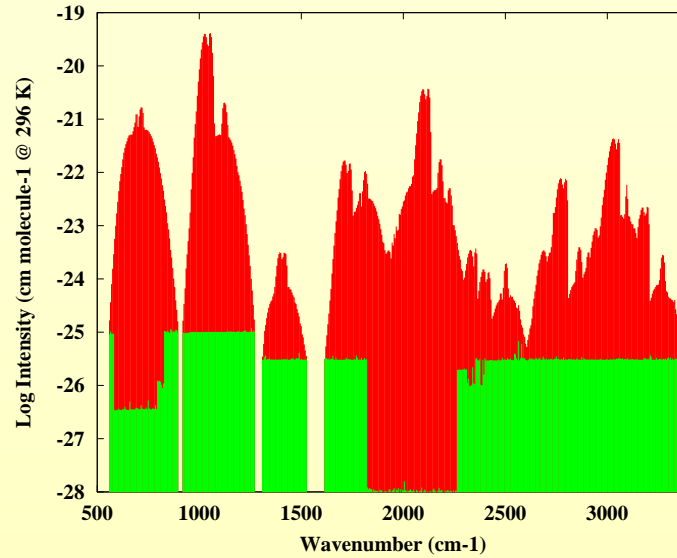
GEISA 1997 for H₂O



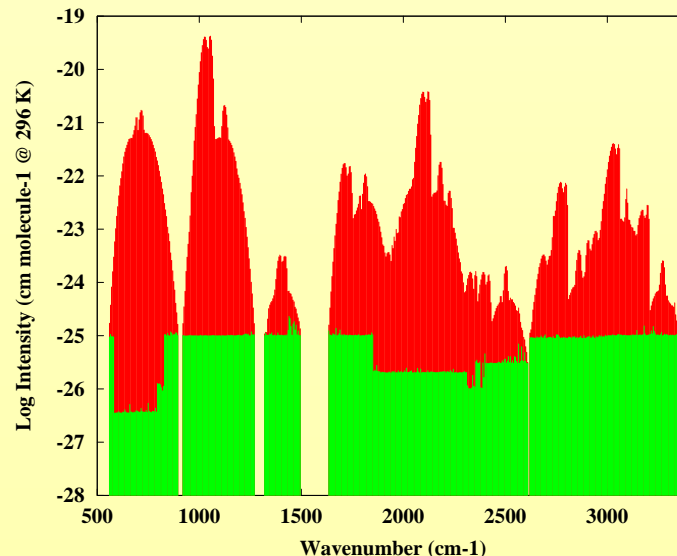


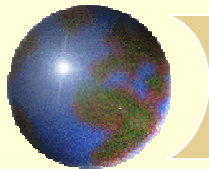
O₃ update in GEISA-03

GEISA 2003 for O₃



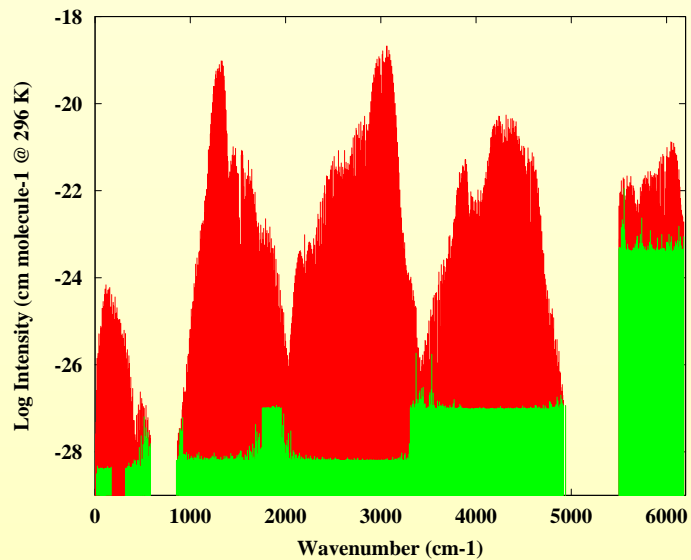
GEISA 1997 for O₃



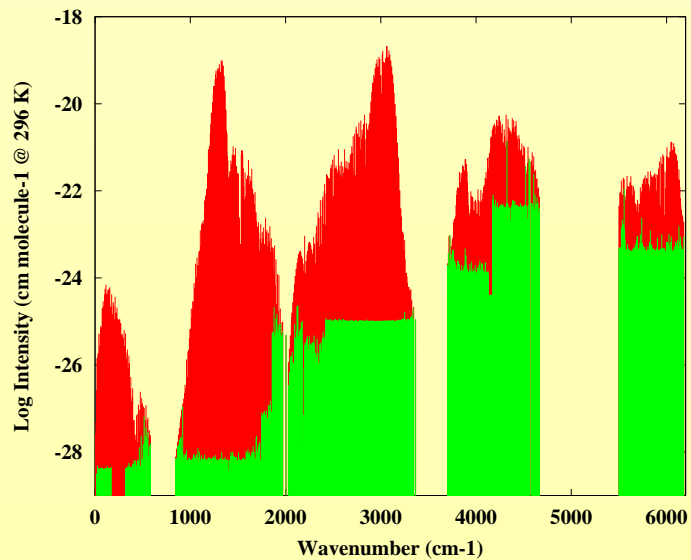


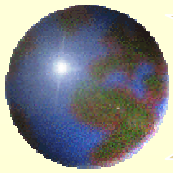
CH₄ update in GEISA-03

GEISA 2003 for CH₄

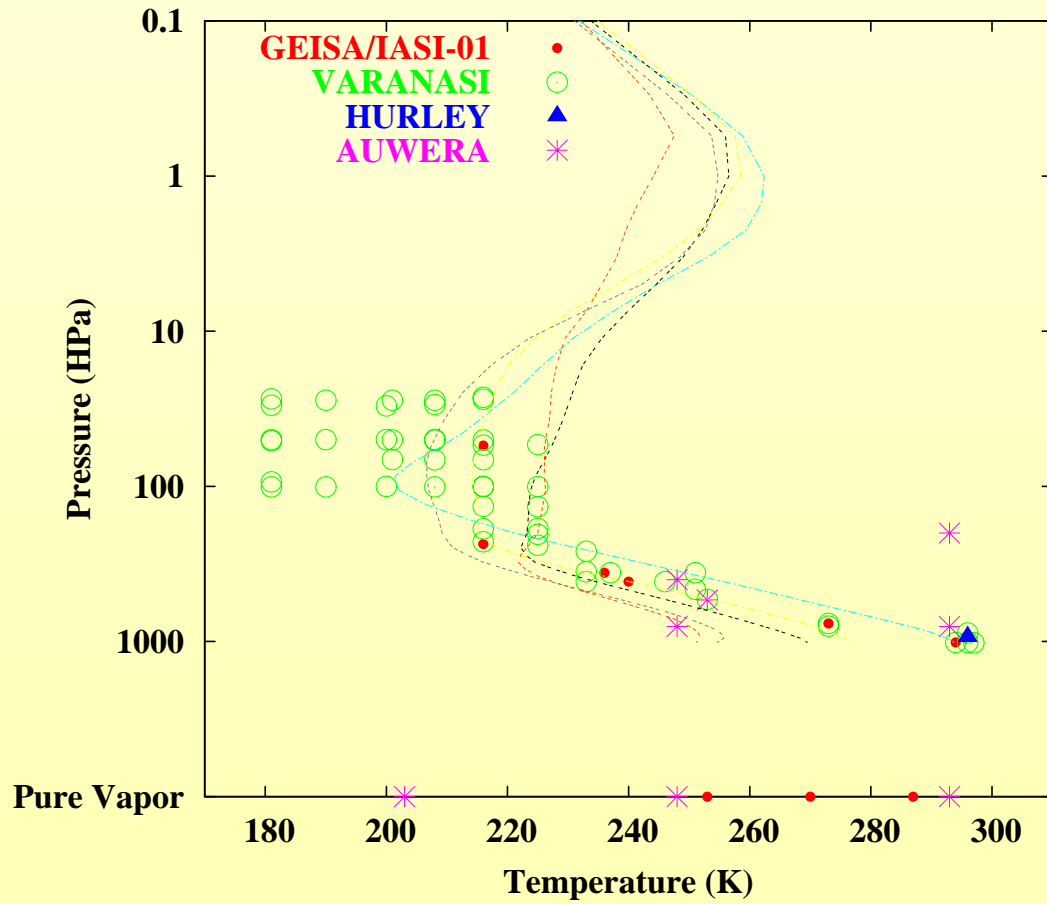


GEISA 1997 for CH₄

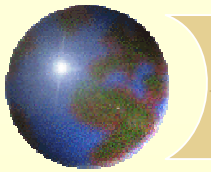




HCFC-22 update in GEISA/IASI-03

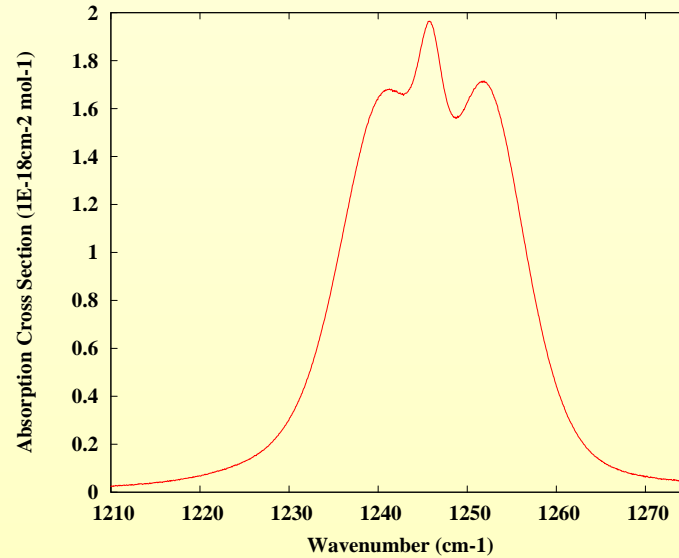


TIGR 2000 Profiles: tropical → polar

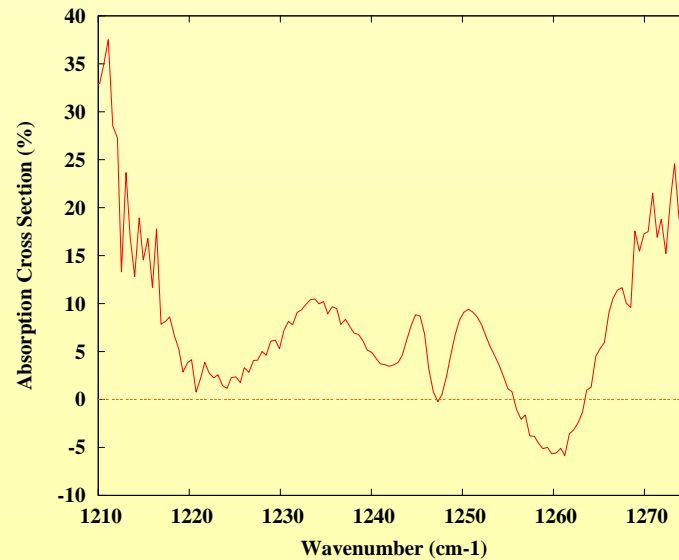


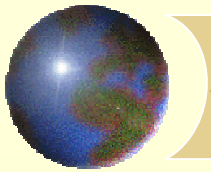
N₂O₅ update in GEISA-03

N2O5 BIRK T=254.1 K P=0 Pa



Difference (BIRK - IASI) / IASI





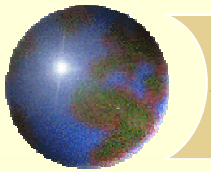
Availability of the GEISA database

The current GEISA database is available with its associated management software, freely from the ARA/LMD group workstations web site:

<http://ara.lmd.polytechnique.fr>
(over 350 registered users)

More complementary information and assistance will be provided upon request from:

jacquinet@lmd.polytechnique.fr



Remaining spectroscopy related problems

Some conclusions of validation exercises, using the 4A-00/LMD Model, in the case of IASI radiative transfer modelling

1. **The water vapour spectroscopic parameters:** still need to be validated;
2. **The water vapour continuum:** more tuning to be done when more situations and situations with high water vapor content become available;
3. **The freons bands at 850 and 920 cm^{-1} :** refine the temperature dependence;
4. **O_3 in the 9.6 micron region:** the spectroscopic parameters still need to be validated;
5. **Some CO_2 – Q branches:** further improvement/tuning of the line mixing

ACKNOWLEDGMENTS

to

**CNES, EUMETSAT and
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