http://ara.abct.lmd.polytechnique.fr

GEISA: Gestion et Etude des Informations Spectroscopiques Atmosphériques; Management and Study of Atmospheric Spectroscopic Information

The GEISA 2015 Spectroscopic Database: Context and New Release

N. JACQUINET, R. ARMANTE, N.A SCOTT, A. CHEDIN,L. CREPEAU

Laboratoire de Météorologie Dynamique, UMR 8539
Ecole Polytechnique, Route départementale 36, F-91128 Palaiseau, France

http://authors.elsevier.com/a/1TUZX54lkPi2w

ACKNOWLEDGMENTS
CNES, CNRS/INSU, UPMC, and EUMETSAT
for their encouragements and supports

With the advent of instruments highly resolved spectrally since the beginning of the 2000's, minimization of the error due to the spectroscopy is more and more essential.

GEISA a computer-accessible Spectroscopic Database with associated management software, designed for the interpretation of various atmospheric remote sensing observations and especially efficient for high spectral resolved Radiative Transfer simulations.

GEISA and RELATIONS TO SPACE MISSIONS (examples)

Atmospheric sounding for scientific study: Meteorology, Climatology, Air quality, Chemestry, astrophysics, ...

Current missions: IASI [on Metop-A (2006) Metop-B (2012), Metop C (2018)]

GEISA reference basis for IASI Level 1 Cal/Val activities @cnes and @lmd

Future missions: IASI-NG, MERLIN, MICROCARB, FLEX

Requirements:
1) remote sensing of the atmosphere at high spectral resolution
FT spectrometers (IASI, IASI-NG)
Grating spectrometers (MICROCARB)
Lidars (MERLIN)
2) evaluations of the performances for:
Missions under exploitation
Missions under development

CURRENT GEISA SYSTEM (created in 1974) Contents and Organization

THREE INDEPENDENT SUB-DATABASES (associated management softwares)

- LINE PARAMETERS: wavenumber, intensity, air broadening pressure half-width (HWHM), energy of the lower transition, quantum identification, temperature dependance of coefficient for HWHM, ...
- ABSORPTION CROSS-SECTIONS: - in the IR (40 molecular species); - in the UV/VIS (17 molecular species)
- MICROPHYSICAL and OPTICAL PROPERTIES of ATMOSPHERIC AEROSOLS

> Minor permanent constituents of the EARTH atmosphere O_3,CH_4,N_2O,CO ...
> Major Permanent constituents of EARTH atmosphere O_2,H_2O,CO_2 ...
> Trace molecules in the EARTH' atmosphere NO, SO_2,NO_2,NH_3, HNO_3, OH,HF, HCl, HBr, HI, ClO, OCS, H_2CO, PH_3
> Molecules in atmospheres of JUPITER, SATURN, URANUS,TITAN, etc.: CH_4, CH_3D, C_2H_2, C_2H_6, GeH_4, HCN, C_2H_6, C_2H_4

DISTRIBUTION, VIZUALIZATION and TOOLS

This new release of GEISA and associated management software facilities will be implemented on AERIS and distributed by its atmospheric chemistry data center "Pôle thématique Ether" http://ara.abct.lmd.polytechnique.fr

http://www.pole-ether.fr/etherType/index.php?id=1450&L=1

GEISA 2015 UPDATED CONTENT

LINE PARAMETERS SUB-DATABASE (Evolution since 1978)

Molecular Species	ID	Contributors to GEISA-2015 update
H_2O	1	L. Coudert, J. Tennyson, A. Campargue, S. Mikhailenko, O.V. Naumenko, J. Orphal, A. Ruth, R.R. Gamache
CO_2	2	V.I. Perevalov, S. Tashkun, R.R. Gamache
O_3	3	A. Barbe, S. Mikhailenko, VI.G. Tyuterev
CH_4	6	V. Boudon, L.R. Brown, A.Campargue, D.C. Benner
O_2	7	S. Yu, B. Drouin
SO_2	9	D. Jacquemart, H.S.P. Müller
NH_3	11	M. Down, J. Tennyson, L.R. Brown
HNO_3	13	A. Perrin
H_2CO	21	D. Jacquemart, H.S.P. Müller
C_2H_2	22	L.R. Brown, K.Y. Sung
CH_3D	23	L.R. Brown, A. Campargue.
C_2H_2	24	D. Jacquemart
C_2H_4	25	J.-M. Flaud
HCN	27	J. Tennyson
C_2N_2	29	A. Jolly.
C_2H_2	30	A. Jolly
CH_3Cl	34	D. Jacquemart, A. Nikitin, J. Buldyreva, N. Lavrentieva
H_2S	36	O.V. Naumenko, L.R. Brown
CH_3Br	43	D. Jacquemart.
HNC	46	J. Tennyson
HDO (NEW)	51	A. Campargue, S. Mikhailenko, O.V. Naumenko, R.R. Gamache
SO_2 (NEW)	52	J. Tennyson, D.S. Underwood

In press N. Jacquinet-Husson et al., J. Mol. Spectrosc. (2016), http://dx.doi.org/10.1016/j.jms.2016.06.007

Summary of GEISA-2015 HDO Update

HDO considered as an independent molecular species in GEISA-2015

HD^{16}O transitions in GEISA-2011

HD^{16}O transitions in GEISA-2015

Isot. ID	Wavenb. min (cm^{-1})	Wavenb. max (cm^{-1})	nlines	Max. Int. (cm molec^{-1}) at 296K	Origin
HD^{16}O 162	0.007002	17080.098	53706	3.175×10^{-21}	IAO, LIPhy
HD^{17}O 172	1234.235	1598.765	175	4.075×10^{-23}	GEISA-2015
HD^{18}O 182	0.197	8748.128	97600	3.694×10^{-21}	5.646×10^{-21} IAO, LIPhy

The new HD^{16}O set, in GEISA-2015, consists of 53,706 transitions in the 0 – 17104 cm^{-1} spectral region, compared to 11,932 transitions between 0 and 13900 cm^{-1} in GEISA-2011

Summary of GEISA-2015 H_2O Update

Log scale graphical display of transition intensities (cm molecule^{-1} at 296 K) included in GEISA-2015 for $H_2{}^{18}O$

Overview of line intensities (at 296 K, in logarithmic scale) in the GEISA-2015 line parameter database for water isotopologues, $H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, between 8850 and 7820 cm^{-1}.

Isot. ID	Wavenb. min (cm^{-1})	Wavenb. max (cm^{-1})	nlines	Max. Int. (cm molecule^{-1}) at 296 K	Origin
$H_2{}^{16}O$ 161	10.713	5098.661	12520	9.974×10^{-19}	LISA, IAO, LIPhy, IAO, UMASS
	5850.0600	7920.3150	18757	1.001×10^{-20}	1.856×10^{-20}
$H_2{}^{17}O$ 171	0.451	1994.5 25	2754	4.857×10^{-20}	9.860×10^{-24} UCL, LIPhy, IAO, SRON, UMASS
	5850.241	7905.615	3659	1.002×10^{-20}	6.939×10^{-24}
	4174.108	4299.793	240	6.46×10^{-23}	4.393×10^{-23}
$H_2{}^{18}O$ 181	895.551	1996.530	974	9.974×10^{-19}	LISA, UCL, SRON, LIPhy, IAO, UMASS
	0.0526	19917.618	39918	8.474×10^{-19}	5.270×10^{-24}
	4177.932	4288.236	478	2.93×10^{-23}	2.440×10^{-23}
	5855.542	7919.033	6641	1.001×10^{-20}	3.647×10^{-21}
$D_2{}^{16}O$ (new) 262	6378.919	6676.140	225	7.31×10^{-24}	2.640×10^{-24} IAO, UMASS
	5.060	7979.072	5746	1.76×10^{-20}	1.75×10^{-20}
$D_2{}^{18}O$ (new) 282	6328.069	6657.658	162	9.41×10^{-24}	5.41×10^{-24} UCC, KIT, UMASS
	0	0	0	0	0

The new H_2O set, in GEISA-2015, consists of 191,846 transitions in the 0 – 25337 cm^{-1} spectral region, compared to 67,789 transitions between 0 and 25232 cm^{-1} in GEISA-2011

ABSORPTION CROSS-SECTIONS SUB-DATABASE

Molecule	# P,T sets	IR range (cm^{-1})
Ethane (update) C_2H_6	14	2545-3315
Propane (update) $CH_3CH_2CH_3$ (C_3H_8)	12	2540-3300
Acetone (update) $(CH_3)_2CO$	19	830-1950
	12	2615-3300
	12	830-1700
Acetonitrile (update) CH_3CN	11	2550-3300
Methanol	12	877-3167
CH_3OH (new)	12	2600-3250
Trifluoromethane CHF_3 (New)	27	950-1500
Acetaldehyde CH_3CHO (new)	16	2400-3400

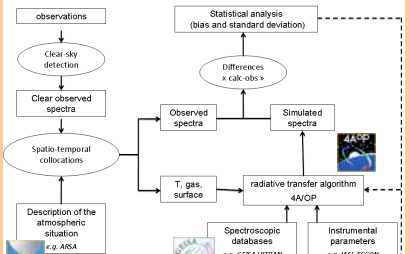
York University
Harrison and Bernath

NIR range (cm^{-1})		Resolution (cm^{-1})	Refs
Acetonitrile	CH_3CN	6014 – 7067	0.001	O'Leary et al., 2012
Methyl iodide	CH_3I	5473 – 7497	0.001	F.P. Farag et al., 2013
Methylmethylacetyl	CH_3O_2	7474 – 7497	0.025	F.P. Farag et al., 2013
Formaldehyde	H_2CO	6547 – 7081	0.001	Daum et al., 2005
Hydroperoxy radical	HO_2	6604 – 6696	0.001	Ibrahim et al., 2007;Jain et al., 2011
Nitrous acid	HONO	6624 – 6665	0.005	Jain et al., 2011
Ammonia	NH_3	6880 – 6997	0.001	O'Leary et al., 2008

VALIDATION of GEISA

The main difficulty in interpreting differences between radiative transfer simulations and observations is to be able to separate errors coming from the different actors of the radiative transfer simulations. For example errors coming from the incomplete knowledge of the atmospheric state and those due to the modeling itself. Based on the calibration/validation procedure developed for thermal infrared observations at Laboratoire de Météorologie Dynamique (http://ara.abct.lmd.polytechnique.fr/), our analysis chain « SPARTE » (Spectroscopic Parameters And Radiative Transfer Evaluation) aims at eliminating the atmospheric effect. SPARTE consists of a detailed statistical analysis of the differences (bias and standard deviation) between simulations and observations (the so-called « residuals ») for a large number of situations.

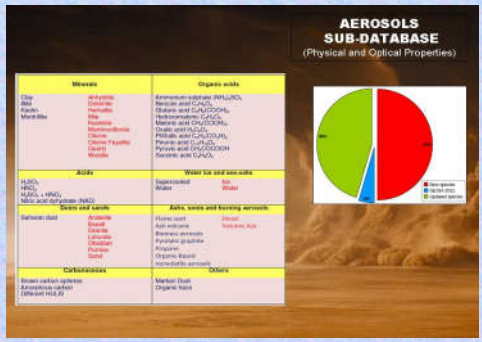
The SPARTE chain at LMD



Using a precise radiative transfer algorithm (here 4A/OP), and observations at high spectral resolution (here from IASI and TCCON), *it has been possible to trace back the impact of the quality of each individual spectroscopic parameter.*

In press as: R. Armante et al., J. Mol. Spectrosc. (2016), http://dx.doi.org/10.1016/j.jms.2016.04.004

AEROSOLS SUB-DATABASE (Physical and Optical Properties)



Spectroscopic validations for the Ultraviolet Visible Near-infrared Shortwave instrument (UVNS)

0.24 – 2.4385 µm

Ground-based data - TCCON network

Fourier transform spectrometer (HR/FTS)
• 2 detectors:
- InGaAs (4000-11000 cm^{-1})
- Si-diode (11000-13000 cm^{-1})
Spectral resolution : 7.5x10^{-3} cm^{-1}

https://tccon-wiki.caltech.edu/

1.6-1.7 µm CH_4 spectral range interest

bad HWHM detected and high impact of the pressure shift observed on H_2O line

(1) H_2O	Position	Intensity	HWHM	E0	P shift
GEISA-2011	6031.89939	7.3020D-26	0.0300	2042.31	-0.00000
GEISA-2015	6031.89940	7.1300D-26	0.0380	2042.31	-0.01106
HITRAN-2012	6031.89939	7.3020D-26	0.0078	2042.31	-0.02200

Use of TCCON high resolved spectra to:

✓ *Control the quality of the proposed updates*
✓ *Be able to discriminate which parameters are involved (shape of the residual)*

(2) CH_4	Position	Intensity	HWHM	E0	P shift
GEISA-2011	6026.22740	5.7210D-22	0.0634	10.4816	-0.0111
GEISA-2015	6026.22710	5.7680D-22	0.0650	10.4817	-0.012
HITRAN-2012	6026.22686	5.7680D-22	0.0682	10.4817	-0.008

Mix of HWHM and pressure shift impacts on CH_4 line

New CH_4 lines added in HITRAN-2012 and GEISA-2015

(3) CH_4	Position	Intensity	HWHM	E0	P shift
GEISA-2011	-	-	-	-	-
GEISA-2015	6029.55760	4.7340D-24	0.066	62.8758	-0.01206
	6029.65580	2.0490D-24	0.066	62.8758	-0.01206
	6029.83250	1.3560D-24	0.060	999.9999	-0.01206
	6029.84520	4.9590D-24	0.060	662.1400	-0.01206
	6029.87310	2.1220D-24	0.060	516.2800	-0.01206
HITRAN-2012	6029.55760	4.7340D-24	0.0637	62.8758	-0.01090
	6029.65580	2.0490D-24	0.0637	62.8758	-0.01090
	6029.83250	1.3560D-24	0.0493	999.9999	-0.01200
	6029.84520	4.9590D-24	0.0523	662.1400	-0.01200
	6029.87310	2.1220D-24	0.0550	516.2800	-0.01200

✓ Alternative updates of both HITRAN (2008, 2012) and GEISA (2011, 2015) databases give the users the possibility to have the best spectroscopic parameters at any time (1)
✓ Study of the residuals makes it possible to validate a dataset provided by a laboratory → feedback before the final version of the GEISA database (2)
✓ It may be possible to identify the parameters which could explain the shape of the residuals even for « minor » parameters such as pressure shift (1) and (3)
✓ validation possible for low intensity lines (3)

The IASI instrument

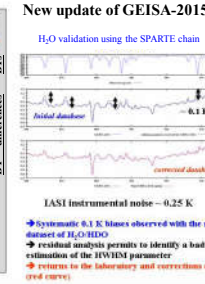
•Developed by CNES, in collaboration with EUMETSAT (EUropean Organisation for the Exploitation of METeorological SATellites)

•IASI (Infrared Atmospheric Sounding Interferometer) is a Fourier Transform Spectrometer which measures the infrared radiation emitted from the Earth.

IASI characteristics :
- 8461 spectral channels between 645 and 2760 cm^{-1} (15.5 - 3.63 µm)
- spectral resolution of 0.5 cm^{-1} after apodisation ("Level 1c" spectra)
- spectral sampling interval is 0.25 cm^{-1}
- nadir FOV: 12 km

New update of GEISA-2015

H_2O validation using the SPARTE chain



IASI instrumental noise ~ 0.25 K

→ Systematic 0.1 K biases observed with the new dataset of H_2O/HDO
→ residual analysis permits to identify a bad estimation of the HWHM parameter
→ returns to the laboratory and corrections done (red curve)

Able to detect bad spectroscopic parameters providing their signature on residuals much lower than instrument noise

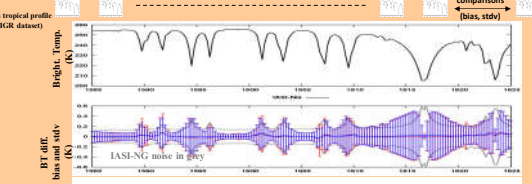
Spectroscopic studies for the Infrared Atmospheric Sounding Interferometer – Next Generation (IASI-NG)

Example of the 6.3 µm band

The aim of this study is to estimate the spectroscopic parameter precision needed for IASI-NG, taking into account the interference between the lines. Simulations have been made using an improvement by a factor 2 of the spectral resolution and of the noise of IASI.

Method : in a given spectral range, a spectroscopic parameter X of GEISA-2015 is randomly perturbated (Gaussian law without bias) for all the lines of a molecule. This action is repeated N times to give at the end N new versions of the GEISA 2015 (perturbated versions).
4A/OP is then run for a given set of atmospheres (from TIGR database) and for the N perturbated databases.
Each run is compared to the reference simulation (original GEISA-2015 spectroscopic parameters)

Exemple of H_2O (GEISA-2015 between 1585-1625 cm^{-1})



A minimum precision around 5% for the intensity or for the HWHM seems to be needed in the center of the 6.3 µm band of H_2O to get a spectroscopy impact error at the same level as the IASI-NG noise