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

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

The GEISA spectroscopic database 2015 edition in the frame of IASI remote sensing applications and IASI-NG phase B studies

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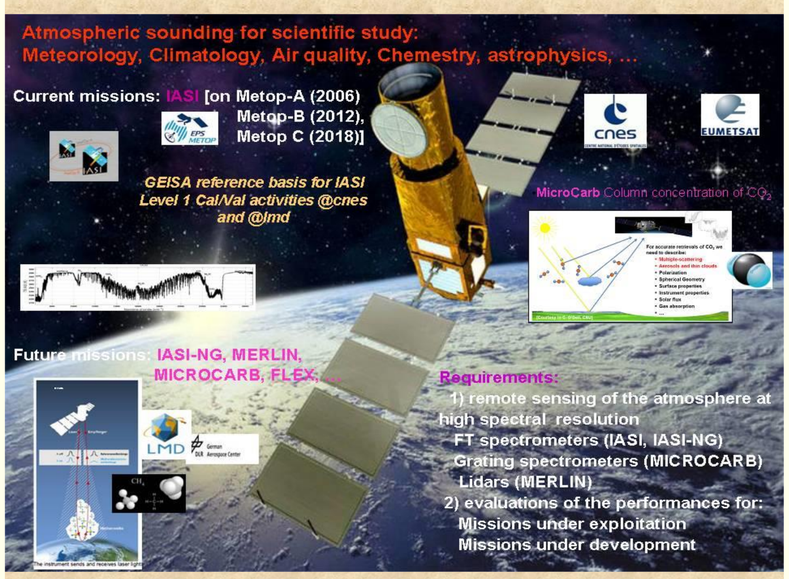
With the advent of instruments highly resolved spectrally since the beginning of the 2000's, minimization of the error due to the spectroscopy is more and more essential.

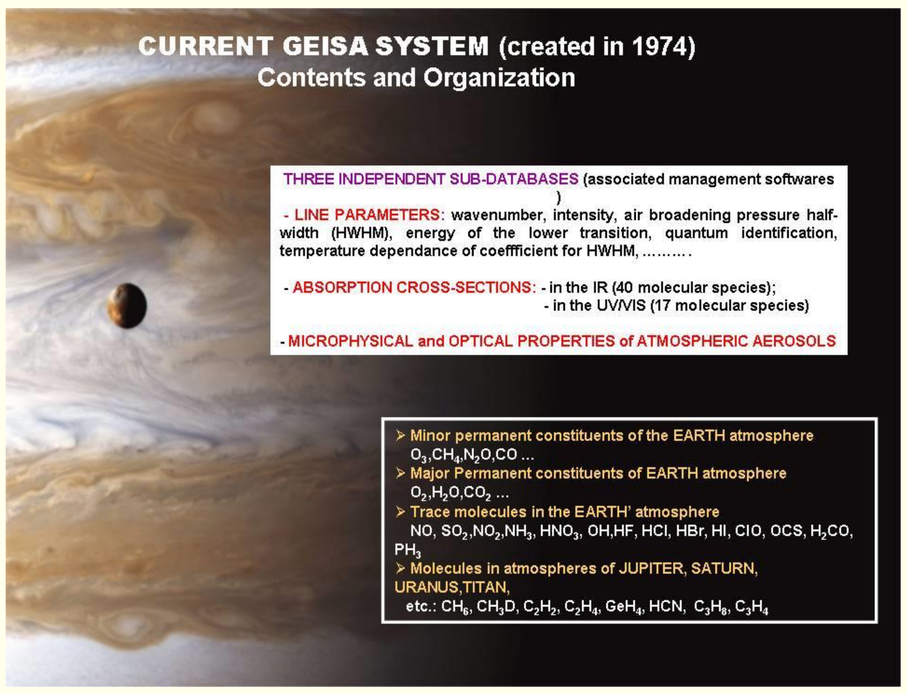
GEISA a computer-accessible Spectroscopic Database with associated management software, designed for the interpretation of various atmospheric remote sensing observations and especially efficient for high spectral resolved Radiative Transfer simulations.

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

GEISA and RELATIONS TO SPACE MISSIONS (examples)



CURRENT GEISA SYSTEM (created in 1974) Contents and Organization

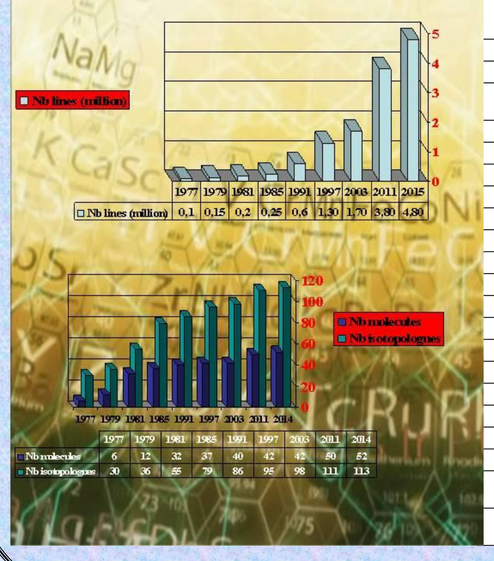


DISTRIBUTION, VIZUALIZATION and TOOLS

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/etherTypo/index.php?id=1450&L=1

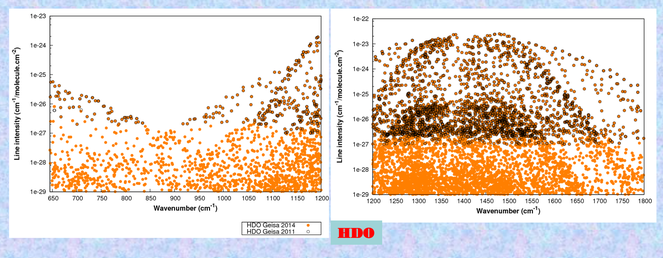
GEISA 2015 UPDATED CONTENT

LINE PARAMETERS SUB-DATABASE (Evolution since 1978)

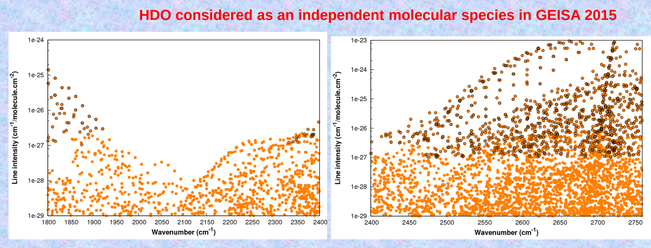


Molecular Species	ID	Contributors to GEISA-2015 update
H_2O	1	L. Coudert, J. Tennyson, A. Campargue, S. Mikhaïlenko, O.V. Naumenko, J. Orphal, A. Ruth, R.R. Gamache
CO_2	2	V.I. Perevalov, S. Tashkun, R.R. Gamache
O_3	3	A. Barbe, S. Mikhaïlenko, Vl.G. Tyuterev
CH_4	6	V. Boudon, L.R. Brown, A.Campargue, 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_6	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_4H_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. Mikhaïlenko, O.V. Naumenko, R.R. Gamache
SO_3 (NEW)	52	J. Tennyson, D.S. Underwood

IASI/IASI-NG Spectral Bands



HDO considered as an independent molecular species in GEISA 2015



Summary of GEISA-2015 HDO Update

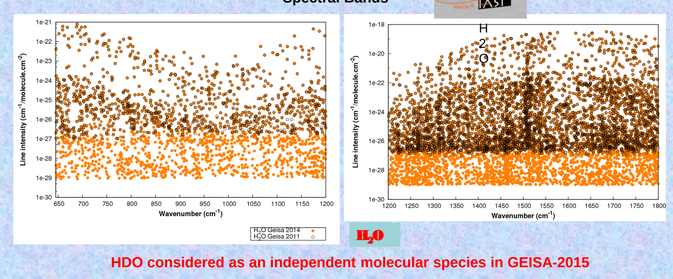
Isotope	Contribution	Wavenb. min (cm^{-1})	Wavenb. max (cm^{-1})	#lines G-14	#lines G-11	Moy. I (cm molec^{-1})	Max. I (cm molec^{-1})
$HD^{16}O$ 162	S. Mikailenko, O.Naumenko (IAO)	0.007002	17080.098180	53706	11932	3.175×10^{-25}	2.700×10^{-22}
$HD^{17}O$ 172	NO new data since GEISA-2011	1234.234730	1598.765470	175	175	4.075×10^{-27}	9.319×10^{-27}
$HD^{18}O$ 182	S. Mikailenko, A. Campargue (IAO, UJF)	0.196882	8748.128100	9760	659	3.694×10^{-27}	5.646×10^{-25}

Line shape parameters revised by G. Gamache

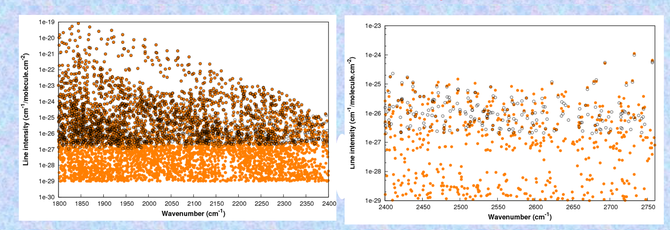
Total = 63641 HDO lines

Total H_2O lines in GEISA-2011 12766

IASI/IASI-NG Spectral Bands



HDO considered as an independent molecular species in GEISA-2015



Summary of GEISA-2015 H_2O Update

Isot. ID	Contribution	Wavenb. min (cm^{-1})	Wavenb. max (cm^{-1})	#lines G-14	#lines G-11	Moy. I (cm molec^{-1})	Max. I (cm molec^{-1})
$H_2{}^{16}O$ 161	L.Coudert (LISA) S. Mikailenko, A. Campargue (IAO, UJF) *Revised and updated by* O.Naumenko (IAO)	0.400560	25335.071700	119885	40920	6.135×10^{-22}	2.656×10^{-18}
$H_2{}^{17}O$ 171	J. Tennyson (UCL) S. Mikailenko, A. Campargue (IAO, UJF) R.A. Scheepmaker et al. (Atmos Meas Tech Discuss (2012)	0.451497	17578.330111	28598	5466	9.595×10^{-25}	9.860×10^{-22}
$H_2{}^{18}O$ 181	J. Tennyson (UCL) L.Coudert (LISA) S. Mikailenko, A. Campargue (IAO, UJF) R.A. Scheepmaker et al. (Atmos Meas Tech Discuss (2012)	0.052583	19917.617846	40074	8352	3.635×10^{-24}	5.270×10^{-21}
$D_2{}^{16}O$ 262	A.Ruth, J.Orphal (Univ. Cork, KIT)	6378.9189	6676.1465	New 225	ABS	5.704×10^{-32}	2.64×10^{-31}
$D_2{}^{18}O$ 282	A.Ruth, J.Orphal (Univ. Cork, KIT)	6328.0684	6637.6582	New 162	ABS	9.411×10^{-35}	5.64×10^{-34}

Line shape parameters revised by G. Gamache

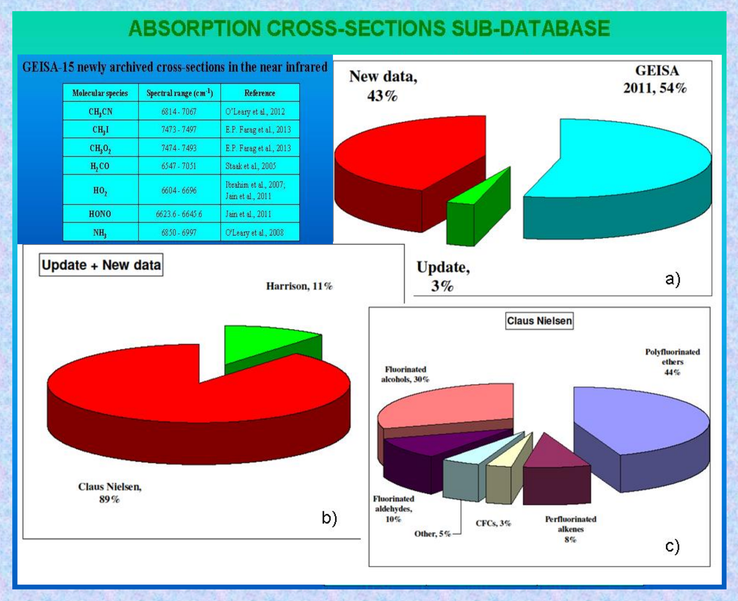
Total = 188944 H_2O lines

Total H_2O lines in GEISA-2011 67504

ABSORPTION CROSS-SECTIONS SUB-DATABASE

GEISA-15 newly archived cross-sections in the near infrared

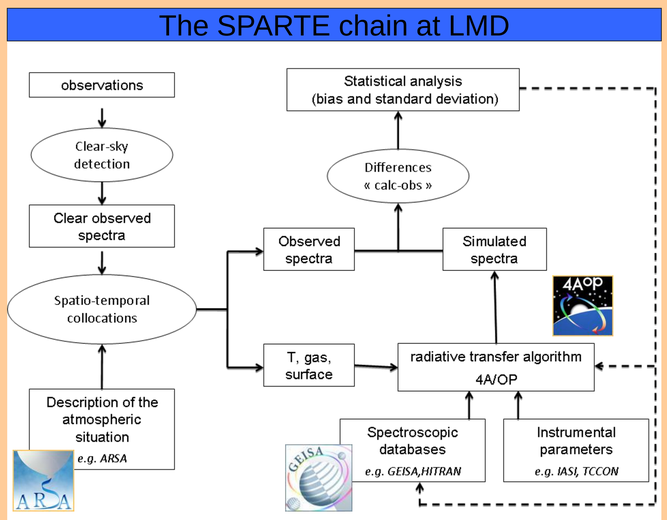
Molecular species	Spectral range (cm^{-1})	Reference
CH_3CN	6814 - 7067	O'Leary et al., 2012
CH_3I	7473 - 7497	E.P. Farag et al., 2013
CH_3O_2	7474 - 7493	E.P. Farag et al., 2013
H_2CO	6547 - 7051	Staak et al., 2005
HO_2	6604 - 6656	Ibrahim et al., 2007; Jain et al., 2011
HONO	6623.6 - 6645.6	Jain et al., 2011
NH_2	6850 - 6997	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.

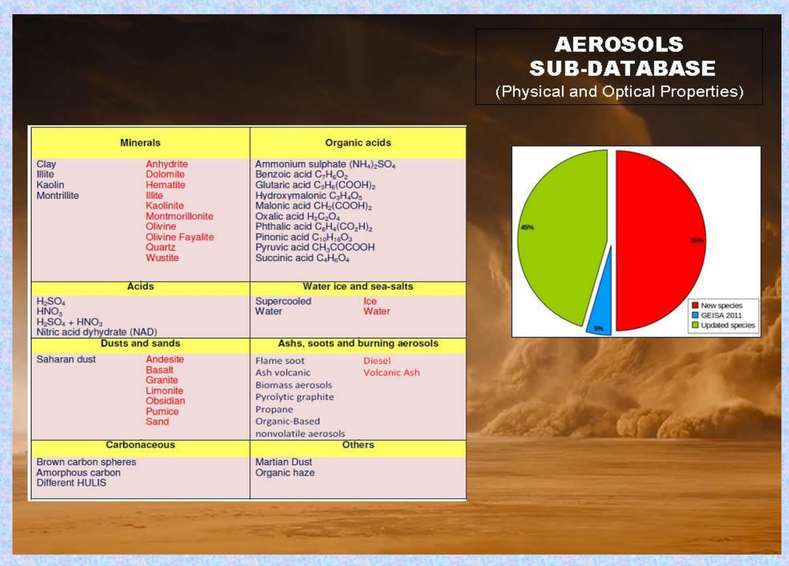
The SPARTE chain at LMD



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.*

(Armante et al, JMS, 2016, SI spectroscopic databases, submitted)

AEROSOLS SUB-DATABASE (Physical and Optical Properties)



Minerals		Organic acids	
Clay, Illite, Kaolin, Montrillite	Anhydrite, Dolomite, Hematite, Illite, Kaolinite, Montmorillonite, Olivine, Olivine Fayalite, Quartz, Wustite	Ammonium sulphate $(NH_4)_2SO_4$, Benzoic acid $C_7H_6O_2$, Glutaric acid $C_3H_6(COOH)_2$, Hydroxymalonic $C_3H_4O_5$, Malonic acid $CH_2(COOH)_2$, Oxalic acid $H_2C_2O_4$, Phthalic acid $C_6H_4(CO_2H)_2$, Pinonic acid $C_{10}H_{16}O_3$, Pyruvic acid $CH_3COCOOH$, Succinic acid $C_4H_6O_4$	
Acids		**Water ice and sea-salts**	
H_2SO_4, HNO_3, $H_2SO_4 + HNO_3$, Nitric acid dyhydrate (NAD)		Supercooled Water, Ice, Water	
Dusts and sands		**Ashs, soots and burning aerosols**	
Saharan dust	Andesite, Basalt, Granite, Limonite, Obsidian, Pumice, Sand	Flame soot, Ash volcanic, Biomass aerosols, Pyrolytic graphite, Propane, Organic-Based nonvolatile aerosols	Diesel, Volcanic Ash
Carbonaceous		**Others**	
Brown carbon spheres, Amorphous carbon, Different HULIS		Martian Dust, Organic haze	

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

Ground-based data - TCCON network

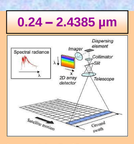
Fourier transform spectrometer (HR/FTS)
- 2 detectors:
  - Ingaas (4000-11000 cm^{-1})
  - Si-diode (11000-13000 cm^{-1})

Spectral resolution : 7.3×10^{-3} cm^{-1}

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)*

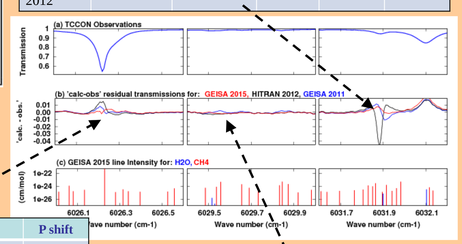
0.24 – 2.4385 µm



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



(2) CH_4	Position	Intensity	HWHM	E0	P shift
GEISA-2011	6026.22740	5.7210D-22	0.0634	10.4816	-0.01111
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

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

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

✓ 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]

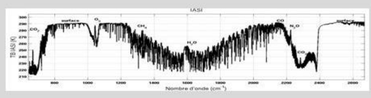
✓ It may be possible to identify the parameters which could explain the shape of the residuals even for « minor » parameters such as pressure shift [1] and [2]

✓ validation possible for low intensity lines [3]

The IASI instrument

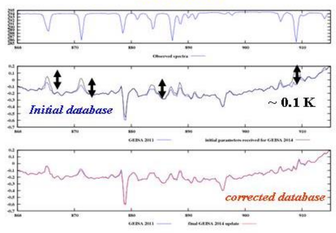
- Developed by CNES, in collaboration with EUMETSAT (EUropean Organisation for the Exploitation of METeorological SATellites)
- IASI (Infrared Atmospheric Sounding Interferometer) is a Fourier Transform Spectrometer which measures the infrared radiation emitted from the Earth.

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

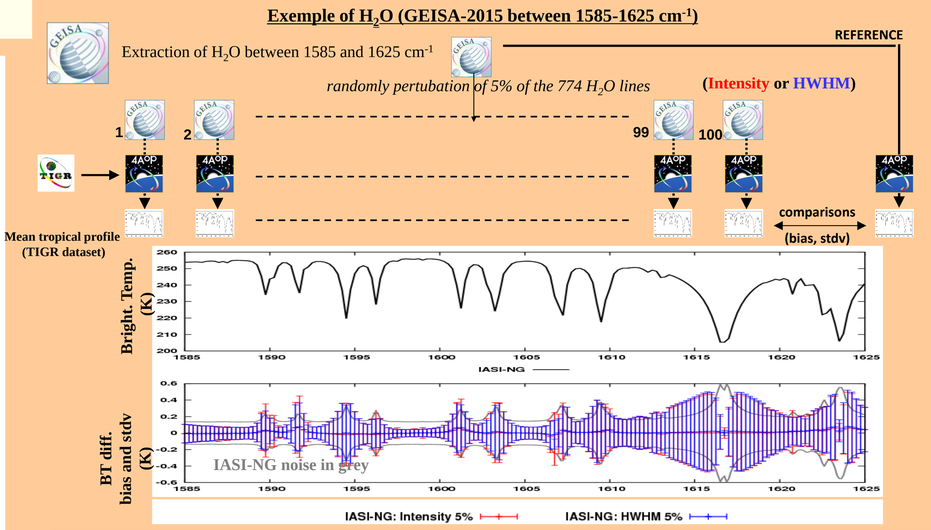
Spectroscopic studies for the Infrared Atmospheric Sounding Interferometer – Next Generation (IASI-NG)

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