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

THE GEISA SPECTROSCOPIC DATABASE IN 2014: CONTEXT AND CONTENTS

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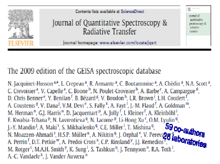

ACKNOWLEDGEMENTS
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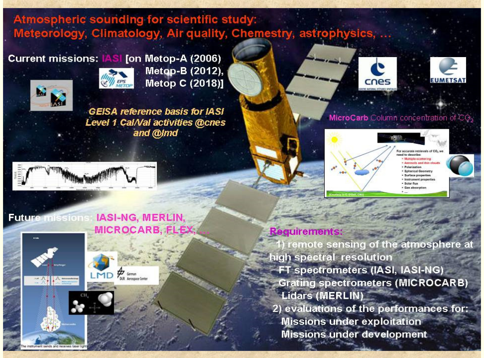
Spectroscopy is at the root of modern planetology, enabling to determine the physical properties of planets remotely.

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.

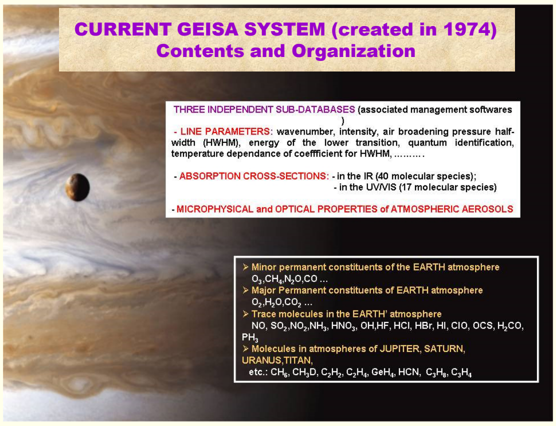
GEISA and RELATIONS TO SPACE MISSIONS (examples)



CURRENT GEISA SYSTEM (created in 1974) Contents and Organization

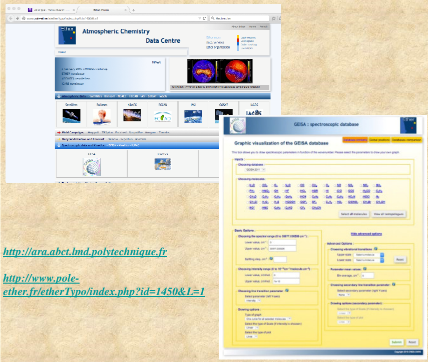
THREE INDEPENDENT SUB-DATABASES (associated management softwares)

- 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_4, GeH_4, HCN, C_3H_8, C_2H_4

DISTRIBUTION, VIZUALIZATION and TOOLS

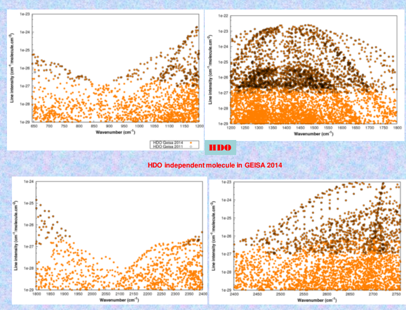


http://ara.abct.lmd.polytechnique.fr

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

GEISA 2014 UPDATED CONTENT

IASI/IASI-NG Spectral Bands



HDO independent molecule in GEISA 2014

Summary of GEISA-2014 HDO Update

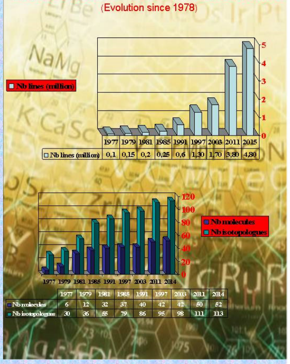
Isotope	Contribution	Wavenb. min (cm⁻¹)	Wavenb. max (cm⁻¹)	#lines G-14	#lines G-11	Moy. I	Max. I
HD16O 161	S. Mikhailenko, O. Naumenko (IAO)	0.007002	17080.098160	53706	11932	3.175x10⁻²²	2.700x10⁻²⁰
HD18O 172	NO new data since GEISA 2011	1234.234730	1598.765470	175	175	4.075x10⁻²⁷	9.319x10⁻²⁶
HD18O 162	S. Mikhailenko, A. Campargue (IAO, UJF)	0.196882	8748.128100	9760	659	3.694x10⁻²⁷	5.646x10⁻²⁵

Line shape parameters revised by G. Gamache

Total = 63641 HDO lines in GEISA-2014

Total H_2O lines in GEISA-2011 12766

LINE PARAMETERS SUB-DATABASE (Evolution since 1978)



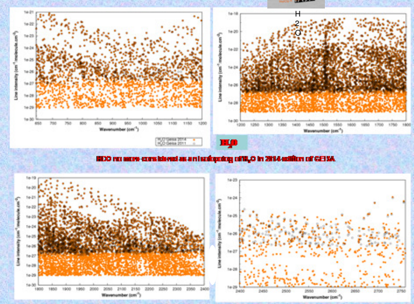
Updated molecules for GEISA 2014 Edition
22 Molecular species

Molecule ID.	Code	Contributors
H_2O	1	L.Coudert, J. Tennyson, S. Mikhailenko, A.Campargue,O. Naumenko, A. Ruth, J.Orphal. HDO no more considered as an isotopologue of H_2O ; individual molecule [coded 51]
CO_2	2	V. Perevalov, R.T. Gamache
O_3	3	S. Mikhailenko
CH_4	6	L.R. Brown, V. Boudon, A.Campargue VI.G. Tyuterev, D.C. Benner
O_2	7	S. Yu, B. Drouin
SO_2	9	D. Jacquemart
NH_3	11	M. Down, J. Tennyson, L.R. Brown
HNO_3	13	A. Perrin ($H^{15}NO_3$ New isotopologue)
H_2CO	21	D. Jacquemart
C_2H_6	22	L. Brown
CH_3D	23	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
H_2S	36	O. Naumenko
CH_3Br	43	D. Jacquemart.
HNC	46	J. Tennyson
HDO (NEW)	51	S. Mikhailenko ,O. Naumenko
SO_3(NEW)	52	J. Tennyson'

Total number of molecules in GEISA-2014: 52

52 Molecular Species in GEISA 2014

IASI/IASI-NG Spectral Bands



HDO no more considered as an isotopologue of H_2O in 2014 edition of GEISA

Summary of GEISA-2014 H_2O Update

Isot. ID	Contribution	Wavenb. min	Wavenb. max	#lines G-14	#lines G-11	Moy. I	Max. I
$H_2^{16}O$ 161	L.Coudert (LISA) S. Mikhailenko, A. Campargue (IAO, UJF) Revised and updated by O.Naumenko (IAO) J. Tennyson (UCL)	0.400560	25335.071700	119885	40820	6.135x10⁻²²	2.656 x10⁻¹⁹
$H_2^{17}O$ 171	S. Mikhailenko, A. Campargue (IAO, UJF) R.A. Schwepmaker et al. (Atmos Meas Tech Discuss (2012) J. Tennyson (UCL)	0.451497	17578.330111	28598	5466	9.595x10⁻²⁶	9.860 x10⁻²³
$H_2^{18}O$ 181	L.Coudert (LISA) S. Mikhailenko, A. Campargue (IAO, UJF) R.A. Schwepmaker et al. (Atmos Meas Tech Discuss (2012)	0.052583	19917.617846	40074	8352	3.635x10⁻²⁵	5.270 x10⁻²²
$D_2^{16}O$ 262	A.Ruth, J.Orphal (Univ. Cork, KIT)	6378.9189	6676.1465	New 225	ABS	5.704 x10⁻²⁶	2.64 x10⁻²⁵
$D_2^{16}O$ 262	A.Ruth, J.Orphal (Univ. Cork, KIT)	6328.0684	6637.6582	New 162	ABS	9.411x10⁻²⁶	5.64 x10⁻²⁵

Line shape parameters revised by G. Gamache

Total = 188944 H_2O lines in GEISA-2014

Total H_2O lines in GEISA-2011 67504

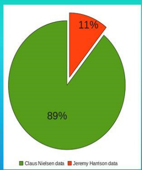
ABSORPTION IR CROSS-SECTIONS SUB-DATABASE

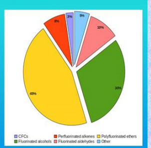
GEISA-15 update cross-sections in the infrared

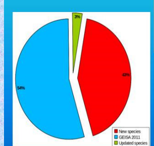
•J. Harrison and P. Bernath, ASA/HITRAN conf., Aug. 2012, Reims

- ✓ Ethane
- ✓ Propane
- ✓ Acetone
- ✓ Acetonitrile
- ✓ Methanol
- ✓ Trifluoromethane
- ✓ Acetaldehyde

•Ø. Hodnebrog, M. Etminan, J.S.Fuglestvedt, G. Marston, G. Myhre, C.J. Nielsen, et al., Rev. of Geophys.,2013





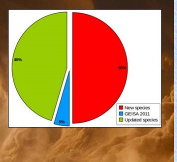


GEISA-15 newly archived cross-sections in the near infrared

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 - 6696	Ibrahim et al., 2007; Jain et al., 2011
HONO	6623.6 - 6645.6	Jain et al., 2011
NH_3	6850 - 6997	O'Leary et al., 2008

AEROSOLS SUB-DATABASE (Physical and Optical Properties)

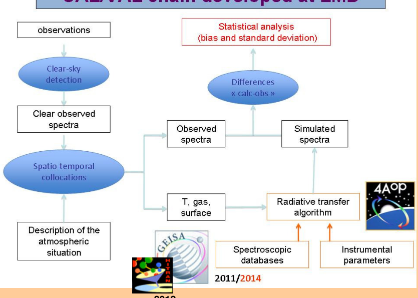
Minerals		Organic acids
Clay, Illite, Kaolin, Montrillite	Anhydrite, Dolomite, Hematite, Illite, Kaolinite, Montmorillonite, Olivine, Olivine Fayalite, Quartz, Wustite	Ammonium sulphate $(NH_4)_2SO_4$, Benzoic acid $C_7H_6O_2$, Glutaric acid $C_3H_6(COOH)_2$, Hydroxymalonic $C_3H_4O_5$, Malonic acid $CH_2(COOH)_2$, 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		**Ash, 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



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 calibartion/validation of level1 procedure developed for thermal infrared observations at Laboratoire de Météorologie Dynamique (http://ara.abct.lmd.polytechnique.fr/), our analysis procedure aims at eliminating the atmospheric effect through the statistical analysis (bias and standard deviation) of numerous situations.
This statistical analysis results in the study of the differences between simulations and observations called "residuals".

CAL/VAL chain developed at LMD

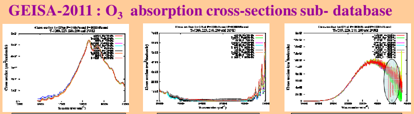


With a precise radiative transfer algorithm like 4A/OP, and with observations at high spectral resolution (like IASI and TCCON), *it has been possible to go back to the quality impact of individual spectroscopic parameters.*

GOME instrument

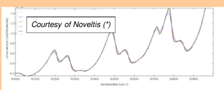
UV/VIS

GEISA-2011 : O_3 absorption cross-sections sub- database



Chappuis band | Huggins band | Hartley's band

cross- sections have to be cleaned of noise effects



Huggins band

Colors correspond to cross-section measurements at different spectral resolutions

➔ Study of the impact of the spectral resolution cross-sections sub-database on GOME instrument simulation

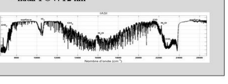
Spectral resolution measured by a laboratory has to be verified ➔ not too low even if the spectral variation of the cross- sections in general is low

The IASI instrument

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

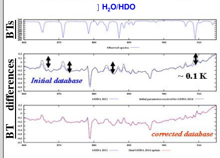
•IASI (Infrared Atmospheric Sounding Interferometer) is a Fourier Transform Spectrometer which measures the infrared radiation emitted from the Earth.

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



TIR

New update of GEISA : 2015
] H_2O/HDO



IASI instrumental noise ~ 0.25 K

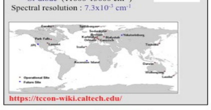
➔Systematic 0.1 K biases observed with the new dataset of H_2O/HDO
➔ residual analysis permits to identify a bad estimation of the HWHM parameter
➔ returns to the laboratory and corrections done (red curve)

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

Ground-based data - TCCON network

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

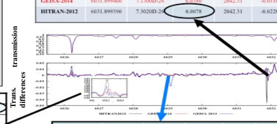
Spectral resolution : 7.3x10⁻³ cm⁻¹



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

SWIR
- ✓ Control the quality of the proposed updates
- ✓ Able to discriminate which parameters are involved
- ✓ Sensitivity of residuals to pressure shift

(1)	Position	Intensity	HWHM	E0	P shift
GEISA-2011	6031.899398	7.3020D-26	0.0688	2842.51	-0.00000
GEISA-2014	6031.899400	7.3300D-26	0.0788	2842.51	-0.01000
HITRAN-2012	6031.899398	7.3020D-26	0.0079	2842.51	-0.02000



(3)	GEISA-2011	GEISA-2014	HITRAN-2012
Position	6026.227400	6026.227100	6026.226461
Intensity	5.7210D-25	5.7660D-25	5.7660D-
HWHM	0.0634	0.0659	0.0682
n	10.4816	10.4817	10.4817
P shift	-0.011115		-0.009100

(2)	Position	Intensity	HWHM	E0	P shift
GEISA-2011	6029.107670	1.1290D-25	0.0655	62.6791	-0.011600
GEISA-2014	6029.107670	1.4290D-25	0.0000	62.9000	-0.013950
HITRAN-2012	6029.107670	1.4290D-25	0.0657	62.6811	-0.012100

MAIN CONCLUSIONS

- Alternative updates of both HITRAN (2008, 2012) and GEISA (2011, 2015) databases give to the users the possibility to have the best spectroscopic parameters at any time (table 1)
- Study of the residuals makes it possible to validate a dataset provided by a laboratory ➔ feedback given before the final version of the GEISA database (table 2)
- For the strongest transitions, it may be possible to identify the parameters which could explain the shape of the residuals (table 3)
- With the new generation of spatial instruments (high spectral resolution), it is needed to take into account « minor » parameters such as the pressure shift (table 3)