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

The GEISA Database

A key tool for atmospheric remote sensing applications

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The 2009 edition of the GEISA spectroscopic database

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59 co-authors
26 laboratories

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GENERAL CONTEXT

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

GEISA a **computer-accessible Spectroscopic Database** and **associated management software**, designed for the interpretation of remote sensing observations (suitable for all instrument categories) and using a line-by-line (atmospheric) layer-by-layer approach.

CURRENT GEISA SYSTEM (created in 1974)
Contents and Organization

(MSG-2 25/01/06)
EARTH

- 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_6, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_8, C_3H_4

(CASSINI-HUYGENS 29/01/06)
TITAN

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 coeffficient for HWHM, …….
- **ABSORBTION CROSS-SECTIONS:** - in the IR (40 molecular species); - in the UV/VIS (17 molecular species)
- **MICROPHYSICAL and OPTICAL PROPERTIES of ATMOSPHERIC AEROSOLS**

GEISA 2014 SYSTEM OVERVIEW

SPACE MISSIONS RELATED TO S PECTROSCOPY AND GEISA (Examples)

Terrestrial atmospheric sounding for scientific study of the atmosphere: METEOROLOGY, CLIMATOLOGY, AIR QUALITY/CHEMISTRY

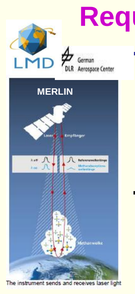
Missions:

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

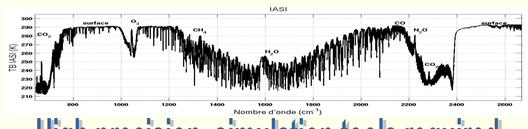
Future: IASI-NG, MERLIN, MICROCARB

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



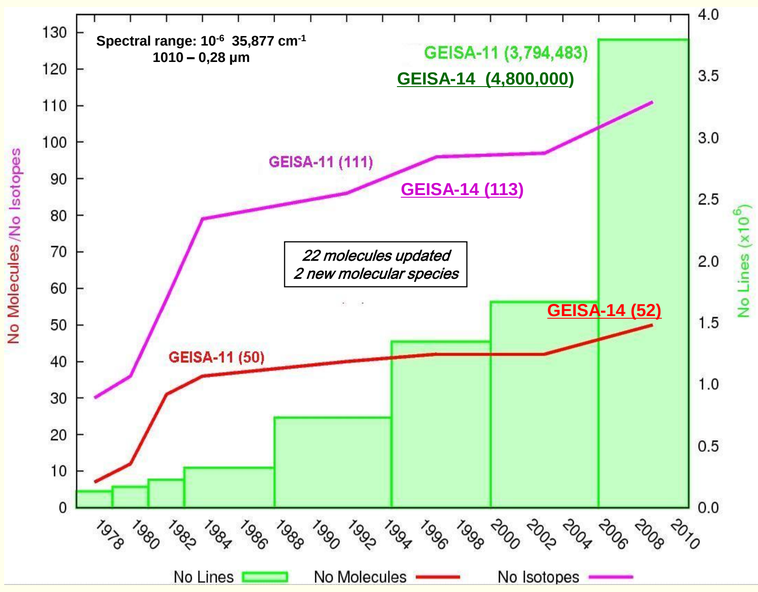
Methane monitoring



High precision simulation tools required

GEISA Reference Basis for IASI Level 1 Cal/Val activities @CNES and @LMD

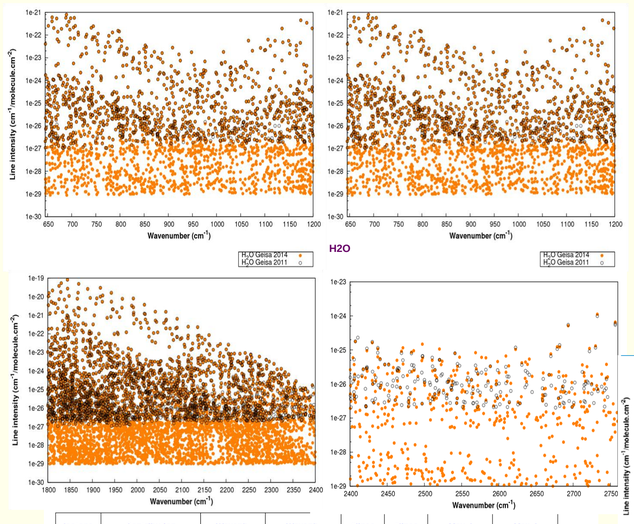
LINE PARAMETERS SUB-DATABASE
(Evolution since 1978)



22 molecular species updated for GEISA 2014 Edition

Molecule ID.	Code	Contributors
H_2O	1	L.Coudert , J. Tennyson, S. Mikhaïlenko, A.Campargue,O. Naumenko, A. Ruth, J.Orphal HDO no more considered as an isotopologue of H_2O ; individual molecule [51]
CO_2	2	R.T. Gamache
O_3	3	S. Mikhaïlenko
CH_4	6	L.R. Brown, V. Boudon, A.Campargue 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. Mikhaïlenko, O. Naumenko
SO_3(NEW)	52	J. Tennyson/

Total number of molecules in GEISA-2014: 52



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. Mikaïlenko, 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. Mikaïlenko, 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 in GEISA-2014

HDO Update for GEISA- 014 SUMMARY

IASI-NG Spectral Bands

H_2O update for GEISA-2014

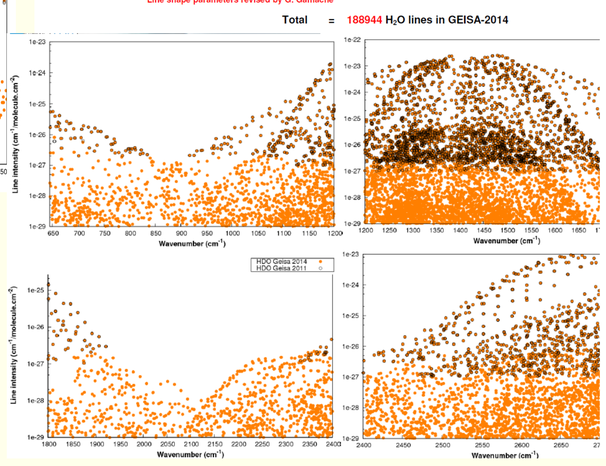
SUMMARY

9 Décembre 2014

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. Mikallenko, 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. Mikallenko, 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. Mikallenko, 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

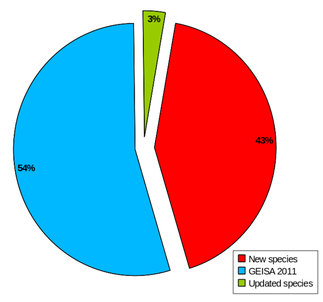
Total = 188944 H_2O lines in GEISA-2014

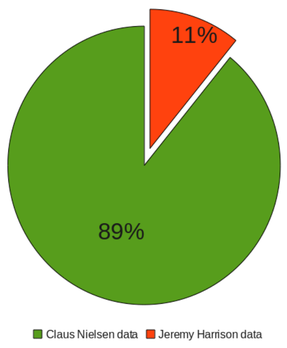


ABSORPTION IR CROSS-SECTIONS SUB-DATABASE

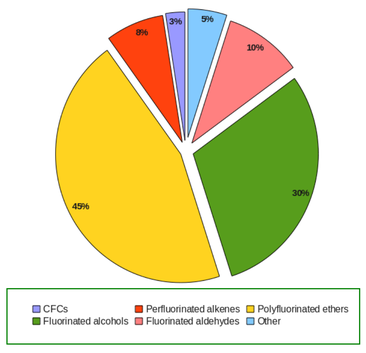
J. Harrison and P. Bernath, ASA/HITRAN conf., Aug. 2012, Reims

Ethane
Propane
Acetone
Acetonitrile
Methanol
Trifluoromethane
Acetaldehyde



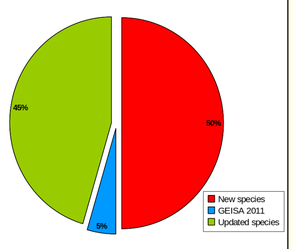


Ø. Hodnebrog, M. Etminan, J.S.Fuglestvedt, G. Marston, G. Myhre, C.J. Nielsen, et al., Rev. of Geophys., 2013



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



Beyond the 2014 GEISA Workshop

2014 GEISA WORKSHOP

Anticipating the future of Molecular Spectroscopy: context and requirements
Improving database contents

- High and very high spectral resolution laboratory measurements.
- Absorption cross sections of atmospheric trace constituents. Of particular interest are the absorption cross sections for gases with greenhouse gas potential.
- Atmospheric aerosol precursors; characterized archives on microphysical and optical properties of aerosols.
- Theoretical spectroscopy: non LTE conditions, line shape models and assessment of associated line parameters.
- Feedback from Metrology groups and from groups developing remote sensing instrumentation on latest needs to improve the precision/accuracy of spectroscopic data.

Databases evolution and user friendly access

"All-purpose" (GEISA, HITRAN, CDMS…) and molecule-specific spectroscopic databases (CDSD, SM&P, CH4…) are concerned:

- Assessment and revision of the contents of each database.
- Feedback from Metrology groups on presently available precision/accuracy of spectroscopic data and on the traceability of spectral reference line data.
- Access: dissemination, adaptability to specific needs from various communities (not necessarily dealing with remote sensing measurements)…

Call for Papers for Special Issue on New Visions of Spectroscopic Databases

Deadline for submission of manuscripts: October 15, 2015

This special issue of the Journal of Molecular Spectroscopy is on "New Visions of Spectroscopic Databases".
It evolved from contributions, discussions and conclusions of the 2014 GEISA Workshop, the aims of which were to assess the current spectroscopic databases and to enhance the interactions between experts from various disciplines, needed to meet the challenges and stringent requirements of future remote sensing instrumentation

GEISA System Distribution