The GEISA 2009 Spectroscopic Database
for Earth and Planetary Atmosphere Studies


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Atmospheric Radiation Analysis Group
Ecole Polytechnique
91128 Palaiseau, France

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


October 3-5, 2011, Reims, France
The 2009 edition of the GEISA spectroscopic database

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[1] GEISA-09 SYSTEM GENERAL CONTEXT
[2] OVERALL DESCRIPTION
[3] GEISA Contents and updates
  ▶ Individual lines sub-database
  ▶ Cross-Sections sub-database
  ▶ Aerosols sub-database

[4] APPLICATIONS
[5] EVALUATION
[6] DISTRIBUTION
The performance of the new generation of hyperspectral sounders such as AIRS in the USA and IASI in Europe, depends ultimately on the accuracy to which the spectroscopic parameters of the optically active atmospheric gases are known, since they constitute an essential input to the forward radiative transfer models that are used to interpret their observations.
Planetary examples include the recent Mars Express, Venus Express and Cassini-Huygens missions, studying the terrestrial planets and Jupiter, Saturn and Titan respectively. Numerous space-based missions continually provide a very large number of spectral observations which produce new revelations in planetology.

For remote sensing of astronomical objects, an essential prerequisite is high accuracy forward radiative transfer modeling.
FROM SATELLITE OBSERVATIONS TO CLIMATE VARIABILITY AND EVOLUTION ANALYSIS: a long process based on RadiativeTransfer

Satellite data
- Desarchiving
- Channel sélection

Data Archive → 100 To
- Cloud detection
- Spatio-temporal collocation

In situ Radiosoundings
- Desarchiving
- Quality control

Radiative Transfer Direct Models
- Clear sky or scattering medium
- Nadir or limb

Radiative Transfer Inverse Models
- Bayesian inference
- Neural Networks
- Clustering

Model/observation bias computation
- Instruments monitoring

GEISA SPECTROSCOPIC DATABASE
- Thermodynamics
- Clouds
- Greenhouse gases
- Continental surfaces
- Aerosols
- etc...

A priori infos

Scientific Themes

Courtesy A. Chédin, Trattoria/CNES
2-3 April 2008

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011
[2] Overall description

Three SUB-DATABASES

- Line transition parameters database
  - 50 molecules (111 isotopic species)
  - 3,807,997 entries in the spectral range 10^-6 and 35,877 cm^-1

- Major Permanent constituents of EARTH atmosphere: O₂, H₂O, CO₂ ...

- Trace molecules in the EARTH's atmosphere:
  - NO, SO₂, NO₂, NH₃, HNO₃, OH, HF, HCl, HBr, HI, ClO, OCS, H₂CO, PH₃

- Molecules in atmospheres of JUPITER, SATURN, URANUS, TITAN etc.:
  - CH₄, CH₃D, C₂H₂, C₂H₄, GeH₄, HCN, C₃H₈, C₃H₄

- Absorption cross-sections database
  - IR: 39 molecular species (mainly CFC's)
  - UV/Visible: 17 molecular species

Aerosol data archive and softwares

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011
GEISA-09 Line transition parameters sub-database evolution since 1978

http://ether.ipsl.jussieu.fr

N. Jacquinet-Husson et al.
DOI 10.1016/j.jqsrt.2011.06.004
GEISA-09 3,807,997 LINES

1,668,371 43%
2,139,626 57%

8 New molecular species
CH₃Br, CH₃OH, NO⁺, HNC, C₆H₆, C₂HD, CF₄, CH₃CN
# GEISA-09: Line transition content

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<th># lines</th>
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50 Molecules  111 isotopes
Total # lines  3,807,997
**Archived Spectroscopic Line Parameters**

A  Wavenumber (cm⁻¹) of the line  
B  Intensity of the line in (cm⁻¹/(molecule.cm²))  
C  Air broadening pressure halfwidth (HWHM) (*) (cm⁻¹.atm⁻¹)  
D  Energy of the lower transition level (cm⁻¹)  
E  Transition quantum identifications for the lower and upper state of the transition  
F  Temperature dependence coefficient n of the air broadening HWHM  
G  Identification code for isotope as in GEISA  
I  Identification code for molecule as in GEISA  
J  Internal GEISA code for the data identification  
K  Molecule number in HITRAN  
L  Isotope number (1=most abundant, 2=second...etc) in HITRAN  
M  Einstein A-coefficient (s⁻¹).  
N  Self broadening pressure HWHM (cm⁻¹.atm⁻¹) (for water)  
O  Air pressure shift of the line transition (cm⁻¹.atm⁻¹)  
R  Temperature dependence coefficient n of the air pressure shift  
A' Estimated accuracy (cm⁻¹) on the line position  
B' Estimated accuracy on the intensity of the line in (cm⁻¹/(molecule.cm²))  
C' Estimated accuracy on the air collision HWHM (cm⁻¹.atm⁻¹)  
F' Estimated accuracy on the temperature dependence coefficient n of the air broadening HWHM  
O' Estimated accuracy on the air pressure shift of the line transition (cm⁻¹.atm⁻¹)  
R' Estimated accuracy on the temperature dependence coefficient n of the air pressure shift  
N' Estimated accuracy on the self broadened HWHM (cm⁻¹.atm⁻¹)  
S  Temperature dependence coefficient n of the self broadening HWHM  
S' Estimated accuracy on the temperature dependence coefficient n of the self- broadening HWHM  
T  Self pressure shift of the line transition (cm⁻¹.atm⁻¹)  
T' Estimated accuracy on the self pressure shift of the line transition (cm⁻¹.atm⁻¹)  
U  Temperature dependence coefficient n of the self pressure shift  
U' Estimated accuracy on the temperature dependence coefficient n of the self pressure shift (*) HWHM: line half-width at half-maximum
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<th>Molecule</th>
<th>Spectral coverage (cm⁻¹)</th>
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39 molecular species, 647 T/P sets

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<th>Pressure range (Pa)</th>
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<td>203 - 297</td>
<td>0 - 65000</td>
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<tr>
<td>SF₅CF₃</td>
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<td>287</td>
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**Acetone (C₃H₅O)**
- 600-1800
- 214-297
- 0-93326
- 21

**PAN**
- 560-2000
- 250-297
- 100
- 3

**C₆H₆**
- 600-6300
- 223-298
- 101325
- 3

**CH₃CN**
- 624-4574
- 276-324
- 101325
- 3

- 4 new molecular species: Acetone, PAN, C₆H₆, CH₃CN
- 5 additives files for SF₅CF₃

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011
GEISA-09: UV-Vis Cross Sections content and updates

17 molecular species, 158 T/P sets

- 10 New molecular species: NO₃, HONO, CHOCHO, IO, OIO,
  C₆H₆, C₇H₈, M-xylene, O-xylene, P-xylene
- 9 updated (additive files) molecular species: NO₂, CS₂, O₃, SO₂,
  O₄, OCIO, H₂CO, OBrO, BrO

Data on microphysical and optical properties of basic aerosol components.

MICROPHYSICAL PROPERTIES
- Size distribution
- Refractive index
- Shape

4 sub-databases included

OPTICAL PROPERTIES
- Extinction coefficient
- Scattering coefficient
- Absorption coefficient
- Single scattering albedo
- Symmetry parameter
- Phase function

A database on refractive indices of basic atmospheric aerosol components (Massie, 2001)
- Solid substances
- Acids
- Water ice
- Water droplets
- Water soluble components
- Thin films
(Update underway)

A Database on atmospheric aerosols from LITMS
(Laboratory for Information Technologies and Mathematical Simulation) (Rublev, 1994)

The software package and database OPAC
(Optical Properties of Aerosols and Clouds) (Hess et al., 1998)

The Global Aerosol Data Set: GADS
(Global Aerosol Data Set) (Koepke et al., 1997)

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011
GEISA : Effective USE

IASI (Infrared Atmospheric Sounding Interferometer) on METOP
(October 19th 2006 launch)

3 Bands
[1] 645-1210 cm\(^{-1}\)
[2] 1210-2000 cm\(^{-1}\)
[3] 2000-2760 cm\(^{-1}\)

Related to
IASI Level 1 Cal/Val activities@ CNES

GEISA (599-3001 cm\(^{-1}\)) used as the reference spectroscopic database

4A/OP co-developed by LMD and Noveltis with the support of CNES (2006)]
Individual spectral lines spectroscopic parameters sub-database
Extraction of GEISA-09 in the spectral range 599 & 3001 cm⁻¹
20 molecules (66 isotopic species):
- H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, HNO₃, OCS, C₂H₂, N₂,
- HCN, NH₃, HCOOH, C₂H₄, CH₃OH, H₂CO

IR absorption cross-sections sub-database (mainly CFC’s)
6 molecular species: CFC-11, CFC-12, CFC-14, CCl₄, N₂O₅, HCFC-22
PAN (peroxyacetyl nitrate)

Microphysical and optical properties of Basic Atmospheric aerosol components sub-database

Continuous update

Related with: IASI measurement capabilities assessment

Associated interest for AIRS
Quantitative comparison between H2O intensity values in GEISA-09 and HITRAN-08

- spectral range 1400 – 2100 cm\(^{-1}\)
- 5626 transitions with common quantum identification in both databases (intensity values larger than 10\(^{-23}\) cm\(^{-1}\)/(molecule cm\(^{-2}\))
- 8% of the strong lines (intensities greater or equal 10\(^{-20}\) cm\(^{-1}\)/(molecule cm\(^{-2}\)) exhibit differences greater that 5%.
Critical evaluation of spectroscopic data quality (following)

- Search for identical transitions, in term of vibro-rotational identification (but not related with a lack of theoretical quantum differentiacion).

- Results of comparisons between simulations (using the LMD radiative transfert code 4A -Scott and Chédin, J. Appl. Met., 1981) and IASI observations.

«Simulations-Observations»
Differences

- Observations over sea (Spectral Interval : 800 – 900 cm⁻¹)
- IASI brightness temperature
- H₂O case; 2003 and 2009 Versions of GEISA/IASI
- July 2007- November 2009 period.

→ What would be obtained with IASI-NG?
FROM CONCLUSIONS OF VALIDATION WITH THE 4A/OP LINE
By LINE RADIATIVE TRANSFER MODEL

- The water vapour spectroscopic parameters: still need to be validated
- The water vapour continuum: more tuning to be done when more validation data (especially with high water vapor content) become available
- The freons bands at 850 and 920 cm⁻¹: refine the temperature dependence
- O₃ in the 9.6 μm region: the spectroscopic parameters still need to be validated
- Some CO₂ – Q, P and R branches: further improvement/tuning of the line mixing

Non exhaustive list
General Spectroscopic Requirement to achieve Forward Model accuracies required for retrievals from IASI and future sounders

Considering the still existing Spectroscopy issues, the following already ongoing specific actions have to be reinforced and maintained:

- **Necessary validation**: Assessment in GEISA/IASI of:
  - spectroscopic molecular species related to IASI trace gas retrievals: HCN, NH₃, HCOOH, C₂H₄, CH₃OH, H₂CO.
  - cross-sections: CFC-11, CFC-12, CFC-14, CCl₄, N₂O₅, HCFC-22 and especially PAN.

- **The still outstanding general spectroscopy-related conclusions for public databases, from ISSWG June 30th - July 2nd 2008, CNES, Paris, France-, to be considered**:
  - Comparison with HITRAN and GEISA, in particular for water vapour, and real IASI spectra, compared to simulations with ECMWF provided radiosondes, lead to the conclusion that:
    - in particular water vapour needs to be validated, and the continuum reinvestigated.
    - IASI related spectroscopy problems with H₂O and CO₂ as first priority

- **Line coupling/mixing modelling (works in progress at LISA)**, (which should be used in conjunction with the molecular data base from which they have been derived) and non-LTE (Local Thermodynamic Equilibrium) effects are areas to be urgently investigated.
[5] REMAINING SPECTROSCOPY RELATED PROBLEMS (following)

NEEDS IN SPACE STUDIES OF OUTER PLANETS AND TITAN
(Courtesy of Athena Coustenis and Bruno Bézard)

- CH$_4$ and CH$_3$D: in the near-infrared region (from 0.8 to 1.3 µm) both from theory and laboratory measurements
  - CH$_3$D: bands around 2 µm
    - Far wings line profiles broadened by N$_2$ at low temperature
- C$_6$H$_2$: at 621 cm$^{-1}$; this band is being studied by Jolly and Bénilan (LISA)
- C$_4$N$_2$: at 472 cm$^{-1}$ (CIRS interest)
- C$_3$H$_6$: needs of bands at 869, 922, 1053 and 1158 cm$^{-1}$
- C$_3$H$_4$: (allene)
- C$_2$H$_6$: need of the spectroscopic parameters for the 1400-1500 cm$^{-1}$ band
  - (observed on Jupiter & Titan), full analysis is ongoing
- For molecules heavier than C$_2$H$_6$ (like C$_6$H$_2$, HC$_5$N) there’s still few data
- CO$_2$ related with VENUS atmosphere:
  - complementary data needed at 1.0, 1.1 and 1.18 µm
  - investigation of continuum

Non exhaustive list

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011
For Titan and the giant planets:

- **Nitriles:**
  - $\text{C}_2\text{N}_2$: no data on the combination band at 735 cm$^{-1}$ (which interferes with $\text{C}_2\text{H}_2$ and $\text{C}_3\text{H}_8$).
  - $\text{CH}_3\text{CN}$ (acetonitrile has been observed in the millimeter range, but also has bands in the mid and far IR)
  - Other nitriles: propionitrile etc...

- **Intensities:**
  - Few things exist in the area (submm) covered by FP1/CIRS on Cassini.
  - Work in progress at LISA laboratory on $\text{C}_2\text{N}_2$ and $\text{C}_4\text{H}_2$.
  - Needs also on: $\text{HC}_3\text{N}$, $\text{C}_6\text{H}_2$, $\text{HC}_5\text{N}$, $\text{C}_4\text{N}_2$.
  - Perhaps also redo intensities on methylacetylene.

For Saturn

$\text{PH}_3$: has improved but further work would be appreciated
Welcome to the Ether website

This website offers various products of French activities linked to the products (see "Login Request"). More information...

Databases

GEISA
RAMCES
ECCAD
Mozac
NDACC
Kinetics

Data

IASI
MIMOSA
ADOMOCA
REPROMUS
Balloon

Services

ARLETY
GIRAFE
Software

Projects

Strapline
GROMON

Ether Products and Services Centre Facilities

http://ether.ipsl.jussieu.fr
GEISA 2009 : Interactive distribution system
http://ether.ipsl.jussieu.fr

The current 2009 edition of GEISA (GEISA-09) is a system comprising three independent sub-databases devoted respectively to:

- **Line transition parameters**
- **Absorption cross-sections**
- **Microphysical and optical properties of atmospheric aerosols (same as GEISA03)**

**GEISA-09 Description**

**GEISA-09 Database Access**

- Interactive access
- FTP access

- R
- UV, VIS

Aerosols
GEISA 2009: Interactive distribution system
Line transition parameters (interactive access)
GEISA 2009: Interactive distribution system
Line transition parameters (interactive access)

GEISA 2009: Lines
- Information
- Content analysis
- Histogram analysis
- Database extract
- Transition analysis
- Transition list

Transition list

Database extract

Histogram analysis

Output file
GEISA09 Lines : Transition List Results

Reading database...

nbr records in this bin file : 3807997

***************
* geisa  geisa *
*  tr  *
* geisa  geisa *
***************

available transitions in geisa2009
spectral interval (cm-1) nu1= 5935.000000  nu2= 7000.000000

extraction of the following molecules and isotopes

3) molecule : o3     quantum number : V1,V2,V3

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The file contains 7789 lines in the spectral range nu1= 5935.000000 and nu2= 7000.000000 cm-1
GEISA 2009: Interactive distribution system
Cross sections + Aerosols

Cross sections

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Aerosols

Table 1: Complex indices of refraction - m-p-iq of basic aerosol components

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<td>Soot</td>
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<td>Volcanic ash</td>
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<tr>
<td>Water-soluble particles</td>
<td>w_s ref</td>
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See headers of data file for format and content description.

Spectroscopy and dynamics of ozone and related atmospheric species, REIMS, FRANCE, 3-5 October 2011.
ACKNOWLEDGMENTS
to
CNES, CNRS/INSU and EUMETSAT
for their Encouragements and Supports

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