Molecular Spectroscopy for Remote Sensing of Planetary Atmospheres Radiative Properties: the GEISA Spectroscopic Database

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OUTLINE

[1] GEISA-11 SYSTEM GENERAL CONTEXT


[3] GEISA and IASI ATMOSPHERIC SOUNDED IMPLICATION

[4] CRITICAL EVALUATION OF SPECTROSCOPIC DATA QUALITY (Examples)

[5] GEISA INTERACTIVE FREE DISTRIBUTION
- **Spectroscopy** is at the root of modern planetology, enabling to determine the physical properties of planets remotely.

- **GEISA** is a computer-accessible Spectroscopic Database designed for accurate forward atmospheric radiative transfer calculations using a line-by-line (atmospheric) layer-by-layer approach.

  spectral range $10^{-6} - 35,877 \, \text{cm}^{-1}$
  $10^{10} - 0.28 \, \mu m$

**GEISA: Gestion et Etude des Informations Spectroscopiques Atmosphériques**
management and study of atmospheric spectroscopic information
Three SUB-DATABASES

- **Line parameters sub-database**
  - 50 molecules (111 isotopic species)
  - 3,794,483 entries in the spectral range 10^{-6} and 35,877 cm^{-1}

  - Major permanent constituents of EARTH atmosphere: O_{2}, H_{2}O, CO_{2} ...
  - Trace molecules in EARTH atmosphere: NO, SO_{2}, NO_{2}, NH_{3}, HNO_{3}, OH, HF, HCl, HBr, HI, ClO, OCS, H_{2}CO, PH_{3} ...
  - Molecules in atmospheres of JUPITER, SATURN, URANUS, TITAN etc.: CH_{4}, CH_{3}D, C_{2}H_{2}, C_{2}H_{4}, GeH_{4}, HCN, C_{3}H_{8}, C_{3}H_{4}

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

- **Microphysical and optical properties of atmospheric Aerosols sub-database**
The performance of the new generation of hyperspectral Earth atmosphere 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.

AIRS: Advanced Infrared Sounding
IASI: Infrared Atmospheric Sounding Interferometer
FROM SATELLITE OBSERVATIONS TO CLIMATE VARIABILITY AND EVOLUTION ANALYSIS: a long process based on Radiative Transfer

Satellite data
- Desearching
- Channel sélection

In situ Radiosoundings
- Desearching
- Quality control

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

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

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

Scientific Themes

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

IRS-2012, Dahlem Cube, Berlin, Germany, 06 – 12 August 2012
## [2-a] GEISA-11: Line Parameters Sub-database Content

<table>
<thead>
<tr>
<th>Mole</th>
<th>Spectral range (cm⁻¹)</th>
<th># lines</th>
<th>Mole</th>
<th>Spectral range (cm⁻¹)</th>
<th># lines</th>
<th>Mole</th>
<th>Spectral range (cm⁻¹)</th>
<th># lines</th>
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<td>413,524</td>
<td>HI</td>
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<td>HF</td>
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<td>CF₄</td>
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<td>CH₃CN</td>
<td>880.052 - 1,650.000</td>
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</tr>
</tbody>
</table>

50 Molecules  111 isotopes  
Total # lines  3,794,483

IRS-2012, Dahlem Cube, Berlin, Germany, 06 – 12 August 2012

http://ether.ipsl.jussieu.fr
# GEISA-11 Line Transition Records

<table>
<thead>
<tr>
<th>252 characters Record</th>
<th>31 Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A) Wavenumber (cm(^{-1})) of the line associated with the vibro-rotational transition</td>
<td></td>
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<tr>
<td>(B) Intensity of the line (cm molecule(^{-1}) at 296K)</td>
<td></td>
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<tr>
<td>(C) Air broadening pressure halfwidth (HWHM) * (cm(^{-1}) atm(^{-1}) at 296K)</td>
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<tr>
<td>(D) Energy of the lower transition level (cm(^{-1}))</td>
<td></td>
</tr>
<tr>
<td>(E) Transition quantum identifications for the lower and upper levels of the transition</td>
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<tr>
<td>(F) Temperature dependence coefficient (n) of the halfwidth</td>
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<tr>
<td>(G) Identification code for isotope</td>
<td></td>
</tr>
<tr>
<td>(I) Identification code for molecule</td>
<td></td>
</tr>
<tr>
<td>(J) Internal GEISA code for data identification</td>
<td></td>
</tr>
</tbody>
</table>

| (N) Self broadening pressure halfwidth (HWHM) (cm\(^{-1}\)atm\(^{-1}\)) at 296K |
| (O) Air pressure shift of the line transition (cm\(^{-1}\)atm\(^{-1}\)) at 296K |

(*) HWHM: line half-width at half-maximum

**Standardized parameter missing values**
GEISA and IASI Atmospheric Sounding Implication

From GEISA-11 to GEISA/IASI-11

- Individual spectral lines spectroscopic parameters sub-database
  - Extraction of GEISA-11 in the spectral range 599 & 3001 cm\(^{-1}\)
  - 20 molecules (66 isotopic species):
    - 14 molecules (53 isotopic species) selected for operational meteorology: \(\text{H}_2\text{O}, \text{CO}_2, \text{O}_3, \text{N}_2\text{O}, \text{CO}, \text{CH}_4, \text{O}_2, \text{NO}, \text{SO}_2, \text{NO}_2, \text{HNO}_3, \text{OCS}, \text{C}_2\text{H}_2, \text{N}_2\)
    - 6 molecules (13 isotopic species) selected for IASI trace gas retrievals: \(\text{HCN}, \text{NH}_3, \text{HCOOH}, \text{C}_2\text{H}_4, \text{CH}_3\text{OH}, \text{H}_2\text{CO}\)

- IR absorption cross-sections sub-database (mainly CFC’s)
  - 6 molecular species: CFC-11, CFC-12, CFC-14, CC\(_4\text{N}_2\text{O}_5\), 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

IRS-2012, Dahlem Cube, Berlin, Germany, 06 – 12 August 2012
GEISA : Effective Use

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

3 Spectral Bands

1. 645 - 1210 cm\(^{-1}\)
   15.50 – 8.26 μm

2. 1210 - 2000 cm\(^{-1}\)
   8.26 – 5.0 μm

3. 2000 - 2760 cm\(^{-1}\)
   5.0 – 3.62 μm

Related to

IASI Level 1 Cal/Val activities @ CNES and @ LMD

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

  4A/OP co-developed by LMD and Noveltis with the support of CNES (2006)]
Evaluation of the impact of H$_2$O spectroscopic archive on IASI radiative transfer modelling

- Radiative transfer simulations with ARA/ABC(t)/LMD radiative transfer models in their latest versions
  - **STANSAC**: line-by-line and layer-by-layer model
    [N.A. Scott, 1974, JQSRT, 14, 691-707]
  - **4A**: (Automatized Atmospheric Absorption Atlas); fast and accurate line-by-line radiative transfer model

- Selected Spectroscopic Databases


  **HITRAN** [Rothman L.S. et al. JQSRT 110 (2009) 533-572] its latest revision

Differences in spectroscopic parameters archives and subsequent IASI radiative transfer modelling, in terms of **Brightness Temperature (K) differences $\Delta BT (K)$**
H₂O Spectroscopy Differences Illustration (1)

IASI brightness temperature BT (K) simulation with GEISA
Differences in BT(K) using GEISA or HITRAN
Evaluation of spectroscopic parameters individual impact on IASI BT modelling differences (2)

IASI Band 3 (15.50 - 8.26 μm)

HWHM impact evaluation

![Graph showing differences in BT measurements for IASI Band 3](image)
H₂O : ΔBT [GEISA - GEISA with HWHM from HITRAN]

H₂O : Content differences for HWHM [GEISA – HITRAN]

For GEISA and HITRAN common lines with intensities > 10⁻²³ cm molecule⁻¹ at 296 K
H₂O Spectroscopy Differences Illustration (4)

For IASI-NG: Spectral Resolution X 2 and Noise divided by 2 comparing with IASI
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

(Restricted to EARTH atmosphere)
CONCLUSIONS FROM THE 2nd INTERNATIONAL IASI CONFERENCE, SEVRIER, France, 25-29 JANUARY 2010

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 of HITRAN or GEISA modelling and real IASI spectra 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 parameters of the data base from which they have been derived) and **non-LTE (Local Thermodynamic Equilibrium) effects** are areas to be urgently investigated.
The GEISA spectroscopic database: Current and future archive for Earth and planetary atmosphere studies

N. Jacquinet-Husson a, *, N.A. Scott a, A. Chédin a, L. Crépeau a, R. Armante a, V. Capelle a, J. Orphal b, A. Coustenis b, C. Boonne d, N. Poulet-Crovisier d, A. Barbe e, M. Birk f, L.R. Brown g, C. Camy-Peyret h, C. Claveau h, K. Chance i, N. Christidis i, G. Chirokov i, M. Dufresne j, P. Drouin j, S. Eglington j, K. Fernandez-Jambrina k, M. Flaud k, R.A. Toth l, J.-M. Flaud m, A. Goldman m, A. Maki m, S. Mikhaiilenko m, C.E. Miller m, T. Mishina m, N. Moazzen-Ahmadi m, H.S.P. Müller m, A. Nikitin m, J. Orphal m, V. Perevalov o, A. Perrin f, D.T. Petkie w, A. Predoi-Cross x, C.P. Rinsland y, J.J. Remedios z, M. Rotger c, M.A.H. Smith y, K. Sung i, S. Tashkun i, J. Tennyson o, R.A. Toth i, A.-C. Vandaele k, J. Vander Auwera n

The 2003 edition of the GEISA/IASI spectroscopic database

N. Jacquinet-Husson a, *, N.A. Scott a, A. Chédin a, L. Crépeau a, R. Armante a, V. Capelle a, J. Orphal b, A. Coustenis b, C. Boonne d, N. Poulet-Crovisier d, A. Barbe e, M. Birk f, L.R. Brown g, C. Camy-Peyret h, C. Claveau h, K. Chance i, N. Christidis i, G. Chirokov i, M. Dufresne j, P. Drouin j, S. Eglington j, K. Fernandez-Jambrina k, M. Flaud k, R.A. Toth l, J.-M. Flaud m, A. Goldman m, A. Maki m, S. Mikhaiilenko m, C.E. Miller m, T. Mishina m, N. Moazzen-Ahmadi m, H.S.P. Müller m, A. Nikitin m, J. Orphal m, V. Perevalov o, A. Perrin f, D.T. Petkie w, A. Predoi-Cross x, C.P. Rinsland y, J.J. Remedios z, M. Rotger c, M.A.H. Smith y, K. Sung i, S. Tashkun i, J. Tennyson o, R.A. Toth i, A.-C. Vandaele k, J. Vander Auwera n

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GEISA 2011 Lines : Database Content

**Information**
Main information of the database to identify for each molecule, the different isotopologues and the corresponding number of lines between a Lower Bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹) with a sampling step : DN (cm⁻¹).

**Content analysis**
Quick analysis of the database contents in any selected spectral range between a Lower Bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹) with a sampling step : DN (cm⁻¹). Default value for sampling step : DN=N2-N1; only one analysis between N1 and N2.

**Histogram analysis**
Plots of intensity (field E) and/or ground level (field D) histograms for one isotopologue of a given molecule in any selected spectral range between a Lower Bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹) with a sampling step : DN (cm⁻¹). Default value for sampling step : DN=N2-N1; only one set of histograms between N1 and N2. No isotopologue specification means considering all the isotopologues of the molecule.

**Database extract**
Extraction of the database contents in any selected spectral range between a Lower bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹) for one or more molecule(s) and isotopologue(s). Extraction of all the isotopologues of a molecule if no isotopologue specification.

**Transition analysis**
Extraction of a set of vib-rotational transitions involved in a specified vibrational transition of one given molecule and a choice of its isotopologues (one or more), in any selected spectral range between a Lower Bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹).

**Transition list**
Complete description of existing vibrational transitions in any selected spectral range between a Lower Bound : N1 (cm⁻¹) and an Upper Bound : N2 (cm⁻¹) for one or more molecule(s).
### July 2012 (see details)

- Line parameters GEISA 2011 sub-database : Supplemental data are now available for molecules: \( \text{H}_2\text{O}, \text{CO}_2, \text{PH}_3, \text{OCS}, \text{H}_2\text{CO} \) and \( \text{SF}_6 \)

### April 2012 (see details)

- GEISA 2009 becomes GEISA 2011.
- Line parameters GEISA 2011 sub-database : slight corrections have been made concerning essentially parameters \( E_3, E_4, E_5 \) for molecules \( \text{H}_2\text{O}, \text{CO}_2, \text{CH}_3\text{CN} \).

### January 2012 (see details)

- The "Transition analysis " option, in the interactive access page, has been improved.

### December 2011 (see details)

- New UV \( \text{O}_2\text{O}_2 \) and \( \text{O}_2\text{H}_2 \) cross-sections files have been added.
- Line parameters GEISA 2011 sub-database : slight corrections have been made concerning essentially parameters \( E_3, E_4, E_5, M \) and \( O \) (GEISA 2011 format for line transition parameters) for molecules \( \text{H}_2\text{O}, \text{CO}_2, \text{N}_2\text{O}, \text{CH}_4, \text{NO}, \text{SO}_2, \text{PH}_3, \text{OH}, \text{HCl, HBr, HI}, \text{HNC}, \text{COF}_2, \text{OCS}, \text{CINO}_2, \text{CF}_6 \) and \( \text{CH}_3\text{CN} \).
ACKNOWLEDGMENTS

to
CNES, CNRS/INSU and EUMETSAT
for their Encouragements and Supports

THANK YOU FOR YOUR ATTENTION