A tool for IASI hyperspectral remote sensing applications: The GEISA/IASI database in its latest edition

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OUTLINE

[1] GEISA SYSTEM GENERAL CONTEXT AND IASI SOUNDING IMPLICATION

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

[3] TOWARDS IASI/NG

[4] GEISA/IASI INTERACTIVE DISTRIBUTION

[5] CONCLUDING COMMENTS
Spectroscopy is at the root of modern planetology, enabling to determine the physical properties of planets remotely.

**GEISA**

Gestion et Étude des Informations Spectroscopiques Atmosphériques; Management and Study of Atmospheric Spectroscopic Information

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

$1010 - 0.28 \, \mu\text{m}$

Line parameters sub-database
3,794,426 entries
50 molecules (111 isotopic species)

Absorption cross-sections sub-database
IR: 39 molecular species
UV/Visible: 17 molecular species

Microphysical and optical properties of atmospheric Aerosols sub-database

GEISA 2013 UPDATE UNDERWAY
Individual spectral lines spectroscopic parameters sub-database

- 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:
    - $\text{CFC-11}$, $\text{CFC-12}$, $\text{CFC-14}$, $\text{CCl}_4$, $\text{N}_2\text{O}_5$, $\text{HCFC-22}$
    - $\text{PAN}$ (peroxyacetyl nitrate)

- Microphysical and optical properties of Basic Atmospheric aerosol components sub-database
The GEISA spectroscopic database: Current and future archive for Earth and planetary atmosphere studies


The 2003 edition of the GEISA/IASI spectr

N. Jacquinet-Husson, N.A. Scott, A. Chédin, K. Gari

The 2009 edition of the GEISA spectroscopic database

**Archived Spectroscopic Line Parameters**

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Wavenumber (cm(^{-1})) of the line</td>
</tr>
<tr>
<td>B</td>
<td>Intensity of the line in (cm(^{-1})/(molecule.cm(^{-2}))</td>
</tr>
<tr>
<td>C</td>
<td>Air broadening pressure halfwidth (HWHM)(*) (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>D</td>
<td>Energy of the lower transition level (cm(^{-1}))</td>
</tr>
<tr>
<td>E</td>
<td>Transition quantum identifications for the lower and upper state of the transition</td>
</tr>
<tr>
<td>F</td>
<td>Temperature dependence coefficient n of the air broadening HWHM</td>
</tr>
<tr>
<td>G</td>
<td>Identification code for isotope as in GEISA</td>
</tr>
<tr>
<td>I</td>
<td>Identification code for molecule as in GEISA</td>
</tr>
<tr>
<td>J</td>
<td>Internal GEISA code for the data identification</td>
</tr>
<tr>
<td>K</td>
<td>Molecule number in HITRAN</td>
</tr>
<tr>
<td>L</td>
<td>Isotope number (1=most abundant. 2= second…etc) in HITRAN</td>
</tr>
<tr>
<td>M</td>
<td>Einstein A-coefficient (s(^{-1})).</td>
</tr>
<tr>
<td>N</td>
<td>Self broadening pressure HWHM (cm(^{-1})atm(^{-1})) (for water)</td>
</tr>
<tr>
<td>O</td>
<td>Air pressure shift of the line transition (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>R</td>
<td>Temperature dependence coefficient n of the air pressure shift</td>
</tr>
<tr>
<td>A′</td>
<td>Estimated accuracy (cm(^{-1})) on the line position</td>
</tr>
<tr>
<td>B′</td>
<td>Estimated accuracy on the intensity of the line in (cm(^{-1})/(molecule.cm(^{-2}))</td>
</tr>
<tr>
<td>C′</td>
<td>Estimated accuracy on the air collision HWHM (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>F′</td>
<td>Estimated accuracy on the temperature dependence coefficient n of the air broadening HWHM</td>
</tr>
<tr>
<td>O′</td>
<td>Estimated accuracy on the air pressure shift of the line transition (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>R′</td>
<td>Estimated accuracy on the temperature dependence coefficient n of the air pressure shift</td>
</tr>
<tr>
<td>N′</td>
<td>Estimated accuracy on the self HWHM</td>
</tr>
<tr>
<td>T</td>
<td>Self pressure shift of the line transition (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>T′</td>
<td>Estimated accuracy on the self pressure shift of the line transition (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>U</td>
<td>Temperature dependence coefficient n of the self pressure shift</td>
</tr>
<tr>
<td>U′</td>
<td>Estimated accuracy on the temperature dependence coefficient n of the self pressure shift broadened HWHM (cm(^{-1})atm(^{-1}))</td>
</tr>
<tr>
<td>S</td>
<td>Temperature dependence coefficient n of the self broadening HWHM</td>
</tr>
<tr>
<td>S′</td>
<td>Estimated accuracy on the temperature dependence coefficient n of the self- broadening</td>
</tr>
</tbody>
</table>

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

Since GEISA-09

Standardized parameter
missing values
CRITICAL EVALUATION OF SPECTROSCOPIC DATA QUALITY (Examples)

Selected molecules:

- [2-a] $\text{H}_2\text{O}$ GEISA-11 and HITRAN-08 comparison
- [2-b] $\text{CH}_4$ (including $\text{CH}_3\text{D}$) GEISA-11 and GEISA-03
Critical Evaluation of Spectroscopic Data Quality

Evaluation of the impact of $\text{H}_2\text{O}$ spectroscopic archive on IASI radiative transfer modelling

- Radiative transfer simulations with ARA/ABC(t)/LMD radiative transfer models in their latest versions
  - STRANSAC; 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

Differences in spectroscopic parameters archives and subsequent IASI radiative transfer modelling, in terms of Brightness Temperature (K) differences $\Delta \text{BT (K)}$
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%.

[2] Quantitative comparison between H\(_2\)O intensity values in GEISA-11 and HITRAN-08
[2-a] H$_2$O Spectroscopy Differences Illustration

IASI brightness temperature BT (K) simulation with GEISA

Differences in BT(K) using GEISA or HITRAN

H$_2$O unique absorbant
[2-a] Evaluation of spectroscopic parameters individual impact on IASI BT modelling differences

IASI Band 1 \((15.50 - 8.26 \, \mu m)\)

Intensity impact evaluation

\[ \Delta BT \, \text{in K} \]

\[ \text{Wavenumbers (cm}^{-1}) \]

- \(TB_G - TB_H\)
- \(TB_G - TB_G\) with H intensities
- \(TB_G - TB_G\) with H HWHM

IASI Noise
[2-a] Evaluation of spectroscopic parameters individual impact on IASI BT modelling differences

IASI Band 3 (15.50 – 8.26 µm)  

HWHM impact evaluation

Differences due to other parameters

\[ \Delta BT \text{ in K} \]

\[ 2000 \quad 2050 \quad 2100 \quad 2150 \quad 2200 \]

Wavenumbers (cm\(^{-1}\))

\( \text{TB}_G - \text{TB}_H \)

\( \text{TB}_G - \text{TB}_G \text{ with H intensities} \)

\( \text{TB}_G - \text{TB}_G \text{ with H HWHM} \)
[2-a] H$_2$O Spectroscopy Differences Illustration

For GEISA and HITRAN common lines with intensities $> 10^{-23}$ cm$^{-1}$/molecule cm$^{-2}$ at 296 K
IASI brightness temperature BT (K) simulation with GEISA: H$_2$O, O$_3$, O$_2$, CO, CH$_4$ and N$_2$O

Differences in BT(K) using GEISA 2011 and GEISA 2003
Impact evaluation of CH$_4$ update on IASI BT modelling differences (1)
Impact evaluation of CH$_4$ update on IASI BT modelling differences (2)

Comparison of intensity perturbations impact with IASI noise

Calculated intensity variation threshold
Wavenumber = 1300 cm⁻¹

- For 1% intensity perturbed => ΔTB=0.1334 K
- For 3% intensity perturbed => ΔTB=0.3992 K
- Noise = 0.1610 K

=> ?? % intensity perturbation.
Impact evaluation of CH$_4$ update on IASI BT modelling differences (3)

Comparison of intensity perturbations impact with IASI noise

Calculated intensity variation threshold

Intensity variation threshold in %

Wavenumbers (cm$^{-1}$)

ΔTB CH$_4$ int

ΔTB CH$_4$ int + 3%

Intensity differences (G11–G03) in %
[3] TOWARDS IASI/NG
[3-a] H_2O Spectroscopy Differences Illustration

**H_2O : ΔBT [GEISA-GEISA with HWHM from HITRAN]**

- With IASI noise display

For IASI-NG: Spectral Resolution X 2 and Noise divided by 2 comparing with IASI
[3-b] CH$_4$ Spectroscopy Differences Illustration

$\Delta$BT [GEISA 2011-GEISA 2011 with CH$_4$ from GEISA 2003] with IASI noise display

For IASI-NG: Spectral Resolution X 2 and Noise divided by 2 comparing with IASI
GEISA/IASI INTERACTIVE DISTRIBUTION

Ether Atmospheric Chemistry Data Centre
CNES/CNRS/IPSL


Close cooperation with Cathy Boonne and Nathalie Poulet-Crovisier
[4] GEISA SYSTEM COMPREHENSIVE DISTRIBUTION


Atmospheric Chemistry
Data Centre

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Atmospheric Data

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Daily Modelisation and Forecast

- Mimosa - Reprobus - Acomida

Spectroscopic data and Kinetics

- GEISA - Kinetics
Adequate tools are required to perform reliable radiative transfer modelling calculations to meet the needs of communities involved in understanding the atmospheres of the Earth and other planets. Among these tools, compilations of spectroscopic parameters are used for a vast array of applications and especially for planetary atmospheric models. In this context, since over three decades, the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie Dynamique) has developed the GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Information) computer-accessible database system (Chédin et al., 1982; Husson et al., 1992; Jaquet-Husson et al., 1999, 2008, 2011). This forward calculation of atmospheric radiative transfer using a line-by-line and (atmospheric) layer-by-layer approach. This effort has proven to be beneficial to the atmospheric scientific community participating in direct and inverse radiative transfer studies.

The role of molecular spectroscopy in modern atmospheric research has entered a new phase with the advent of highly sophisticated spectroscopic instruments and computers. For example, the performance of Earth atmospheric sounders like AIRS in the USA, and IASI in Europe, which have a better vertical resolution and accuracy, compared to the previous existing satellite infrared vertical sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases, since these are essential input in the forward models used to simulate recorded radiance spectra. Consequently, a strong demand exists for highly comprehensive, well validated, efficiently operational, and desirably interactive computer-based spectroscopic databases to benefit the research in direct and inverse radiative transfer.

In this purpose, GEISA is currently involved in activities related to the assessment of the capabilities IASI through the GEISA/IASI database, extensively described in Jaquet-Husson et al. (2005). Since the Metop European polar satellite launch (October 19th 2006), GEISA-IASI is the reference spectroscopic database for the validation of the level-1 IASI data, using the 4A (Automated Atmospheric Absorption Atlas) radiative transfer model (Scott, 1974; Scott and Chédin, 1981; 4A/LMD, 4A/CP co-developed by LMD and Noveltis with the support of CNES).
GEISA : ETHER distribution
Database access page

GEISA09 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 : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) with a sampling step : DNU (cm⁻¹).

Content analysis
Quick analysis of the database contents in any selected spectral range between a Lower Bound : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) with a sampling step : DNU (cm⁻¹). Default value for sampling step : DNU= NU2-NU1, only one analysis between NUI and NU2.

Histogram analysis
Plots of intensity (field B) and/or ground level (field D) histograms for one isotope of a given molecule, in any selected spectral range between a Lower Bound : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) with a sampling step : DNU (cm⁻¹).
Default value for sampling step : DNU= NU2-NU1 : only one series of histograms between NUI and NU2. No isotope specification means considering all the isotopes of the molecule.

Database extract
Extraction of the database contents in any selected spectral range between a Lower Bound : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) for one or more molecule(s) and isotope(s). Extraction of all the isotopes of a molecule if no isotope specification.

Transition analysis
Extraction of a set of vibro-rotational transitions involving one 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 : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹).

Transition list
Complete description of existing vibrational transitions in any selected spectral range between a Lower Bound : NUI (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) for one or more molecule(s).

3 Sub-databases :
- Line by line
- Cross sections
- Aerosols

Line by line sub-database :
- Content description
  - General content
  - Format description
  - Overall description

- Data access (FTP)

- Data access (Interactive)
  - Information
  - Content analysis
  - Histogram analysis
  - Database extract
  - Transition analysis
  - Transition list
3rd IASI Conference, Hyères, France, 4–8 February 2013

GEISA: ETHER distribution
Graphical Tools

Descriptions of updates and changes related to GEISA

GEISA data archives and facility tools


The role of molecular spectroscopy in modern atmospheric research has entered a new phase with the advent of highly sophisticated spectroscopic instruments and computers. For example, the performance of Earth atmospheric sounders like AIRS, in the USA, and IASI in Europe, which have a better vertical resolution and accuracy compared to the previous existing satellite infrared vertical sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases, since these are essential input in the forward models used to simulate observed radiance spectra. Consequently, a strong demand exists for highly comprehensive, well validated, efficiently operational, and desirable interactive computer-based spectroscopic databases to benefit the research in direct and inverse radiative transfer.

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[5] CONCLUDING COMMENTS
GEISA: ETHER distribution
Graphical Tools

- Global positions of transitions
- Database content
- Databases comparison
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
- \(\text{O}_3\) in the 9.6 \(\mu\text{m}\) region: the spectroscopic parameters still need to be validated
- Some \(\text{CO}_2/\text{CH}_4\) – Q, P and R branches: further improvement/tuning of the line mixing

NON EXHAUSTIVE LIST

(Restricted to EARTH atmosphere)
General Spectroscopic Requirement to achieve Forward Model accuracies required for retrievals from IASI and future sounders (specific actions 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.
ACKNOWLEDGMENTS

CNES, CNRS/INSU, EUMETSAT, and Ether (Atmospheric Chemistry data Centre) for their encouragements and supports.

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