ASSESSMENT OF THE GEISA AND GEISA/IASI SPECTROSCOPIC DATA QUALITY: through comparisons with other public database archives

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Diapositive 1

<table>
<thead>
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<th>husson; 14/10/2005</th>
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<td>h18</td>
<td>husson; 14/10/2005</td>
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OUTLINE

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II) DATABASE FORMATS

III) UPDATING SPECTROSCOPIC PARAMETERS: examples of issues

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2) Differences between GEISA (GEISA/IASI-03) and HITRAN-04
3) Differences between GEISA(GEISA/IASI-03) and MIPAS-03

IV) EVALUATION OF THE IMPACT OF SPECTROSCOPIC ARCHIVE DIFFERENCES ON RADIATIVE TRANSFER SIMULATIONS

V) CONCLUDING COMMENTS
Data bases involved in comparisons

- **GEISA**

- **GEISA/IASI-03**

- **HITRAN-04**
  Rothman et al. JQSRT 96 (2005) 139-204.

- **MIPAS Dedicated Spectroscopic Database**

*Evaluation of the differences in contents and subsequent radiative transfer modelling impacts*
DATABASES OVERVIEW
The GEISA-2003 system

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

Three SUB-DATABASES

- Line transition parameters database
  - 42 molecules (96 isotopic species)
  - 1,668,371 entries between 0 and 35,877 cm⁻¹

- Absorption cross-sections database
  - IR: 32 molecular species (mainly CFC’s)
  - UV/Visible: 11 molecular species

- Aerosol data archive and softwares

ASSOCIATED MANAGEMENT SOFTWARES
(For each sub-database)
### SUMMARY CONTENTS OF HITRAN-04 AND GEISA-03 INDIVIDUAL LINE LISTS

<table>
<thead>
<tr>
<th>Molecule</th>
<th>GEISA-03 # lines</th>
<th>HITRAN-04 # lines</th>
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<tr>
<td>H2O</td>
<td>58726</td>
<td>63196</td>
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<td>CO2</td>
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<td>O3</td>
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<tr>
<td>NO+</td>
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<th>Molecule</th>
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<th>HITRAN-04 # lines</th>
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<tr>
<td>C2H6</td>
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<td>CH3D</td>
<td>35518</td>
<td>isotope of CH4</td>
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<td>C2H2</td>
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<td>SF6</td>
<td>11520</td>
<td>22901 Supl.</td>
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<td>C3H4</td>
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<td>HO2</td>
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<td>ClONO2</td>
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<td>HOBr</td>
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<tr>
<td>CH3OH</td>
<td>HITRAN specific</td>
<td>19899</td>
</tr>
</tbody>
</table>
GEISA/IASI-03 database: **extraction** (spectral range 599-3001 cm\(^{-1}\)) and **partial update** of GEISA-03 Spectroscopic database

- Maintained and developed with the purpose of assessing the IASI measurements capabilities, within the ISSWG, in the frame of the CNES/EUMETSAT European Polar System (EPS) preparation, by simulating high resolution radiances and/or using experimental data.

- IASI mainly designed for operational meteorological soundings with a very high level of accuracy. Measurement technique based on passive IR remote sensing using an accurately calibrated Fourier Transform Spectrometer operating in the 3.7- 5.5 µm spectral range.

**Continuous update**

**Associated interest for AIRS**

- **IASI**: Infrared Atmospheric Sounding Interferometer
- **AIRS**: Advanced InfraRed Sounder
- **ISSWG**: IASI Sounding Science Working Group
- **CNES**: Centre National d’Etude Spatiales, France
- **EUMETSAT**: EUROpean organization for the exploitation of METeorological SATEllites

9th HITRAN conference, 26-28 June 2006, Cambridge, MA, USA
MIPAS Dedicated Spectroscopic Database

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment operating on board the ENVISAT satellite since March 2002

- Recording emission limb sounding spectra at 0.025 cm\(^{-1}\) (unapodized) in the spectral range 685-2410 cm\(^{-1}\)
- Starting from HITRAN-96 and GEISA-97, and updated in 2001 and 2003 with specific spectroscopic studies or from spectroscopic studies prior to their publications
- 32 molecules retained from the HITRAN list (O, NO+, HOBr, C\(_2\)H\(_4\), CH\(_3\)OH, H\(_2\)CO, CH\(_3\)OH discarded)
- Molecular line parameters updated for: H\(_2\)O, CO\(_2\), O\(_3\), N\(_2\)O, CH\(_4\), NO\(_2\), HNO\(_3\), HOCl, COF\(_2\)

Validation through ATMOS and MIPAS recorded spectra
DATABASE FORMATS
# GEISA-03 Line Transitions Records

**A-J fields**  
Mainly specific of GEISA management software

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A)</td>
<td>Wavenumber (cm⁻¹) of the line associated with the vibro-rotational transition.</td>
</tr>
<tr>
<td>(B)</td>
<td>Intensity of the line (cm molecule⁻¹ at 296K).</td>
</tr>
<tr>
<td>(C)</td>
<td>Lorentzian collision halfwidth (cm⁻¹ atm⁻¹ at 296K).</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 levels of the transition.</td>
</tr>
<tr>
<td>(F)</td>
<td>Temperature dependence coefficient $n$ of the halfwidth.</td>
</tr>
<tr>
<td>(G)</td>
<td>Identification code for isotope.</td>
</tr>
<tr>
<td>(I)</td>
<td>Identification code for molecule.</td>
</tr>
<tr>
<td>(J)</td>
<td>Internal GEISA code for data identification.</td>
</tr>
</tbody>
</table>

**K-Q fields in the GEISA format**  
Mainly HITRAN-01 format inter-compatibility related

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(K)</td>
<td>Molecule number as in HITRAN.</td>
</tr>
<tr>
<td>(L)</td>
<td>Isotope number as in HITRAN.</td>
</tr>
<tr>
<td>(M)</td>
<td>Transition probability (in debye²).</td>
</tr>
<tr>
<td>(N)</td>
<td>Self broadening pressure halfwidth (HWHM) (cm⁻¹ atm⁻¹) at 296K (for water).</td>
</tr>
<tr>
<td>(O)</td>
<td>Air pressure shift of the line transition (cm⁻¹ atm⁻¹) at 296K.</td>
</tr>
<tr>
<td>(P)</td>
<td>Accuracy indices for wavenumber, intensity and halfwidth.</td>
</tr>
</tbody>
</table>
| (Q)   | Indices for lookup of references for wavenumber, intensity and halfwidth.
### GEISA-03 Line Transitions Records (following)

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
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<tbody>
<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 halfwidth (HWHM) (cm$^{-1}$atm$^{-1}$)</td>
</tr>
<tr>
<td>(F')</td>
<td>Estimated accuracy on the temperature dependence coefficient $n$ of the air broadening HW</td>
</tr>
<tr>
<td>(O')</td>
<td>Estimated accuracy on the air pressure shift of the line transition (cm$^{-1}$atm$^{-1}$) @296K</td>
</tr>
<tr>
<td>(R')</td>
<td>Estimated accuracy on the temperature dependence coefficient $n$ of the air pressure shift</td>
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</table>

**Water specific**

<table>
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<th>Field</th>
<th>Description</th>
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<tbody>
<tr>
<td>(N')</td>
<td>Estimated accuracy on the self broadened (HWHM) (cm$^{-1}$atm$^{-1}$) @296K</td>
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<tr>
<td>(S)</td>
<td>Temperature dependence coefficient $n$ of the self broadening halfwidth</td>
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<tr>
<td>(S')</td>
<td>Estimated accuracy on the temperature dependence coefficient $n$ of the self broadening HW</td>
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<td>(T)</td>
<td>Self pressure shift of the line transition (cm$^{-1}$atm$^{-1}$) @296K</td>
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<tr>
<td>(T')</td>
<td>Estimated accuracy on the self pressure shift of the line transition (cm$^{-1}$atm$^{-1}$) @296K</td>
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<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</td>
</tr>
</tbody>
</table>

**209 Characters record**
HITRAN-04 Line Transition Records

160-character records of the HITRAN-04 line-by-line section

- **M**: Molecule number
- **I**: Isotopologue number
- **\(v\)**: Vacuum wavenumber \(\text{cm}^{-1}\)
- **\(S\)**: Intensity \(\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^2)\) at 296K
- **\(R\)**: Weighted square of the transition moment, \(\text{Debye}^2\)
- **\(A\)**: Einstein A-coefficient \(\text{s}^{-1}\)
- **\(\gamma_{\text{air}}\)**: Air-broadened half-width, HWHM at 296K, \(\text{cm}^{-1}\text{atm}^{-1}\)
- **\(\gamma_{\text{self}}\)**: Self-broadened half-width, HWHM at 296K, \(\text{cm}^{-1}\text{atm}^{-1}\)
- **\(E'\)**: Lower-state energy \(\text{cm}^{-1}\)
- **\(\eta_{\text{air}}\)**: Temperature-dependence exponent for \(\gamma_{\text{air}}\)
- **\(\delta_{\text{air}}\)**: Air pressure-induced line shift \(\text{cm}^{-1}\text{atm}^{-1}\) at 296K
- **\(V'\)**: Upper-state “global” quanta
- **\(V''\)**: Lower-state “global” quanta
- **\(Q'\)**: Upper-state “local” quanta
- **\(Q''\)**: Lower-state “local” quanta
- **\(I_{\text{err}}\)**: Uncertainty indices
- **\(I_{\text{ref}}\)**: Reference indices
- **\(*)\**: Flag: Availability of program and data for the case of line mixing
- **\(g'\)**: Statistical weight of the upper state
- **\(g''\)**: Statistical weight of the lower state
The format of the MIPAS database as well as the numbering of the molecules and of the isotopic species is the same as in HITRAN-96 and HITRAN-2K
UPDATING OF SPECTROSCOPIC PARAMETERS: examples of issues
1) Updating of H₂O in GEISA and GEISA/IASI-03
H2O GEISA/IASI-03 updating and alternative archive

Toth’s (2000, 2002)
599.681 - 2819.848 cm\(^{-1}\)

RAL/ EUMETSAT
700.032 - 1299.980 cm\(^{-1}\)

Choice for GEISA/IASI-03 update

Alternative choice for GEISA/IASI-03 update
H2O updating in GEISA/IASI-03: TOTH VS RAL

Halfwidths (%)

Intensity (%)

H2O RAL / geisa+toth halfwidth differences:
\[ \text{HWdif} = \left[ \text{HW(RAL)} - \text{HW(GS+TOT)} \right] \text{ in percent} \]

H2O RAL / geisa+toth Intensity differences:
\[ \text{Idif} = \left[ \text{I(RAL)} - \text{I(GS+TOT)} \right] \text{ in percent} \]
2) DIFFERENCES BETWEEN GEISA (GEISA/IASI-03) and HITRAN-04
H$_2$O Intensity Differences

GEISA/IASI 03 (Toth’s data) and HITRAN 04 comparisons for air-broadened half-widths (HW) and intensities (I)

\[
\% \text{10 cm}^{-1} \text{ HW Average difference} \\
= \frac{(\text{HW}_{H04} - \text{HW}_{G03})}{(\text{HW}_{H04 \text{ max}} + \text{HW}_{G03 \text{ max}})^{2} \times 100}
\]

\[
\% \text{10 cm}^{-1} \text{ Intensity Average difference} \\
= \frac{(\text{I}_{H04} - \text{I}_{G03})}{(\text{I}_{H04 \text{ max}} + \text{I}_{G03 \text{ max}})^{2} \times 100}
\]
CO₂ Intensity Differences

GEISA/IASI 03 and HITRAN 04 comparisons for intensities

New data for GIA-03
LTS
LPMA

% 10 cm⁻¹ Intensity Average difference

\[
\frac{(I_{H04} - I_{G03})}{(I_{H04\ max} + I_{G03\ max})} \times 100
\]
**O₃ Intensity Differences**

GEISA/IASI 03 and HITRAN 04 comparisons for intensities

New data for GIA-03

GSMA, LPMA, LPPM (LISA), LTS, NASA (Langley), JPL

Wavenumber (cm⁻¹)

HITRAN more Complete MIPAS data?

% 10 cm⁻¹ Intensity Average difference

\[
\frac{(I_{H04} - I_{G03})}{(I_{H04 \ max} + I_{G03 \ max})} \times 2 \times 100
\]
N₂O Collision Half-Width Differences

GEISA/IASI 03 and HITRAN 04 comparisons for air-broadened half-widths

% 10 cm⁻¹ HW Average difference
(HW H04 – HW G03) / (HW H04 max + HW G03 max) * 2 * 100
3) DIFFERENCES BETWEEN GEISA (GEISA/IASI-03) and MIPAS-03
H₂O Intensity Differences

![Graph 1](image1)

![Graph 2](image2)

![Graph 3](image3)
H₂O Collision Half-Width Differences
CO$_2$ Collision Half-Width Differences

\[\text{Halide unit} \times \text{atm}^{-1}\]

![Graphs showing CO$_2$ collision half-width differences.](image-url)
O₃ Intensity Differences

![Graph 1](image1)

![Graph 2](image2)

![Graph 3](image3)

![Graph 4](image4)
Evaluation of the Impact of Spectroscopic Archive Differences on Radiative Transfer Simulations
Spectroscopic data involved in comparisons

**GEISA/IASI-03**

599 - 3,001 cm\(^{-1}\)

14 molecules: H\(_2\)O, CO\(_2\), O\(_3\), N\(_2\)O, CO, CH\(_4\), O\(_2\), NO, SO\(_2\), NO\(_2\), HNO\(_3\), OCS, C\(_2\)H\(_2\), N\(_2\)

**MIPAS database**

597 – 2,503 cm\(^{-1}\)

Version pf3.1

**HITRAN-04**

extractions in GEISA/IASI and MIPAS databases common spectral intervals

---

6 Molecular species selected for comparisons, i.e.:

H\(_2\)O, CO\(_2\), O\(_3\), N\(_2\)O, CO, CH\(_4\)
Five atmospheric profiles; mean of each of 5 air mass class the Thermodynamic Initial Guess Retrieval (TIGR) data set, in its latest version, a climatological library of about 2300 representative atmospheric situations selected by statistical methods from 80,000 radiosonde reports [Chédin et al., 1985; Achard, 1991; Chevallier et al., 1998].

- Mc Clatchey profiles

- Three IASI spectral Bands: 645-1210 cm\(^{-1}\); 1210-2000 cm\(^{-1}\); 2000-2760 cm\(^{-1}\)


- Mean thermodynamic Parameters for each TIGR air-mass
Spectroscopy issues and IASI sounding Channels Selection (H$_2$O exemple)

IASI Stransac-2000 simulations with RAL or TOTH spectroscopy
HITRAN and GEISA H$_2$O DIFFERENCE IMPACT

STRANSAC-2000 IASI Simulation

Tropical TIGR-2000 atmosphere
HITRAN and GEISA $\text{O}_3$ DIFFERENCE IMPACT

**STRANSAC-2000 IASI Simulation**

- IASI resolution 4A-2000: simulation of all molecules (green) vs. H2O (red) (Tigr2000 tropical)
- GEISA/IASI $\text{O}_3$ + HITRAN 04 for $\text{O}_3$
- Difference

Tropical TIGR-2000 atmosphere
HITRAN and GEISA N₂O DIFFERENCE IMPACT

Tropical TIGR-2000 atmosphere

GEISA/IASI 03 + HITRAN 04 for n2o

Brightness temperatures (K)

Wavenumbers (cm⁻¹)

Brightness temperature difference (K)

Wavenumbers (cm⁻¹)
IASI 4A-2000 Band-2 Simulation
TIGR-2000 Polar 2

9th HITRAN conference, 26-28 June 2006, Cambridge, MA, USA
IASI 4A-2000 Band-3 Simulation
TIGR-2000 Tropical

Tigr2000 Tropical

Wavenumber (cm⁻¹)

Brightness temperature difference (K)

Geisa/IASI/MIPAS - Geisa/IASI
Hitran04 - Geisa/IASI
IASI noise at Tb
Standard IASI noise at T=280K

Tigr2000 Tropical

Wavenumber (cm⁻¹)

Brightness temperature difference (K)

Hitran - Geisa/IASI/Mipas
IASI noise at Tb
Standard IASI noise at T=280K
CONCLUDING COMMENTS
Remaining spectroscopy related problems

Some conclusions of validation exercises, using e.g.: the 4A-00/LMD Model, in the case of IASI radiative transfer modelling

1. The water vapour spectroscopic parameters: still need to be validated;
2. The water vapour continuum: more tuning to be done when more validation data (especially with high water vapor content) become available;
3. The freons bands at 850 and 920 cm\(^{-1}\): refine the temperature dependence;
4. O\(_3\) in the 9.6 micron region: the spectroscopic parameters still need to be validated;
5. Some CO\(_2\) – Q branches: further improvement/tuning of the line mixing
GEISA/IASI and associated facilities are being implemented on the **Ether (CNRS/IPSL)** Products and Services Centre (CPS)

**Effective fall 2006**

**Ether Products and Services Centre Facilities:**

- **measurement data** from French laboratories, as well as from many international centres,
- **forecasts** such as Potential Vorticity,
- **modelling results**,
- downloadable **procedures**,
- **browse images**, on-line **processing software** (which can be activated through the Ether interface)
IAI INSTRUMENT STATUS

Launch 17 July 2006

IAI Level 1 Cal/Val activities

- GEISA/IAI used as the reference spectroscopic database
- It is expected that validation can be achieved using a Line by line RTM (4A will be used for validation at 3 wavenumbers in each 3 bands)
ACKNOWLEDGMENTS

to

CNES and EUMETSAT

for their Encouragements and Supports