EVALUATION OF SPECTROSCOPY for IASI THROUGH the GEISA /IASI-2009 DATABASE

Jacquinet-Husson N., Crépeau L., Armante R, Boutammine C., Chédin A., Scott N.A. Crevoisier C., Capelle V.

Laboratoire de Météorologie Dynamique
Atmospheric Radiation Analysis Group
Ecole Polytechnique
91128 Palaiseau, France

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

4th ISSWG-2, ECMWF, Reading, UK, 7-8 October 2010
The performance of the second generation vertical sounding, high-resolution, sophisticated infrared spectroscopic instruments, such as AIRS in the USA and IASI in Europe, highly depends on the accuracy in the spectroscopic parameters of the optically active atmospheric gases, since such data constitute an essential input in the forward models that are used to interpret the recorded spectral radiances.

FROM SATELLITE OBSERVATIONS TO CLIMATE VARIABLES: a long process based on Radiative Transfer

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

A priori infos

GEISA SPECTROSCOPIC DATABASE

Scientific Themes

- Thermodynamics
- Clouds
- Greenhouse gases
- Continental surfaces
- Aerosols
- etc…

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

4th ISSWG-2, ECMWF, Reading, UK, 7-8 October 2010
Submitted September 15th 2010

Manuscript Number: JQSRT-D-10-00265

Title: The 2009 edition of the GEISA spectroscopic database

First Author: Nicole Jacquinet-Husson

59 co-authors

26 Institutions or Laboratories
GEISA-09 LINE TRANSITION PARAMETERS
SUB-DATABASE EVOLUTION SINCE 1978

http://ara.lmd.polytechnique.fr/
http://ether.ipsl.jussieu.fr

+ 2,139,626 entries
THE GEISA-2009 SYSTEM

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: 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_4, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_6, C_3H_4

- Absorption cross-sections database
  - IR: 43 molecular species (mainly CFC's)
  - UV/Visible: 19 molecular species

- Aerosol data archive and softwares
FROM GEISA-09 TO GEISA/IASI-09

- **Individual spectral lines spectroscopic parameters sub-database**
  - Extraction of GEISA-09 in the spectral range 599 - 3001 cm\(^{-1}\)
  - 20 molecules (66 isotopic species):
    - \(\text{H}_2\text{O}, \text{CO}_2, \text{O}_3, \text{N}_2\text{O}, \text{CO}, \text{CH}_4, \text{O}_2, \text{NO}, \text{SO}_2, \text{NO}_2, \text{HNO}_3, \text{OCS}, \text{C}_2\text{H}_2, \text{N}_2, \)
    - \(\text{HCN}, \text{NH}_3, \text{HCOOH}, \text{C}_2\text{H}_4, \text{CH}_3\text{OH}, \text{H}_2\text{CO}\)

- **IR absorption cross-sections sub-database (mainly CFC’s)**
  - 6 molecular species: CFC-11, CFC-12, CFC-14, \(\text{CCl}_4, \text{N}_2\text{O}_5, \text{HCFC-22}\)
  - PAN (peroxyacetyl nitrate)

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

- **Continuous update**

Associated interest for AIRS
GEISA/IASI EFFECTIVE USE

Related to

IASI Level 1 Cal/Val activities@ LMD
(with the support of CNES)

- 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)]
Operational Meteorology selection

11 Molecules updated
H₂O, CO₂, O₃, CH₄, N₂O, NO, SO₂, NO₂, HNO₃, C₂H₂, N₂

3 Molecules non updated: CO, O₂, OCS

+473,165 entries
Since GEISA/IASI-03
**Additional selection for Chemistry and Climate**

**Related with IASI Trace Gas Retrievals**

- NH₃
- HCN
- CH₃OH
- C₂H₄
- HCOOH
- H₂CO

**148,620 Additional lines**

- nh₃: 14278
- ch₄: 12682
- hcn: 20004
- hcooh: 55876
- ch₃oh: 15234
- h₂co: 30546

**2009**

**2003**

4th ISSWG-2, ECMWF, Reading, UK, 7-8 October 2010
GEISA/IASI Content Evolution since the 2003 Edition

GEISA/IASI-09  1,324,335 LINES

GEISA/IASI 2003
Addition in 2009

702,550
53%

621,785
47%

VG-2, ECMWF, Reading, UK, 7-8 October 2010
GEISA/IASI-09 Line Transitions Records

252 characters Record
31 Parameters

(A) Wavenumber (cm⁻¹) of the line associated with the vibro-rotational transition.
(B) Intensity of the line (cm molecule⁻¹ at 296K).
(C) Lorentzian collision halfwidth (cm⁻¹ atm⁻¹ at 296K).
(D) Energy of the lower transition level (cm⁻¹).

(E) **Transition quantum identifications for the lower and upper levels of the transition**

(F) Temperature dependence coefficient \( n \) of the halfwidth

(G) Identification code for isotope.

(I) Identification code for molecule.

(J) Internal GEISA code for data identification.

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<th>B</th>
<th>C</th>
<th>D</th>
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<td>I2</td>
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</tbody>
</table>

(M) Einstein A-coefficient

(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
GEISA/IASI 2009 UPDATE EVALUATION

Spectroscopy Changes in GEISA/IASI-09
Impact evaluation

Example for H$_2$O, N$_2$O, CH$_4$

_stransac/4A-OP Brightness Temperatures Modelization (K)_
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, N2O, HCFC-22 and especially PAN.

- **The still outstanding general spectroscopy-related conclusions for public databases, from ISSWG -30, June-2 July 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 re-investigated.
  - IASI related spectroscopy problems with H2O and CO2 as first priority

- **Line coupling/mixing modelling:** (which should be used in conjunction with the molecular parameters of the data base from which they have been derived); work in progress with J.M. Hartman

- **non-LTE** (Local Thermodynamic Equilibrium) effects are areas to be urgently investigated (not especially related with spectroscopic parameters)
Welcome to the Ether website

This website offers various products of French activities in national and international projects. The access rights vary according to the products (see "Login Request"). More information...

Databases
- RAMCES
- LECA

Data
- IASI
- ODIOS

Services
- AEPLTY

Links
- StratoPolE

Ether Products and Services Centre Facilities
http://ether.ipsl.jussieu.fr
The GEISA-09 sub-database on line transition parameters

The GEISA-09 sub-database of line transition parameters involves 50 molecules (111 isotopic species) and contains 3,807,202 entries, in the spectral range from 10^{8} to 35,877 cm^{-1}. This represents an increase of: 8 molecular species, 14 isotopic species and 2,135,944 entries since the GEISA-03 edition. The newly archived molecular species are: CH3Br, CH3OH, NO+, HNC, C6H6, C2H4, CF4, CH3CN.

The included molecules are constituents of the atmospheres of Earth (major permanent and trace molecules) and of other Planets (such as: C2H4, GeH4, C3H5, C2N2, C4H2, HC3N, H2S, HCOOH and C3H4, for the Giant Planets). Among the 31 spectroscopic parameters archived in GEISA, the most important for atmospheric radiative transfer modelling are: the wavenumber (cm^{-1}) of the line associated with a vibro-rotational transition, the intensity of the line (cm molecule^{-1} at 296K), the Lorentzian collision halfwidth (cm^{-1} atm^{-1} at 296 K), with associated self - pressure broadening parameter, the energy of the lower level of the transition (cm^{-1}), the transition quantum identifications for the lower and upper levels of the transition, the temperature dependence coefficient of the halfwidth, the database management identification codes for isotopes and for molecules.

- General content
- GEISA-09 format for line transition parameters
- Overall description of available vibrational transitions
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 : NU1 (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 : NU1 (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 NU1 and NU2.

**Histogram analysis**
Plots of intensity and/or ground level histograms for one isotope of a given molecule in any selected spectral range between a Lower Bound : NU1 (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 NU1 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 : NU1 (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) for one or more molecule(s) and isotope(s).

**Transition analysis**
Extraction of a set of vibro-rotational transitions involved in a specified vibrational transition of one given molecule and one of its isotopes, in any selected spectral range between a Lower Bound : NU1 (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹). Maximum field length: 25 digits for upper and lower level vibrational quantum code identification. See GEISA-09 format for line transition parameters and Overall description of available vibrational transitions for proper selection and description of vibrational transitions of interest.

**Transition list**
Complete description of existing vibrational transitions in any selected spectral range between a Lower bound : NU1 (cm⁻¹) and an Upper Bound : NU2 (cm⁻¹) for one or more molecule(s).
Histograms of H$_2$O Intensities  Spectral Interval 800 – 900 cm$^{-1}$

Differences between 2009 and 2003 GEISA/IASI versions

log$_{10}(B)$ 800.000$<\nu<900.000$ for molecule h$_2$o isotope(s) 161
ACKNOWLEDGMENTS

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for their Encouragements and Supports

THANK YOU FOR YOUR ATTENTION