



SPECATMOS : "Spectroscopy and Atmosphere: Measurements and Modelling" International Summer School

Spectroscopic Databases Tutorial

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Introduction

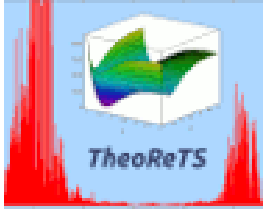


- Adequate tools are required to perform reliable radiative transfer modelling calculations to meet the needs of communities involved in understanding the atmospheres of the Earth and other planets, especially with the emergence of highly sophisticated spectroscopic instruments (OCO-2, IASI-NG, Merlin...).
- Among these tools compilations of spectroscopic parameters are used for a vast array of applications and especially for planetary atmospheric remote sensing.
- There is an acute need for comprehensive, trustworthy and operational interactive spectroscopic databases to benefit the research in direct and inverse radiative transfer.
- The goal of spectroscopic databases is to have a self-consistent set of parameters.

Specific databases

Global/general databases

Pure *ab initio* databases



Molecular linelists (O₃, CO₂...)

S&MPO

CDS-4000



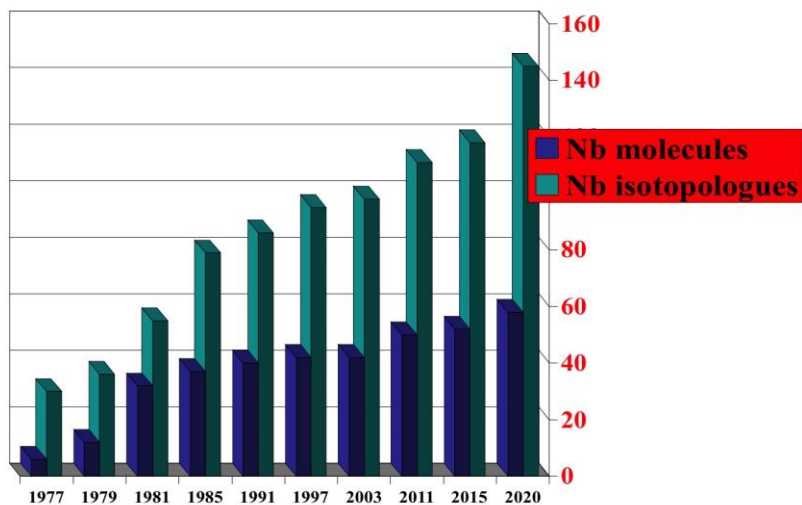
Mix of experimental and theoretical data



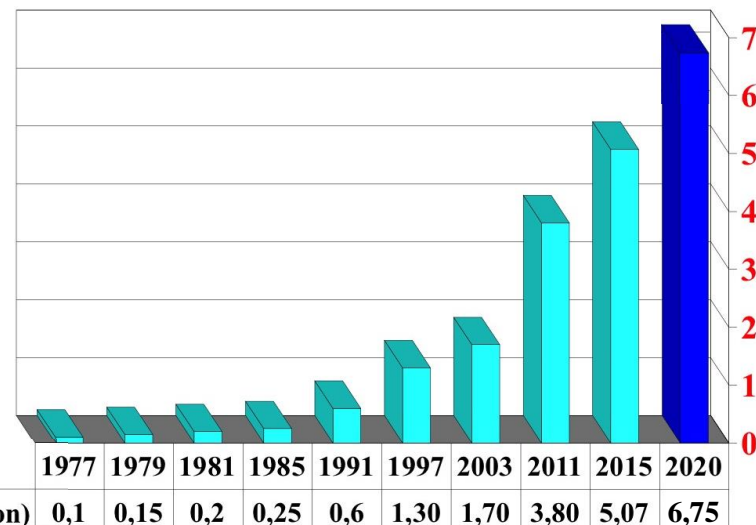
GEISA2020 update



- GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques), is developed and maintained at LMD since 1974.
- Use as reference database for several space missions: IASI, IASI-NG, MicroCarb, Merlin...
- Compilation of three databases: line-parameters, cross-sections and aerosols properties.
- **GEISA-2020 line-parameter database:** 6,746,987 lines (+33% vs GEISA-2015) on the spectral range 10^{-6} - $35,877$ cm^{-1} .
- 23 updated and 6 new molecules (HONO, COFCl, CH_3F , CH_3I , RuO_4 , $\text{H}_2\text{C}_3\text{H}_2$ (isomer of C_3H_4) - total of 145 isotopologues.



	1977	1979	1981	1985	1991	1997	2003	2011	2015	2020
Nb molecules	6	12	32	37	40	42	42	50	52	58
Nb isotopologues	30	36	55	79	86	95	98	111	118	145



	1977	1979	1981	1985	1991	1997	2003	2011	2015	2020
Nb lines (million)	0,1	0,15	0,2	0,25	0,6	1,30	1,70	3,80	5,07	6,75



<https://geisa.aeris-data.fr/>

A screenshot of a web browser displaying the GEISA Spectroscopic database website. The browser tab is titled 'GEISA - Spectroscopic database' and the address bar shows 'https://geisa.aeris-data.fr/'. The website header includes a logo, navigation links for 'DATABASE ACCESS', 'GEISA 2020', 'GEISA 2015', 'GEISA 2011', and 'DOCUMENTATION', and a 'LEGALS MENTIONS' link. The main content area features a large banner image of Earth from space with the text 'GEISA Spectroscopic database'. Below the banner, there are three columns: 'GEISA data archives and facility tools' with a paragraph of text, a 'Search' box with a search input field and a 'Search' button, and 'GEISA NEWS' with a 'NEWS' tag and a headline 'Corrections for CH4, CO, O2 and HCl'.



GEISA access



Main database access

<https://geisa.aeris-data.fr/>

GEISA specific version description and access

The screenshot shows the GEISA website interface. A red arrow points from the text 'Main database access' to the 'DATABASE ACCESS' button. Another red arrow points from 'GEISA specific version description and access' to the 'GEISA 2020', 'GEISA 2015', and 'GEISA 2011' buttons. A third red arrow points from 'Database files and content description' to the 'DOCUMENTATION' button. The website header includes the GEISA logo, a navigation menu with 'DATABASE ACCESS', 'GEISA 2020', 'GEISA 2015', 'GEISA 2011', and 'DOCUMENTATION', and a 'LEGALS MENTIONS' link. The main banner features the text 'GEISA Spectroscopic database'. Below the banner, there is a section titled 'GEISA data archives and facility tools' with a paragraph of text. To the right, there is a search bar and a 'GEISA NEWS' section with a 'NEWS' button and a snippet of text: 'Corrections for CH4, CO, O2 and HCl'.



GEISA line parameters



- GEISA2020 line parameters: 6,746,987 lines (+33% vs GEISA-2015) on the spectral range 10^{-6} - 35,877 cm^{-1} .
- 23 updated and 6 new molecules (HONO, COFCl, CH_3F , CH_3I , RuO_4 , $\text{H}_2\text{C}_3\text{H}_2$ (isomer of C_3H_4) - total of 58 molecules and 145 isotopologues.



LEGALS MENTIONS

DATABASE ACCESS

GEISA 2020

GEISA 2015

GEISA 2011

DOCUMENTATION

Interactive access

[Homepage](#) / [Interactive access](#)

Select option

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}).

Select Database

2020

Choosing molecules (from database 2020)

[Show/Hide isotopologues](#)

[Select all](#)

[Unselect all](#)

- | | | | | | | | | | | | | | | |
|-------------------------------|-------------------------------|-------------------------------|--------------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|---------------------------------|---------------------------------|--------------------------------|-------------------------------|
| <input type="checkbox"/> h2o | <input type="checkbox"/> co2 | <input type="checkbox"/> o3 | <input type="checkbox"/> n2o | <input type="checkbox"/> co | <input type="checkbox"/> ch4 | <input type="checkbox"/> o2 | <input type="checkbox"/> no | <input type="checkbox"/> so2 | <input type="checkbox"/> no2 | <input type="checkbox"/> nh3 | <input type="checkbox"/> ph3 | <input type="checkbox"/> hno3 | <input type="checkbox"/> oh | <input type="checkbox"/> hf |
| <input type="checkbox"/> hcl | <input type="checkbox"/> hbr | <input type="checkbox"/> hi | <input type="checkbox"/> clo | <input type="checkbox"/> ocs | <input type="checkbox"/> h2co | <input type="checkbox"/> c2h6 | <input type="checkbox"/> ch3d | <input type="checkbox"/> c2h2 | <input type="checkbox"/> c2h4 | <input type="checkbox"/> geh4 | <input type="checkbox"/> hcn | <input type="checkbox"/> c3h8 | <input type="checkbox"/> c2n2 | <input type="checkbox"/> c4h2 |
| <input type="checkbox"/> hc3n | <input type="checkbox"/> hocl | <input type="checkbox"/> n2 | <input type="checkbox"/> ch3cl | <input type="checkbox"/> h2o2 | <input type="checkbox"/> h2s | <input type="checkbox"/> hcooh | <input type="checkbox"/> cof2 | <input type="checkbox"/> sf6 | <input type="checkbox"/> c3h4 | <input type="checkbox"/> ho2 | <input type="checkbox"/> clono2 | <input type="checkbox"/> ch3br | <input type="checkbox"/> ch3oh | <input type="checkbox"/> no+ |
| <input type="checkbox"/> hnc | <input type="checkbox"/> c6h6 | <input type="checkbox"/> c2hd | <input type="checkbox"/> cf4 | <input type="checkbox"/> ch3cn | <input type="checkbox"/> hdo | <input type="checkbox"/> so3 | <input type="checkbox"/> hono | <input type="checkbox"/> cofcl | <input type="checkbox"/> ch3i | <input type="checkbox"/> ch3f | <input type="checkbox"/> ruo4 | <input type="checkbox"/> h2c3h2 | | |

Choosing the spectral range in cm^{-1} μm Ghz (from 0 to 35877.030506)

Lower Bound

Upper Bound

Choosing intensity range (0 to $1\text{E-}16\text{cm}^{-1}/\text{molecule.cm}^{-2}$)

Lower Bound

Upper Bound

Submit



GEISA line parameters



- Download the full database: Database Access -> Interactive access -> Download GEISA files
- The user can choose the version (2020, 2015, 2011) and download the full database or specific molecule files (ASCII format).

Full database

Interactive access

LEGALS MENTIONS

DATABASE ACCESS GEISA 2020 GEISA 2015 GEISA 2011 DOCUMENTATION

Homepage / Interactive access

Select option

Download GEISA files

Choose molecules or download the whole database: **Download**

Select Database

2020

Choosing molecules (from database 2020) Select all Unselect all

<input type="checkbox"/> h2o	<input type="checkbox"/> co2	<input type="checkbox"/> o3	<input type="checkbox"/> n2o	<input type="checkbox"/> co	<input type="checkbox"/> ch4	<input type="checkbox"/> o2	<input type="checkbox"/> no	<input type="checkbox"/> so2	<input type="checkbox"/> no2	<input type="checkbox"/> nh3	<input type="checkbox"/> ph3	<input type="checkbox"/> hno3	<input type="checkbox"/> oh	<input type="checkbox"/> hf
<input type="checkbox"/> hcl	<input type="checkbox"/> hbr	<input type="checkbox"/> hi	<input type="checkbox"/> clo	<input type="checkbox"/> ocs	<input type="checkbox"/> h2co	<input type="checkbox"/> c2h6	<input type="checkbox"/> ch3d	<input type="checkbox"/> c2h2	<input type="checkbox"/> c2h4	<input type="checkbox"/> geh4	<input type="checkbox"/> hcn	<input type="checkbox"/> c3h8	<input type="checkbox"/> c2n2	<input type="checkbox"/> c4h2
<input type="checkbox"/> hc3n	<input type="checkbox"/> hocl	<input type="checkbox"/> n2	<input type="checkbox"/> ch3cl	<input type="checkbox"/> h2o2	<input type="checkbox"/> h2s	<input type="checkbox"/> hcooh	<input type="checkbox"/> cof2	<input type="checkbox"/> sf6	<input type="checkbox"/> c3h4	<input type="checkbox"/> ho2	<input type="checkbox"/> clono2	<input type="checkbox"/> ch3br	<input type="checkbox"/> ch3oh	<input type="checkbox"/> no+
<input type="checkbox"/> hnc	<input type="checkbox"/> c6h6	<input type="checkbox"/> c2hd	<input type="checkbox"/> cf4	<input type="checkbox"/> ch3cn	<input type="checkbox"/> hdo	<input type="checkbox"/> so3	<input type="checkbox"/> hono	<input type="checkbox"/> cofcl	<input type="checkbox"/> ch3i	<input type="checkbox"/> ch3f	<input type="checkbox"/> ruo4	<input type="checkbox"/> h2c3h2		

Submit

or molecule selection

- The user can also extract a part of the database in the 'Database extract' tab.



- GEISA database
<https://geisa.aeris-data.fr/>
- Radis package
<https://github.com/radis/radis>
- Simple spectrum calculation (RADIS-app)
<https://www.radis.app/>
- Online environment for advanced spectrum processing and comparison with experimental data (RADIS-Lab)
<https://radis.github.io/radis-lab/>
- Anaconda python distribution (for simple Radis installation)
<https://www.anaconda.com/products/distribution>
install RADIS using 'cmd prompt' executing 'pip install radis -v'



Spectrum simulation



- For online spectrum simulation purpose, GEISA is interfaced with RADIS.

<https://github.com/radis/radis>

- RADIS is a fast line-by-line code for high resolution infrared molecular spectra (emission / absorption) based on GEISA/HITRAN/HITEMP/ExoMol.
- It includes post-processing tools to compare experimental spectra and spectra calculated with RADIS or other spectral codes.



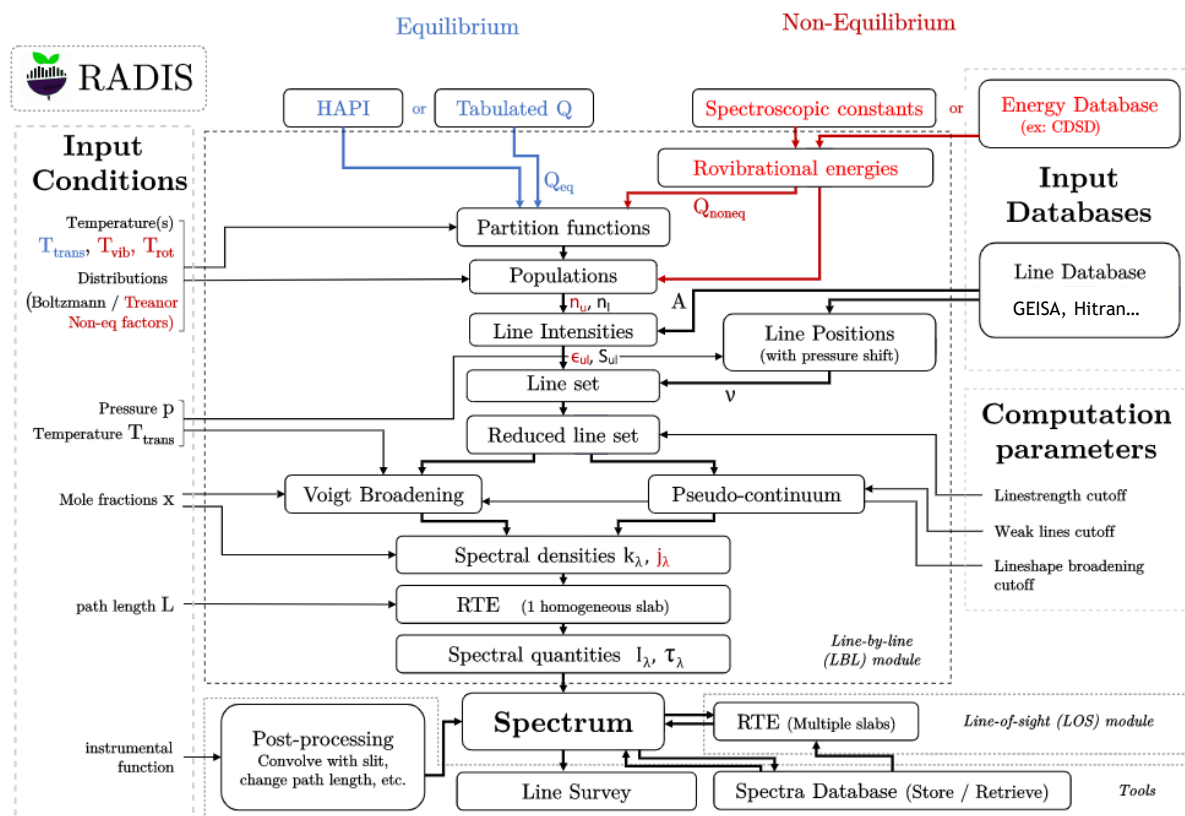
Journal of Quantitative Spectroscopy and Radiative Transfer

Volumes 222–223, January 2019, Pages 12–25



RADIS: A nonequilibrium line-by-line radiative code for CO₂ and HITRAN-like database species

Erwan Pannier , Christophe O. Laux





- Simple online spectrum calculation RADIS-app (GEISA available in some days).
- Flexible gaz mixture configuration <https://www.radis.app/>

RADIS app

Mode
Transmittance

Wavenumber range (cm⁻¹)
6075 6079

Tgas	Pressure	Path length
296	K 1,01325 bar	100 cm

HITRAN 2020 Molecule	Mole Fraction	
CH ₄	0,000002	+
H ₂ O	0,002	×
CO ₂	0,0004	×

Use non-equilibrium calculations

Simulate a 1.5 nm instrumental slit

CALCULATE SPECTRUM

Spectrum for CH₄ (X_{CH₄} = 0.000002), H₂O (X_{H₂O} = 0.002), CO₂ (X_{CO₂} = 0.0004)

Transmittance

Wavenumber (cm⁻¹)

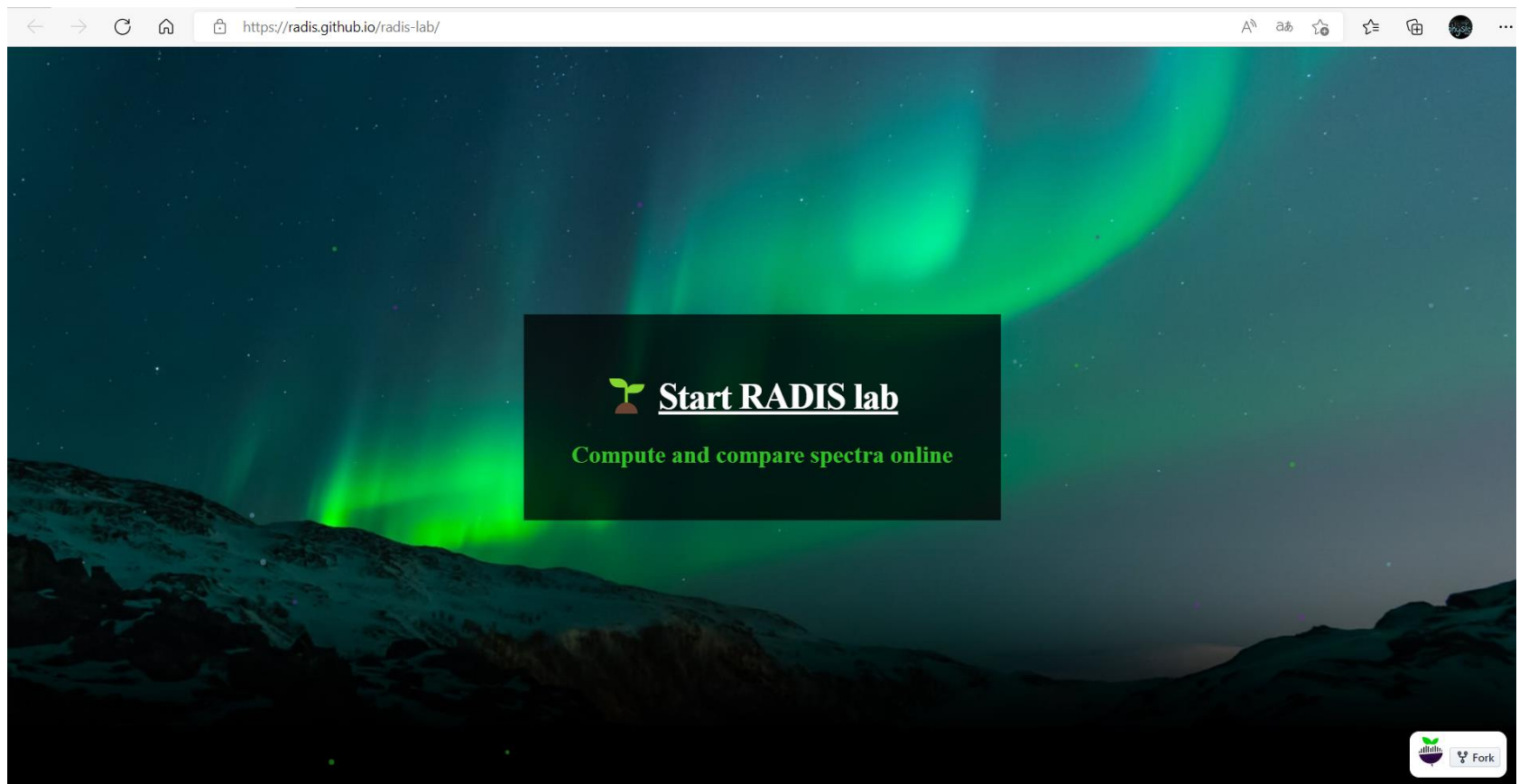


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- Online environment for advanced spectrum processing and comparison with experimental data (RADIS-Lab)

<https://radis.github.io/radis-lab/>





After the notebook is loaded, just drag and drop the following 4 files at the root:

The screenshot shows the JupyterLab interface with a file explorer on the left and a Windows File Explorer window open in the center. The File Explorer window displays the contents of the 'Spectro_databases_tuto' folder, with four files highlighted in a red box:

Nom	Modifié le	Type	Taille
Databases_tuto_links.pdf	17/05/2022 12:30	Foixit PDF Reader ...	107 Ko
experiment.txt	17/05/2022 10:02	Document texte	196 Ko
Starting_TP.ipynb	17/05/2022 11:36	Fichier IPYNB	47 Ko
TP_compare_with_experiment.ipynb	17/05/2022 15:43	Fichier IPYNB	172 Ko
TP_post-process-spectra.ipynb	17/05/2022 11:50	Fichier IPYNB	5 836 Ko

A red arrow points from the 'radi.json' file in the JupyterLab file explorer to the red box in the File Explorer window.



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