Spectroscopic Databases for the VAMDC Portal: New Tools and Improvements

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HITRAN conference

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Dijon databases

- 6 spectroscpic **molecular** databases (http://vamdc.icb.cnrs.fr)

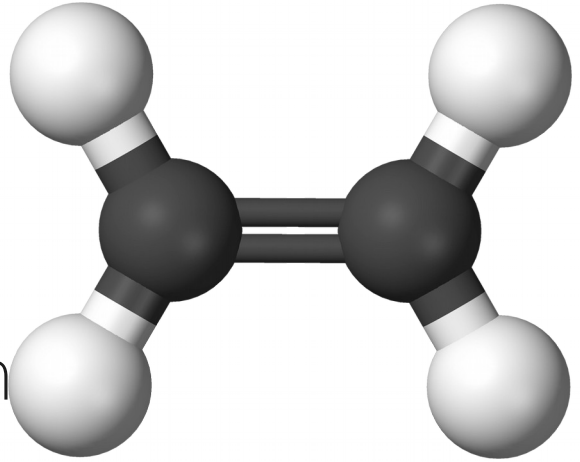
  → CH_4, C_2H_4, SF_6, CF_4, RuO_4 et GeH_4

- Calculated databases (positions + intensities)

  → Large amount of transitions

  → Large amount of known parameters that can be described in a XSAMS file

ECaSDa (620-1525 cm^{-1})



Ethene database

Naturally occurring molecule playing a role in the atmosphere of the Earth as a tropospheric polluant

Last update : 2016

File format produced different from HITRAN

→ HITRAN : J K_a K_c from assymetric top

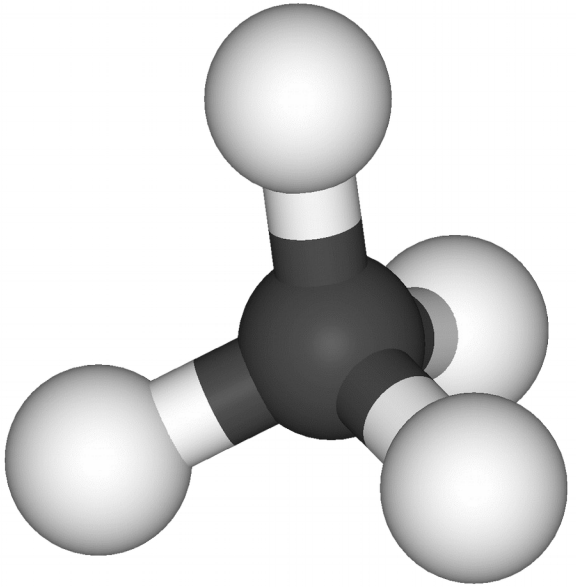
→ EcaSDa : J C α from tensorial formalism

MeCaSDa (0-6773 cm^{-1})

Methane database

Greenhouse molecule –

Astrophysical interest



Last update : 2017

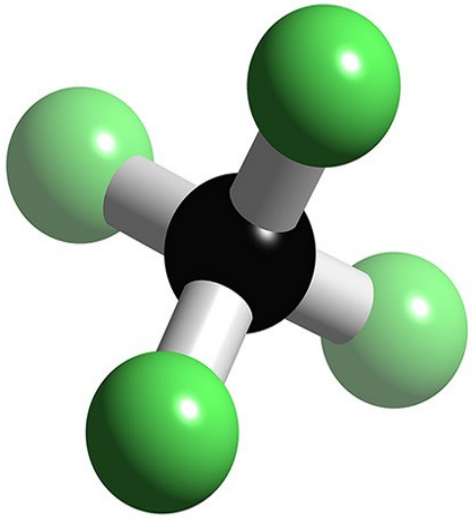
→ 16 548 849 transitions

TFMeCaSDa (1-1697 cm^{-1})

CF_4 database

Powerful greenhouse gaz mainly of anthropogenic origin

Estimated lifetime of more than 50000 years



Last update : 2017

→ 1 093 813 transitions

SHeCaSDa (271-2858 cm^{-1})

SF_6 database

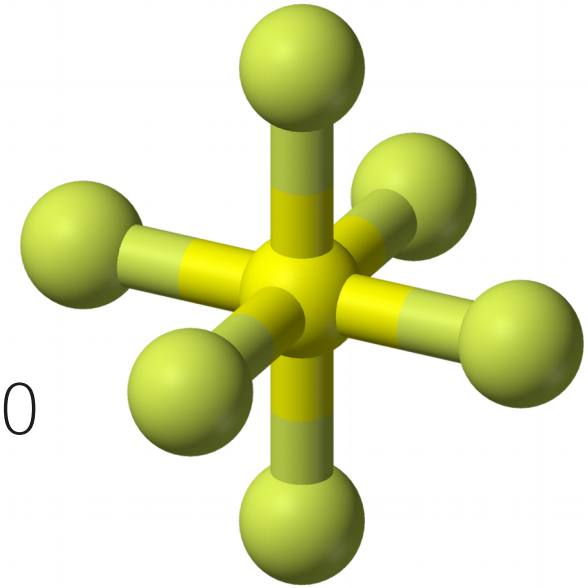
Powerful greenhouse

Estimated lifetime of more than 3000 years

Analysis in progress but a lot of hot bands

→ A lot of transitions

Expected update : 2018



See talk TF02, TF03

GeCaSDa (1928-2266 cm^{-1})

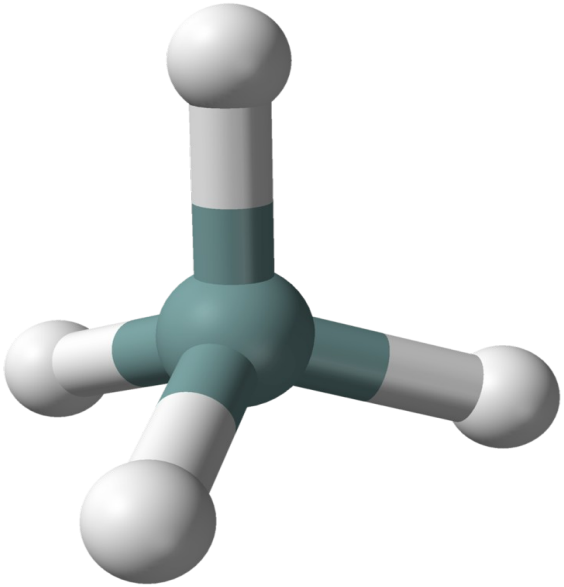
Germane database

Molecule of interest for planetology

→ Strong presence in gas giants

→ Juno probe

5 isotopologues



See talk TJ02

Last update : 2017

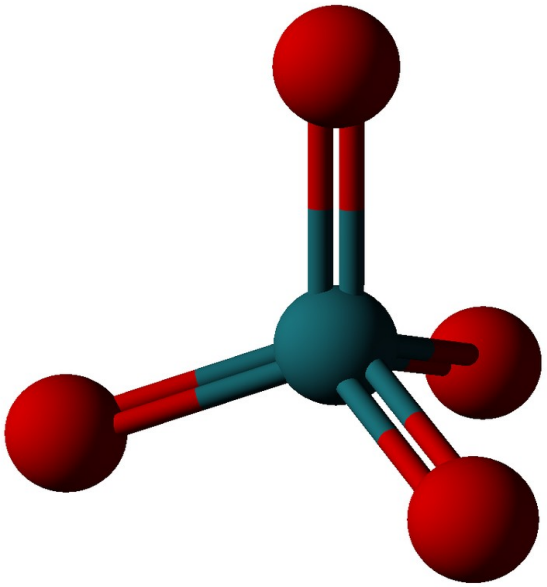
RuCaSDa (891-948 cm^{-1})

RuO_4 database

Fission product of uranium

Can bu used as a marker during a severe nuclear reactor accident with air ingress

9 isotopologues



See talk WC02, WH08

Dernière mise à jour : 2017

News

- 2 new databases (RuO_4 and GeH_4)
- Website refactoring
- New viewer tool
- New conversion tool XSAMS → HITRAN

Website refactoring

Calculated Spectroscopic Databases (CaSDa) at 296K

Molecule HITRAN ID	Molecule Formula	Database Name
06	CH_4	MeCaSDa
30	SF_6	SHeCaSDa
38	C_2H_4	ECaSDa
42	CF_4	TFMeCaSDa
52	GeH_4	GeCaSDa
--	RuO_4	RuCaSDa

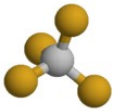
Website refactoring

VAMDC consortium

Calculated TFMeCaSDa line list extraction at 296K

Isotope(s)

☑ 12CF4 [1.173 -> 1696.643 cm^{-1}]



Characterisation

◉ electric dipole [1.000e-30 -> 8.442e-20 cm^{-1}/(molecule cm^{-2})]

○ polarizability [0.000e+0 -> 0.000e+0 arbitrary unit]

Type of Data

◉ line by line

○ cross sections with a step of: 1 cm^{-1}

Wavenumber Range

Lower wavenumber: 0 cm^{-1}

Upper wavenumber: 1700 cm^{-1}

Intensity Threshold

Threshold: 0

Extract

The extraction can last several minutes

Website refactoring

VAMDC consortium

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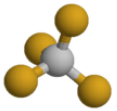

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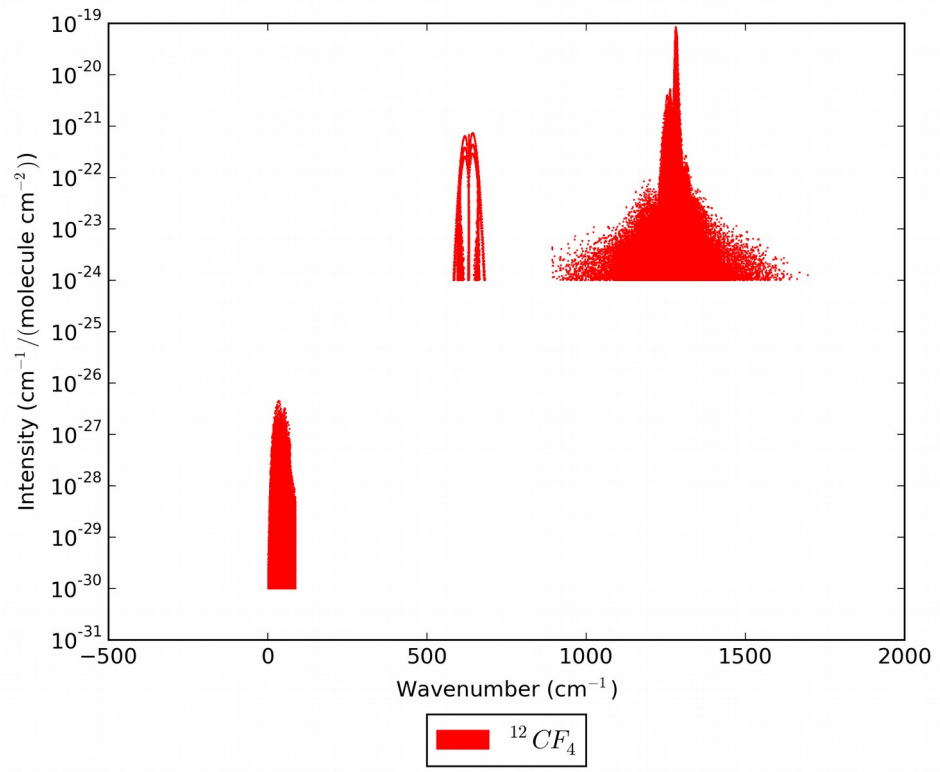
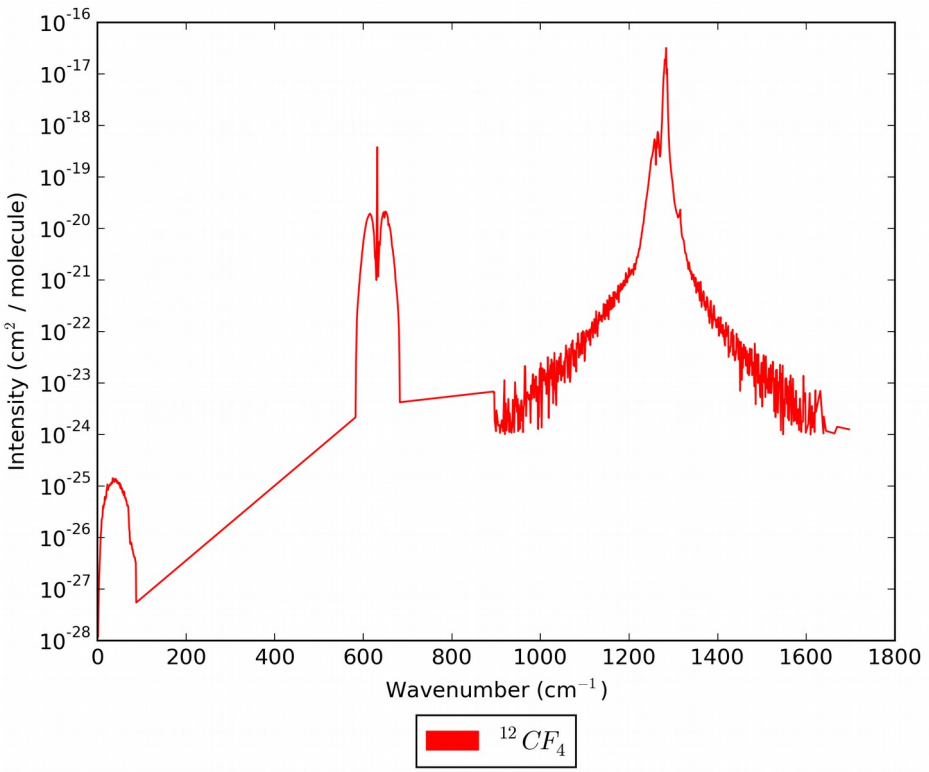
Spectrum viewer

Transitions



Cross sections



Format : HITRAN 2004 (160-character) Format : 2 columns

Conversion XSAMS to Hitran

Spectroscopists, planetary and atmospheric science, work with HITRAN format

→ Flat files

→ Last revision in 2004

→ Molecules chronologically numbered into the database

For example, for the main isotopologue of methane: 61

```
61    0.001063 1.358E-36 8.643E-24.06500.079   62.87570.730.000000    0 0 0 0 1A1    0 0 0 0 1A1    3F2  1        3F1  1     534330453738 7 1 0    21.0   21.0
61    0.002348 1.062E-37 9.564E-24.05300.068  689.70520.640.000000    0 0 0 0 1A1    0 0 0 0 1A1   11F2  1       11F1  1     534330453738 7 1 0    69.0   69.0
61    0.003384 1.339E-36 7.257E-23.05600.073  470.71680.650.000000    0 0 0 0 1A1    0 0 0 0 1A1    9F2  1        9F1  1     534330453738 7 1 0    57.0   57.0
```

XSAMS to Hitran conversion

Available on the VAMDC portal

Results by node

Name	View data	Response	Last database update	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
MeCaSDa - Methane Calculated Spectroscopic Database	** XSAMS to Hitran Display	OK	Not available	XSAMS file	1	3457	1918	1918	0	0
HITRANonline	XSAMS to Hitran Display	OK	Not available	XSAMS file	1	2	6	6	0	0

Good points:

→ Main databases handled

→ Add of HITRAN units in the XSAMS format

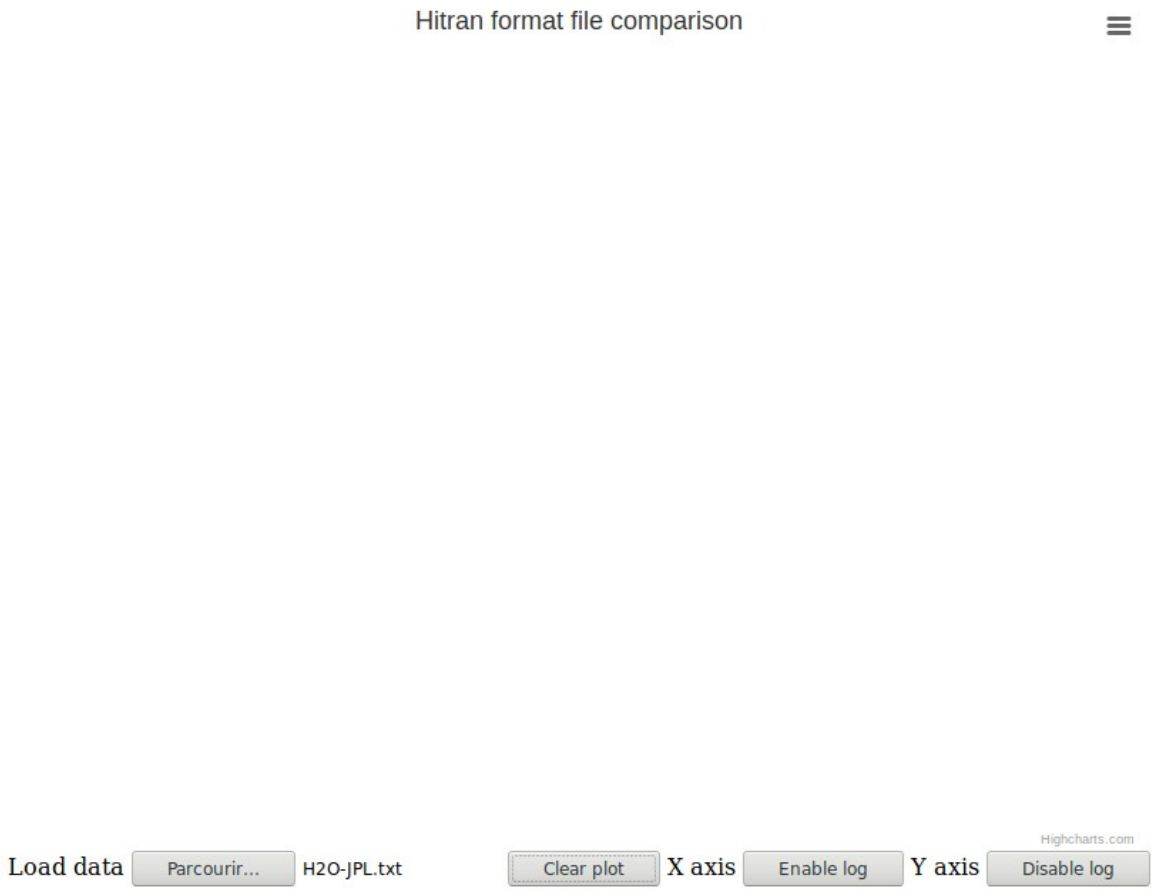
→ JPL and CDMS have added a new field for intensity consistencity of XSAMS format

Bad points:

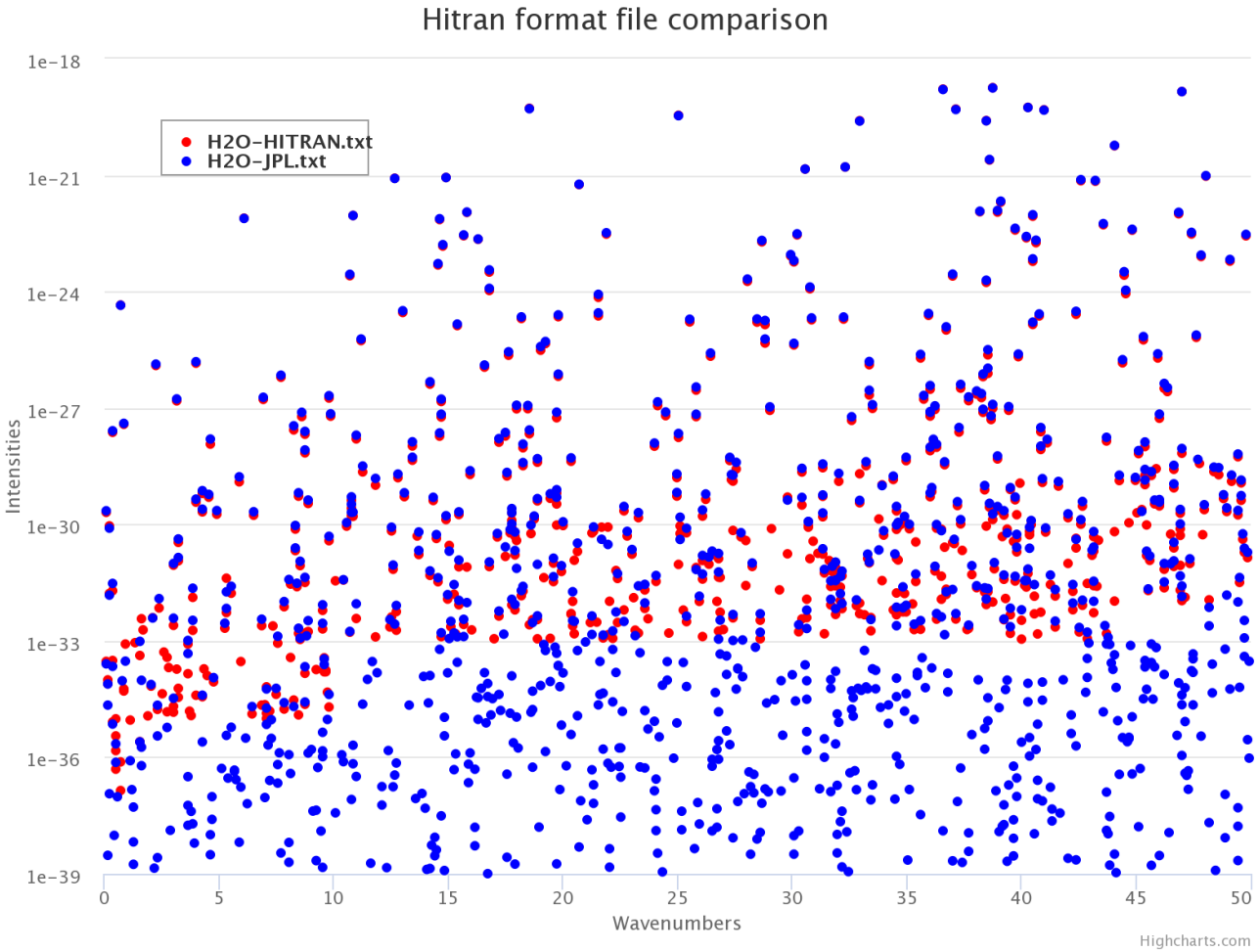
→ Inhomogeneities in some files for the same molecule: need to be fixed on a "case by case" basis.

→ Truncated files when database is too big

New tool developed for VAMDC

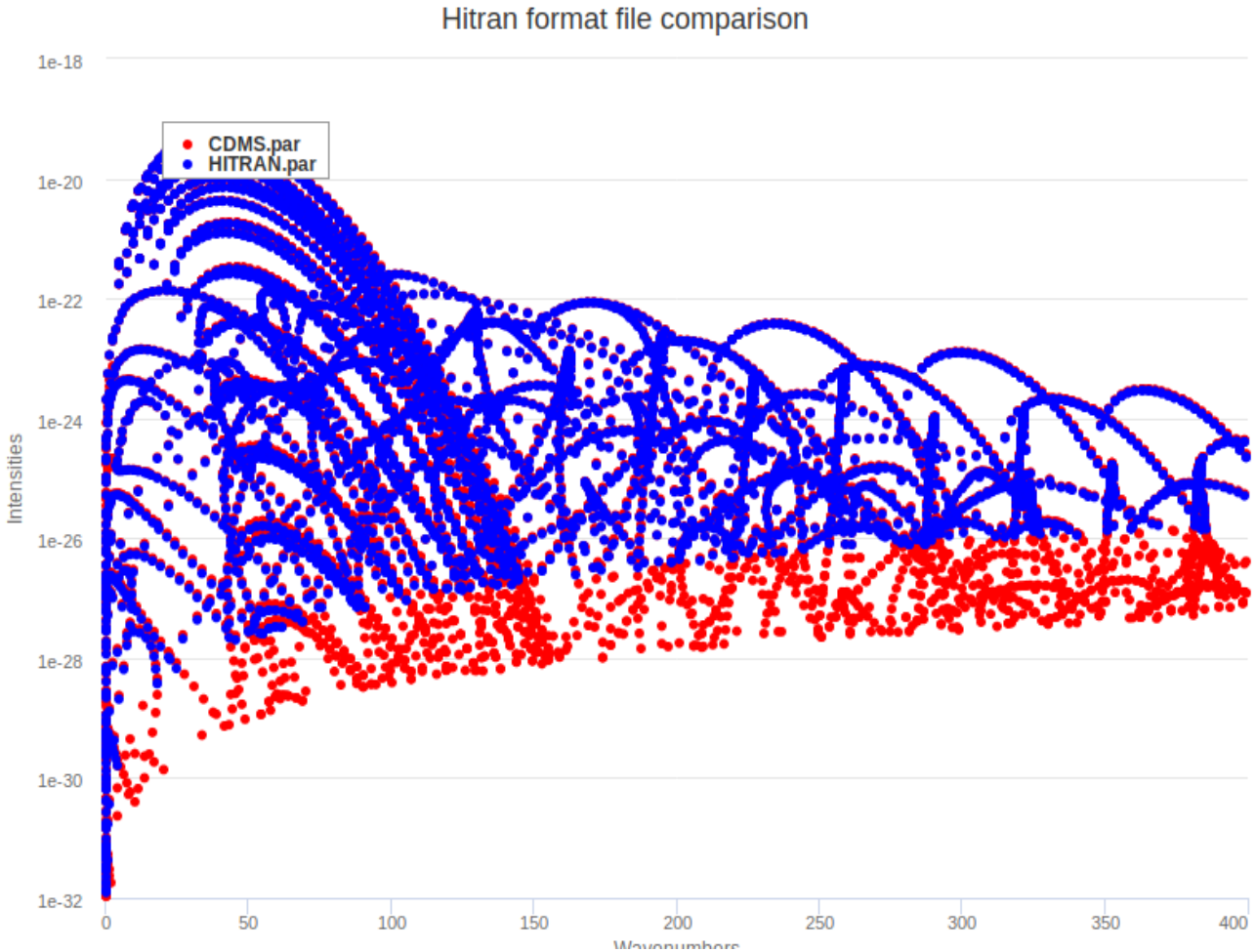


Compare data : H_2O



Compare data : H_2CO

www.vamdc.org/hitran-display



Possible improvements

Databases can be huge :

→ Several **million** of transitions for **MeCaSDa**

→ Several **billion** of transitions for CH_4 in **ExoMol**

There's a limit yet in the XSASMS filesize one can download :

→ Truncated files (limited to 10 000 transitions in most cases)

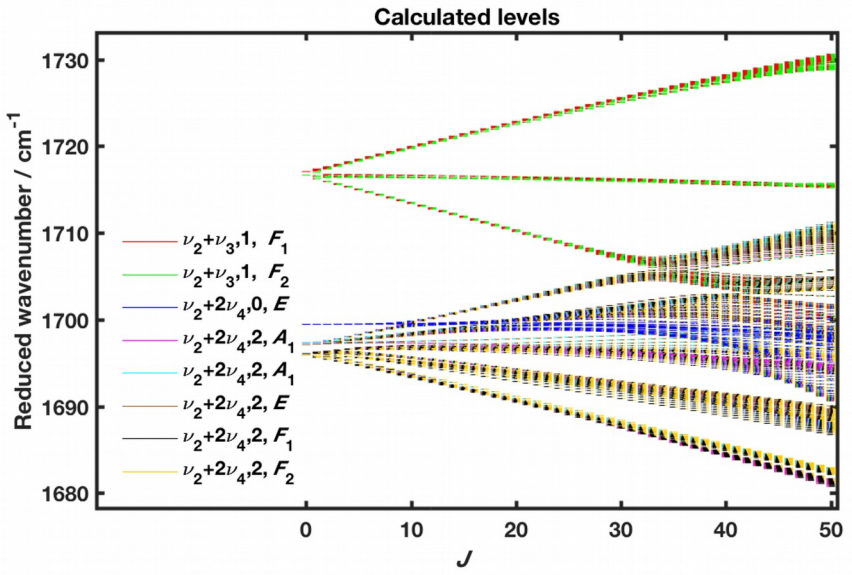
Need asynchronous requests + email

Perspectives

Dijon databases are the only ones to propose the complete decomposition of the eigenvectors :

→ levels viewer

→ porting this tool to VAMDC



Integrate GEISA to VAMDC

Write a new code to convert XSAMS to GEISA