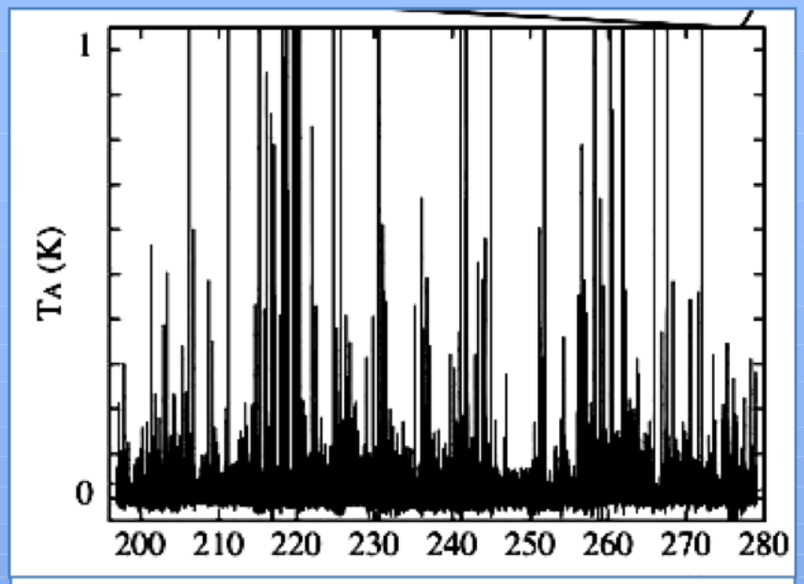
Feedbacks from user-oriented tools: CASSIS

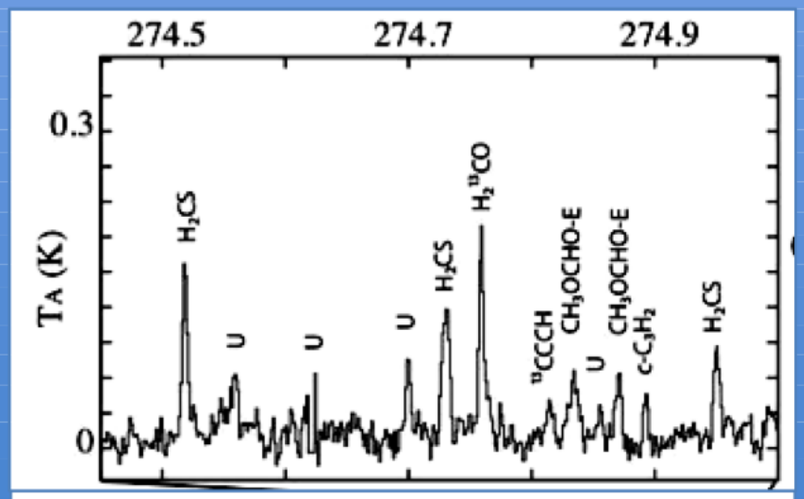
Charlotte Vastel
for the CASSIS team:
Jean-Michel Glorian & Mickael Boiziot
Emmanuel Caux & Sandrine Bottinelli

VAMDC annual meeting, 10-13 June 2020, Virtual

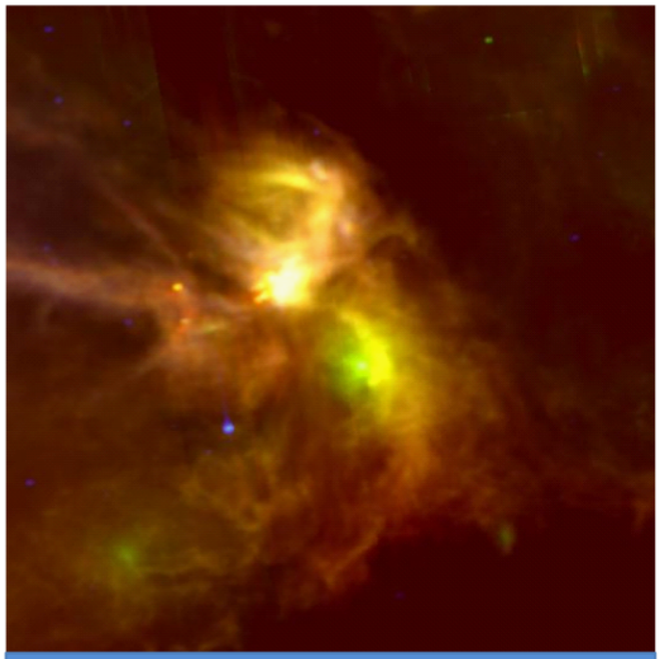
OBSERVATIONS



STEP1: Observe the spectrum of the source.
Tool: telescope

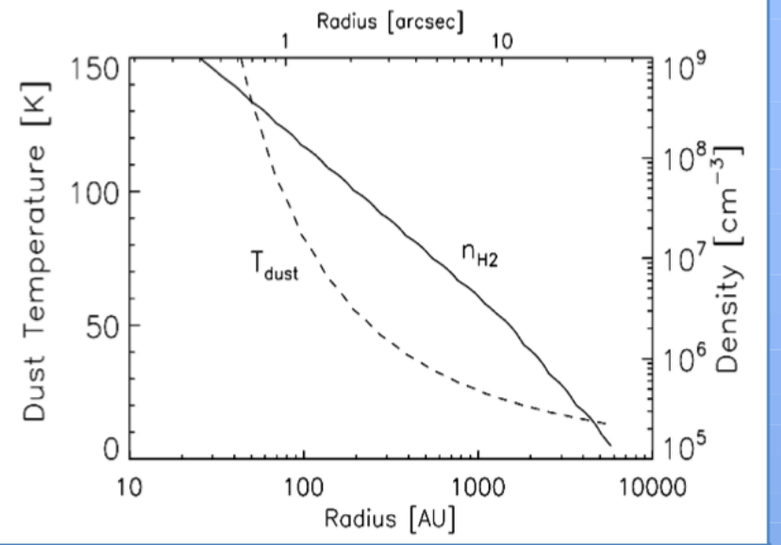


STEP2: Identify the lines and species.
Tool: spectroscopic data

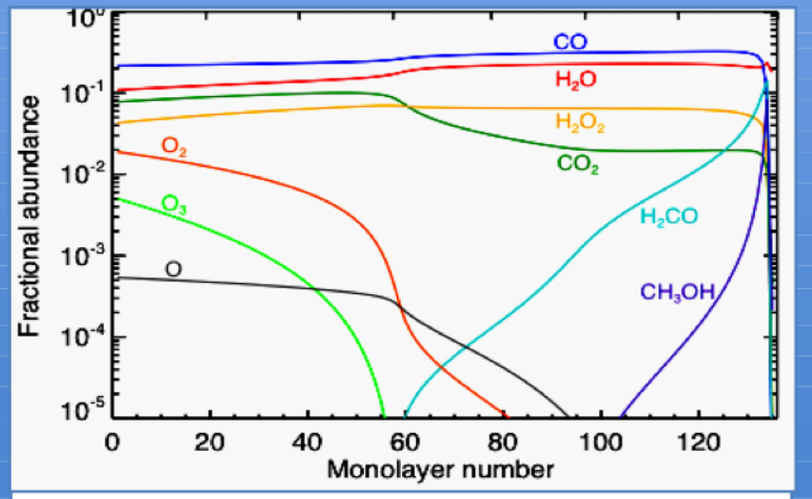


ASTROPHYSICAL OBJECT

TOOLS & MODELS



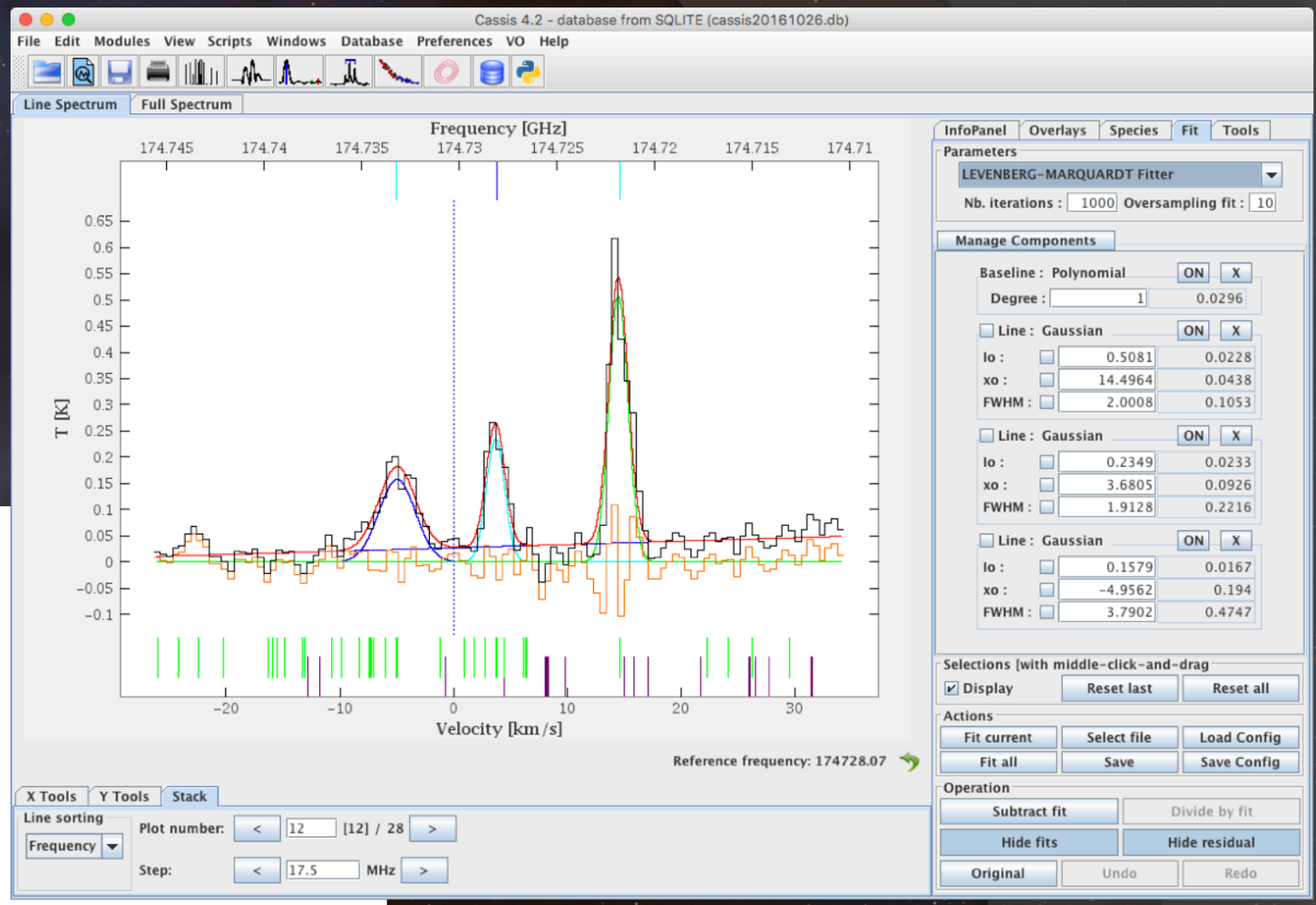
STEP3: Derive the physical and chemical structure.
Tool: radiative transfer models



STEP4: Understand the chemical structure.
Tool: astrochemical models

CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques):

http://cassis.irap.omp.eu/



Astrophysical template
(fixed parameters N, T_k, T_{ex}, N_{H2}, Δv, choice of the molecule…)

Observed spectra
(laboratory or telescope)
SSAP protocol (IVOA)

CASSIS

- **LTE model and Radex**
- **Parameters to vary: N, T_k, T_{ex}, n_{H2}, Δv, choice of the molecule and telescope, beam dilution…**

Spectroscopic and molecular databases (JPL, CDMS, NIST)

TAP protocol (IVOA)

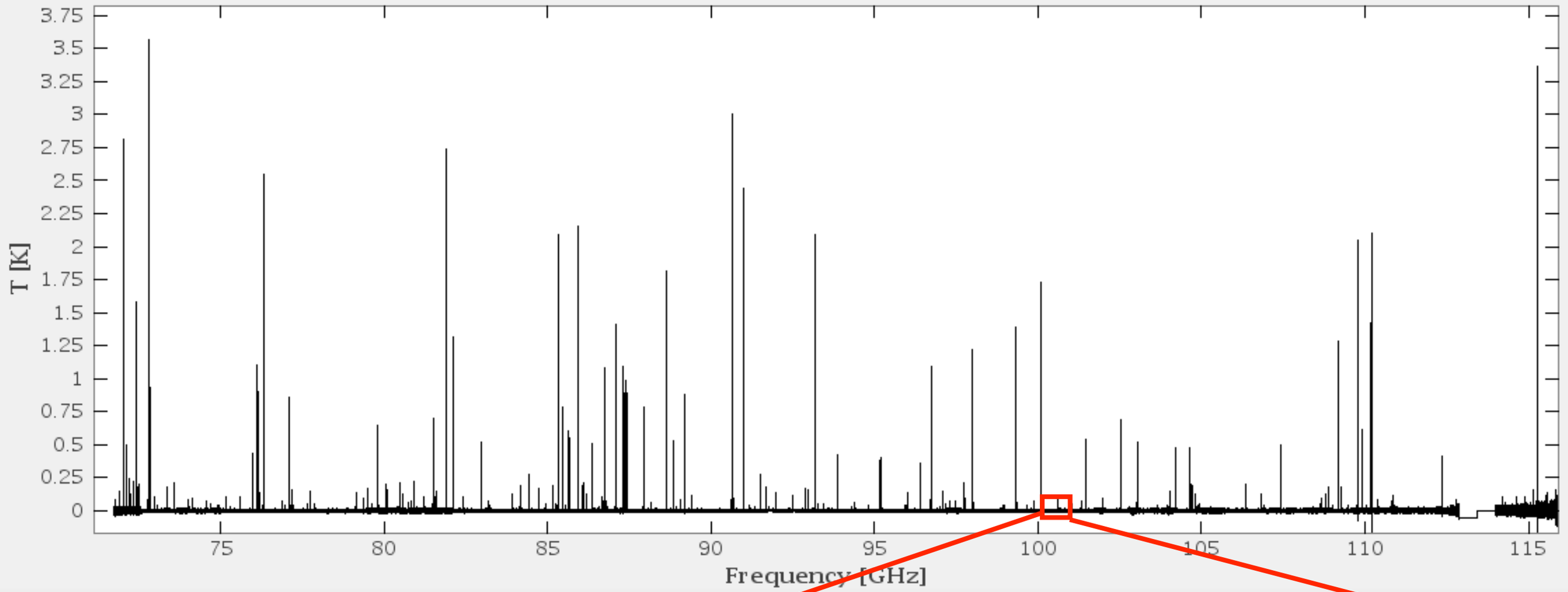
VAMDC
Virtual Atomic and Molecular Data Centre

+ CASSIS own databases with:

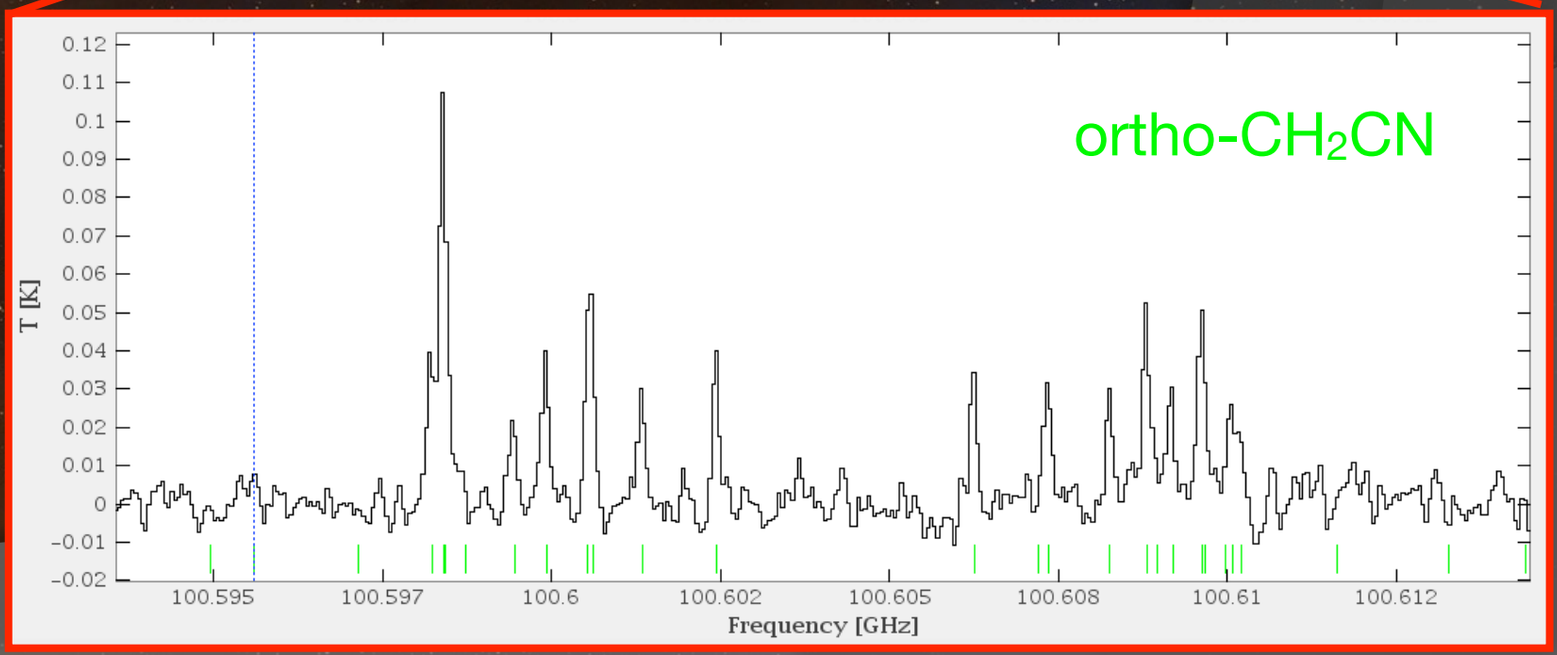
1) ortho / para / A / E separation
2) HFS
3) ~80 entries for Radex compatible collisional files

Synthetic spectra, Line identification, Automatic adjustment (MCMC, χ^2), Rotational diagram

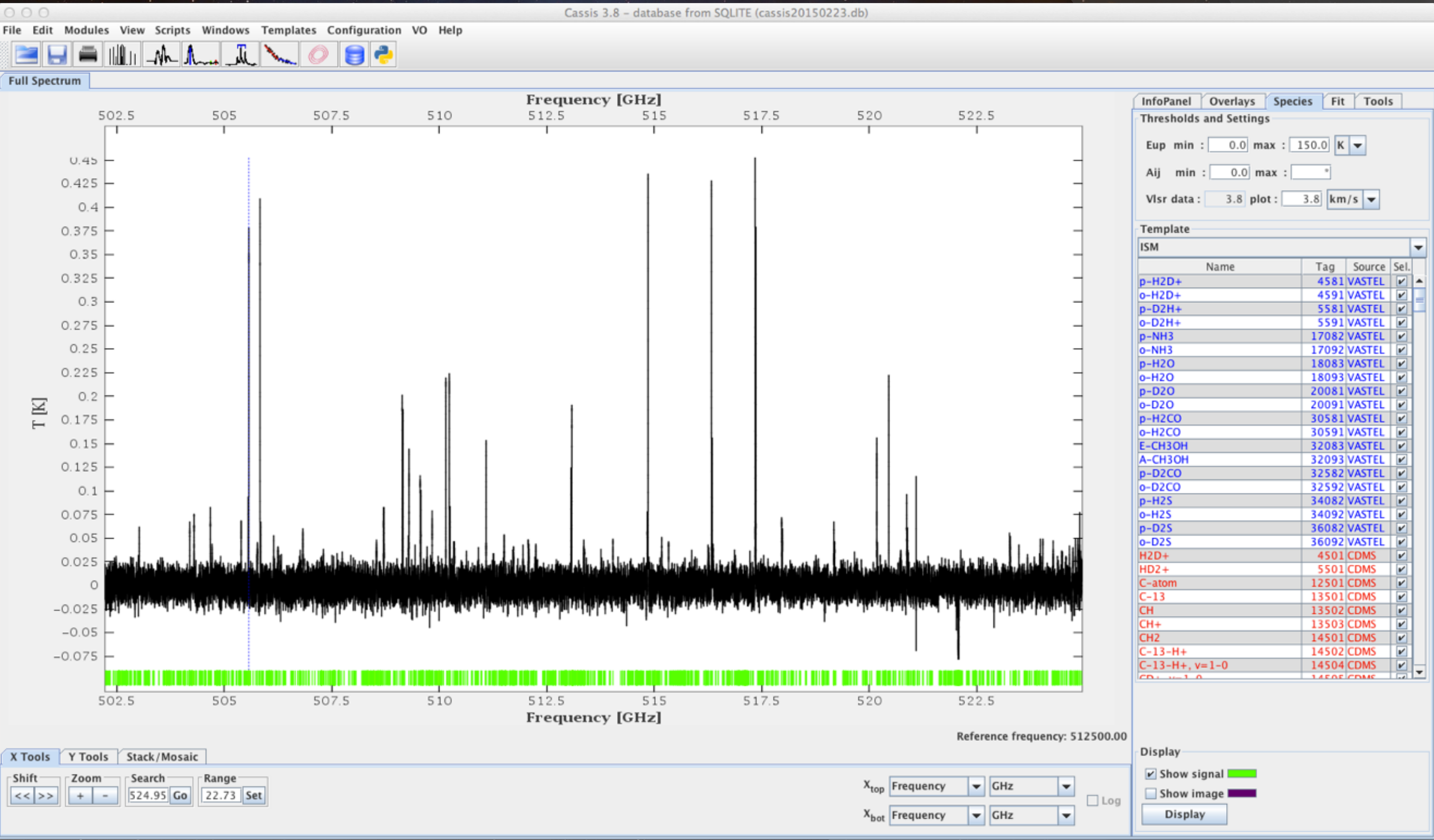
Line Identification



- JPL
- CDMS
- NIST/VALD
- Your own database
- VAMDC



Line Identification



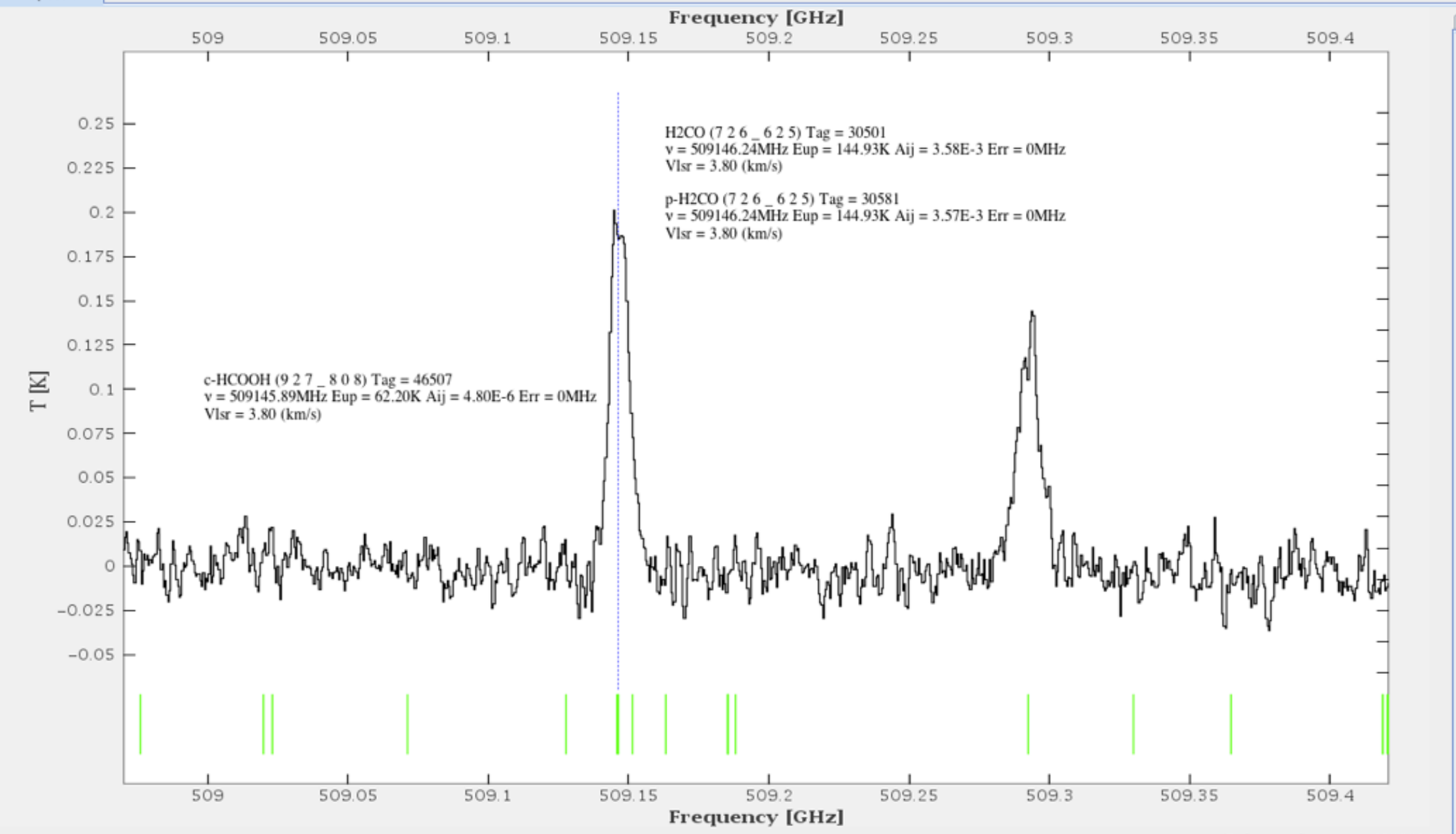
SQLite database

Line Identification

Cassis 3.8 – database from SQLITE (cassis20150223.db)

ile Edit Modules View Scripts Windows Templates Configuration VO Help

Full Spectrum



Reference frequency: 509000.20

InfoPanel | Overlays | Species | Fit | Tools

Thresholds and Settings

Eup min : 0.0 max : 150.0 K

Aij min : 0.0 max :

Vlsr data : 3.8 plot : 3.8 km/s

Template: ISM

Name	Tag	Source	Sel.
p-H2D+	4581	VASTEL	✔
o-H2D+	4591	VASTEL	✔
p-D2H+	5581	VASTEL	✔
o-D2H+	5591	VASTEL	✔
p-NH3	17082	VASTEL	✔
o-NH3	17092	VASTEL	✔
p-H2O	18083	VASTEL	✔
o-H2O	18093	VASTEL	✔
p-D2O	20081	VASTEL	✔
o-D2O	20091	VASTEL	✔
p-H2CO	30581	VASTEL	✔
o-H2CO	30591	VASTEL	✔
E-CH3OH	32083	VASTEL	✔
A-CH3OH	32093	VASTEL	✔
p-D2CO	32582	VASTEL	✔
o-D2CO	32592	VASTEL	✔
p-H2S	34082	VASTEL	✔
o-H2S	34092	VASTEL	✔
p-D2S	36082	VASTEL	✔
o-D2S	36092	VASTEL	✔
H2D+	4501	CDMS	✔
HD2+	5501	CDMS	✔
C-atom	12501	CDMS	✔
C-13	13501	CDMS	✔
CH	13502	CDMS	✔
CH+	13503	CDMS	✔
CH2	14501	CDMS	✔
C-13-H+	14502	CDMS	✔
C-13-H+, v=1-0	14504	CDMS	✔

X Tools | Y Tools | Stack/Mosaic

Shift << >> Zoom + - Search 511.72 Go Range 4.36 Set

X_{top} Frequency GHz

X_{bot} Frequency GHz

Log

Display

Show signal

Show image

Display

SQLite database

Line Identification

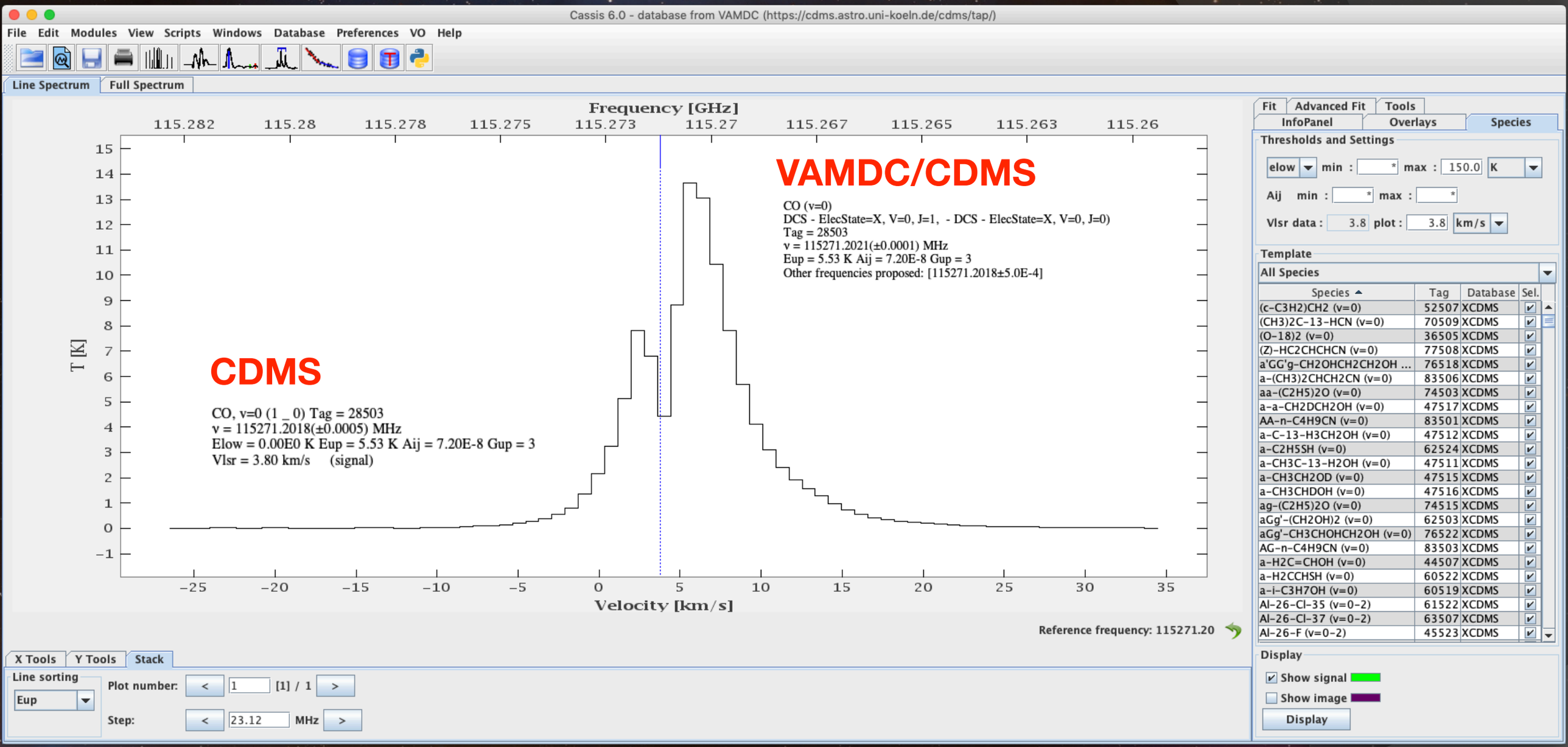
Databases and interoperability

The astronomers need: atomic, molecular databases

Local database (SQLite), built on CDMS, JPL, NIST, and private databases (lab or computations), database with nuclear spin state (ortho, para, A and E): *very quick*
CASSIS sometimes finds incoherences in the databases

Access to the CDMS, JPL and VALD databases linked through VAMDC: *very slow*
Questions:
1) How is the update done through VAMDC? Regularly?
2) Within CASSIS, we must retrieve everything, references included: not useful! Too time consuming. Solution: json?
3) Through the portal, is it possible to select a database only? And define criteria?

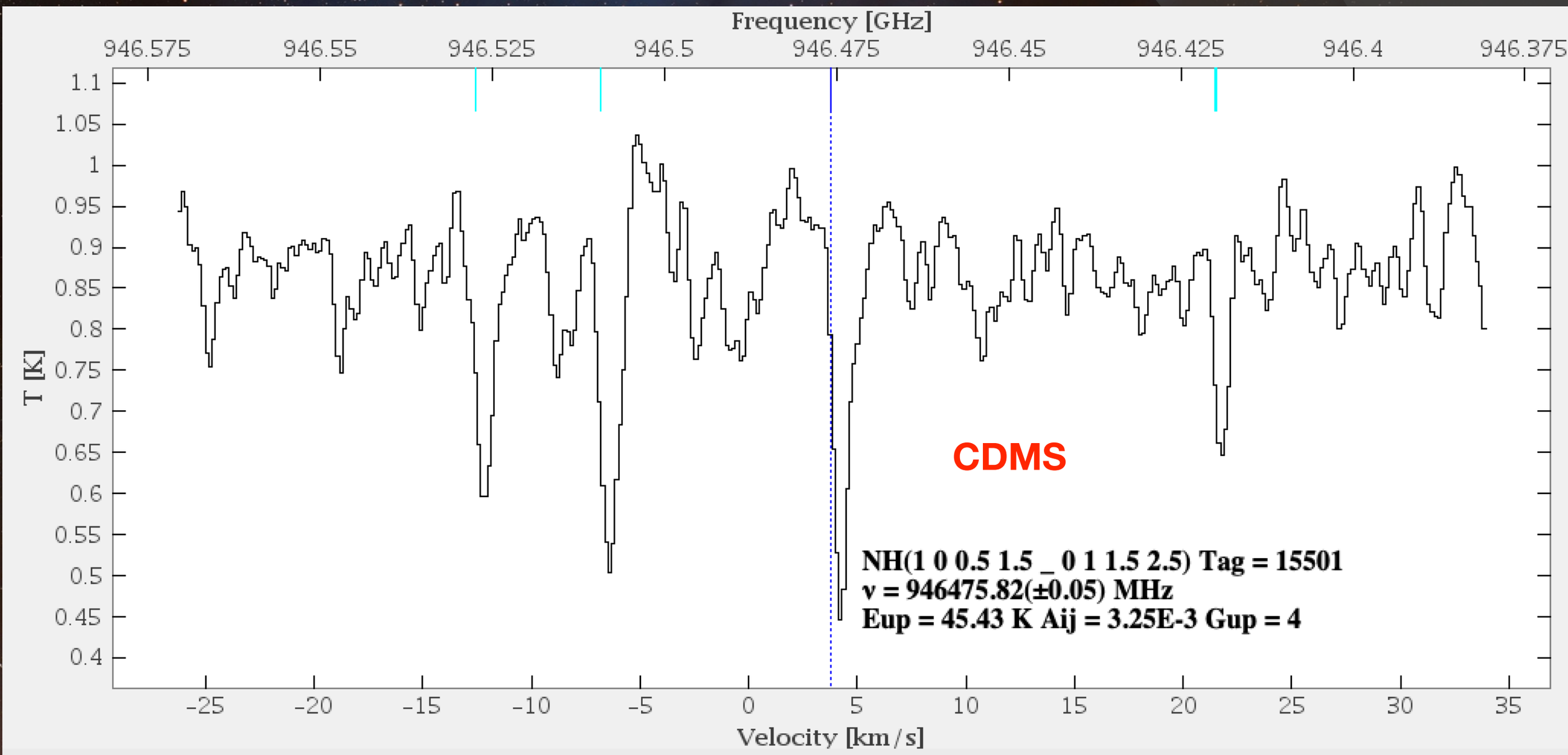
Line Identification: VAMDC Access to CDMS



When many frequencies available, we choose the one one with the lowest uncertainty.

VAMDC: not limited for example for the 3 digit limit on the statistical weigh

Line Identification: VAMDC Access to CDMS



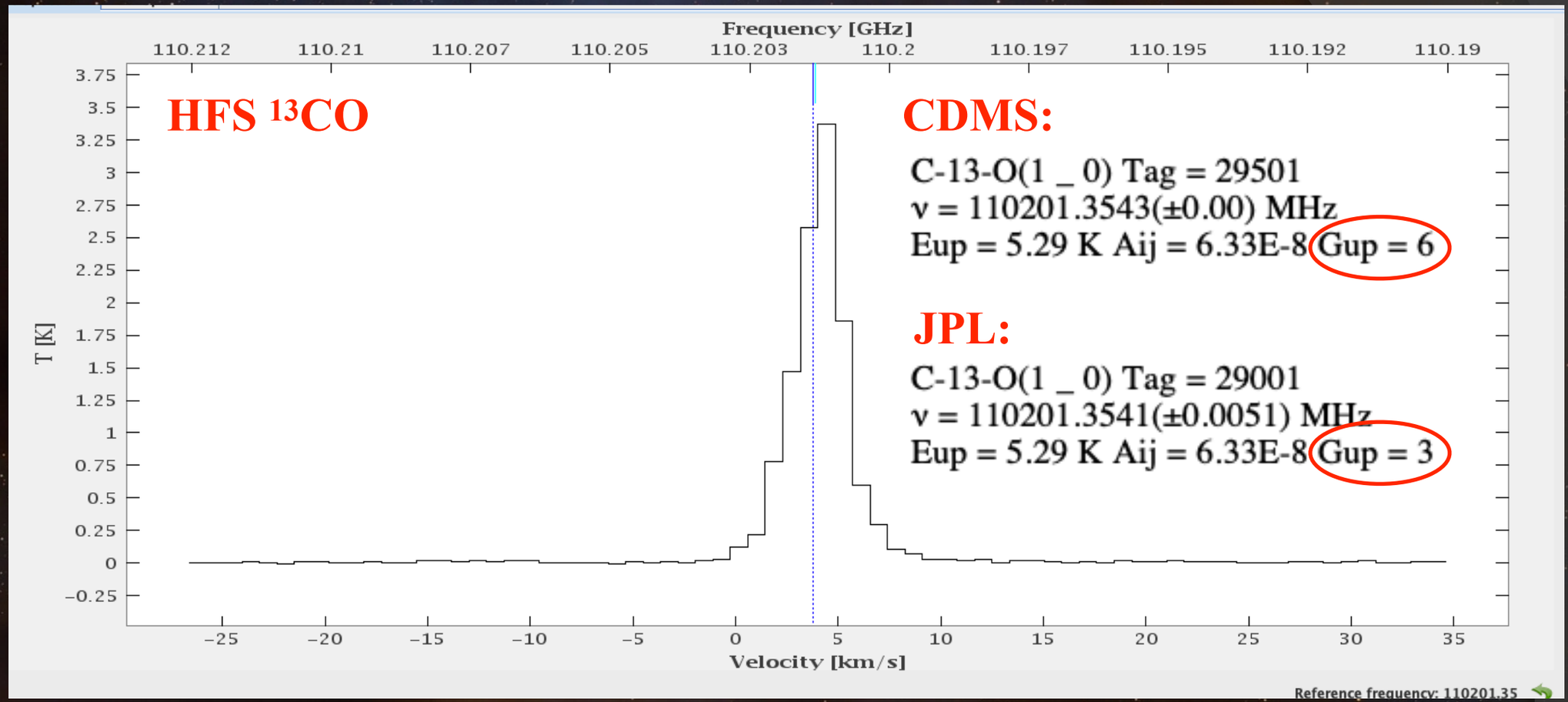
NH from VAMDC decoded in CASSIS:

NH (v=0)(
HUNDB - ElecState=X, S=1.0, F1NuclearSpinRef=N, V=0, FValue=1.5, J=0.0, F1Value=0.5, FNuclearSpinRef=H, N=1, -
HUNDB - ElecState=X, S=1.0, F1NuclearSpinRef=N, V=0, FValue=2.5, J=1.0, F1Value=1.5, FNuclearSpinRef=H, N=0,)
Tag = 15501
ν = 946475.8538(±0.033) MHz
Eup = 45.43 K Aij = 3.25E-3 Gup = 4
Other frequencies proposed: [946475.82±0.05]

4 quantum numbers in CDMS

NH in VAMDC (15mn to download in VAMDC portal):

Line Identification: VAMDC Access to CDMS



VAMDC/CDMS

- **DCS - ElecState=X, V=0, FValue=1.5, J=1, FNuclearSpinRef=C-13, - DCS - ElecState=X, V=0, FValue=0.5, J=0, FNuclearSpinRef=C-13**

ν = 110201.3707(±0.0001) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 4

Other frequencies proposed: [110201.37039±6.6E-4]

- **DCS - ElecState=X, V=0, J=1, - DCS - ElecState=X, V=0, J=0,**

ν = 110201.3543(±0.00) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 6

- **DCS - ElecState=X, V=0, FValue=0.5, J=1, FNuclearSpinRef=C-13, - DCS - ElecState=X, V=0, FValue=0.5, J=0, FNuclearSpinRef=C-13**

ν = 110201.3216(±0.0002) MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 2

Other frequencies proposed: [110201.3218±7.0E-4]

VAMDC/JPL:

- **DCS - ElecState=X, V=0, J=1, - DCS - ElecState=X, V=0, J=0,)**

ν = 110201.3541(±0.0051) MHz

Eup = 5.29 K Aij = 6.33E-8 Gup = 3

Radiative transfert should be easier through VAMDC, but however much slower

Line Identification: Atomic databases

1 simple species, many different frequencies and A_{ij}, f_{ji}, S_{ik}

CHIANTI: 1 4 1215.670 5.550e-01 6.260e+08 1s 2S1/2 - 2p 2P3/2 Lyman alpha

Chianti/VAMDC:

<SpeciesRef>Xchianti-1</SpeciesRef><Probability><TransitionProbabilityA><Value units="1/s">626000000.0</Value></TransitionProbabilityA><WeightedOscillatorStrength><Value units="unitless">0.555</Value></WeightedOscillatorStrength></Probability>

<ProcessClass></ProcessClass></RadiativeTransition><RadiativeTransition id="Pchianti-R10"><EnergyWavelength><Wavelength methodRef="Mchianti-EXP"><Value units="A">1215.67</Value></Wavelength><Wavelength methodRef="Mchianti-THEO"><Value units="A">1215.02</Value></Wavelength></EnergyWavelength><UpperStateRef>Schianti-3000001</UpperStateRef><LowerStateRef>Schianti-1000001</LowerStateRef>

NIST:

Observed	Ritz Wavelength	Aij									
1215.6699	1215.668237310	6.2648e+08	AAA	0.0000000000-2	259.2850014	1s	2S	1/2	2p	2P°	3/2

NIST/VAMDC: ATTENTION: There was an error in making the XML output and at least one item in the following parts was skipped: Atoms RadTran

VALD/VAMDC:

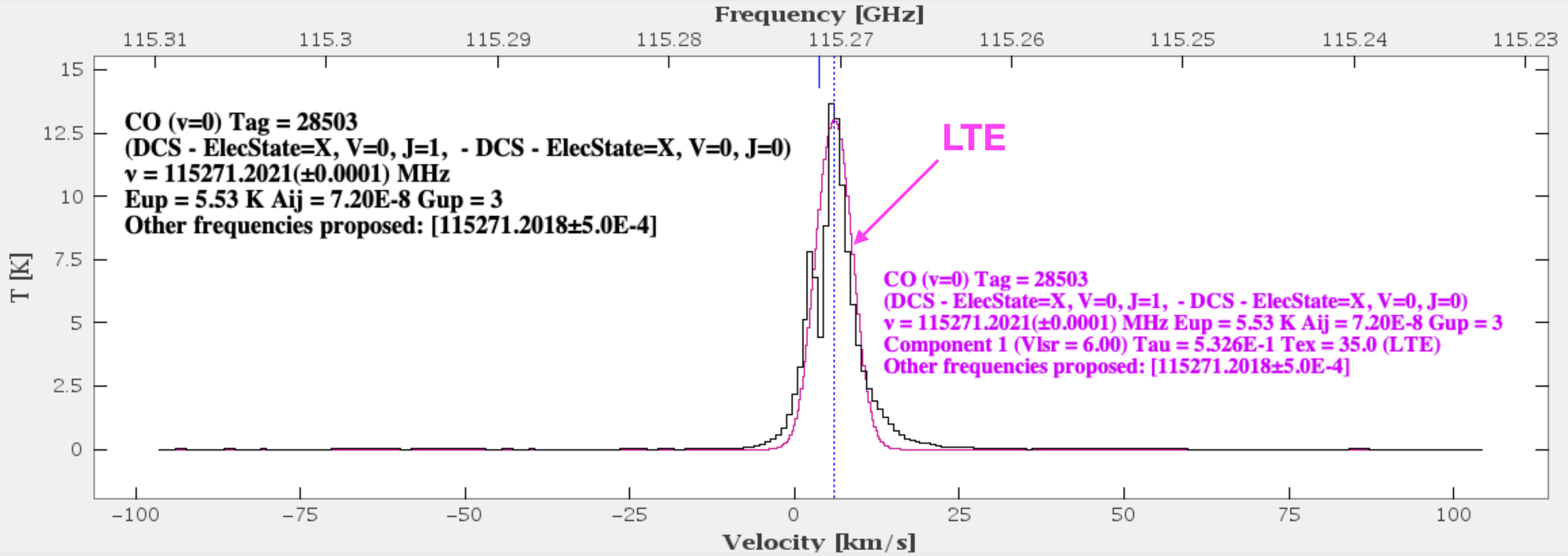
<SpeciesRef>Xvald-1</SpeciesRef><Probability><Log10WeightedOscillatorStrength><SourceRef>Bvald-CDROM18</SourceRef><Value units="unitless">-0.801</Value></Log10WeightedOscillatorStrength></Probability><ProcessClass></ProcessClass><Broadening name="natural" envRef="Evald-natural"><Comments>Natural Broadening</Comments><SourceRef>Bvald-CDROM18</SourceRef><Lineshape name="lorentzian"><LineshapeParameter name="log(gamma)"><Value units="1/s">8.77</Value></LineshapeParameter></Lineshape></Broadening></RadiativeTransition><RadiativeTransition id="Pvald-R154476610" process="excitation"><EnergyWavelength><Wavelength><Comments>Vacuum wavelength from state energies (RITZ)</Comments><SourceRef>Bvald-CDROM18</SourceRef><Value units="A">1215.67100000</Value><Wavelength><Wavelength><Comments>Vacuum wavelength from measurements (non-RITZ)</Comments><SourceRef>Bvald-CDROM18</SourceRef><Value units="A">1215.67089746</Value></Wavelength></EnergyWavelength><UpperStateRef>Svald-1105790</UpperStateRef><LowerStateRef>Svald-1021407</LowerStateRef>

Kentucky database (Not in VAMDC):

-LAMBDA-VAC-ANG-	-SPECTRUM--	TT	--------TERM---------	---J---	----LEVEL ENERGY--CM-1----
1215.6700	H I	E1	1-2	1/2-*	0.00 - 82259.11

Radiative transfer: LTE

1) Line identification through VAMDC
2) LTE modelling using the partition function, Aij, gu, frequencies given by VAMDC



Radiative transfer: non-LTE

Collisional databases

Line Analysis 1

Data
Load | 'IRAS16293_SS/iram.bas | Vlsr data: 3.8 km/s | in: REST | Telescope ???

Tuning
Range min: 79.9948749 max: 281.004874 GHz | Band: 60.0 km/s

Threshold
Eup min: 0.0 max: 150.0 K | Aij min: 0.0 max: *
Jup min: * max: * | Kup min: * max: * | Lup min: * max: * | Mup min: * max: *

Template: All Species

Name	Tag	Sel.
C-13-N	27004	
C-13-N	27505	
C-13-N-15	28505	
C-13-O	29001	
C-13-O	29501	✓
C-13-O+	29519	
C-13-O-17	30503	
C-13-O-18	31502	
C-13-O-1...	31511	
C-13-S	45001	
C-13-S, v...	45501	

Load config | Display | Save config

LTE-RADEX ✓

Telescope: apex | Tmb->Ta *
Observing Mode: PSw/DBSw
Background: Tbg: 2.73 K
Noise: rms: 0.0 mK
Oversampling: Oversampling: 3.0

Continuum | ✓ Component 1 X | +

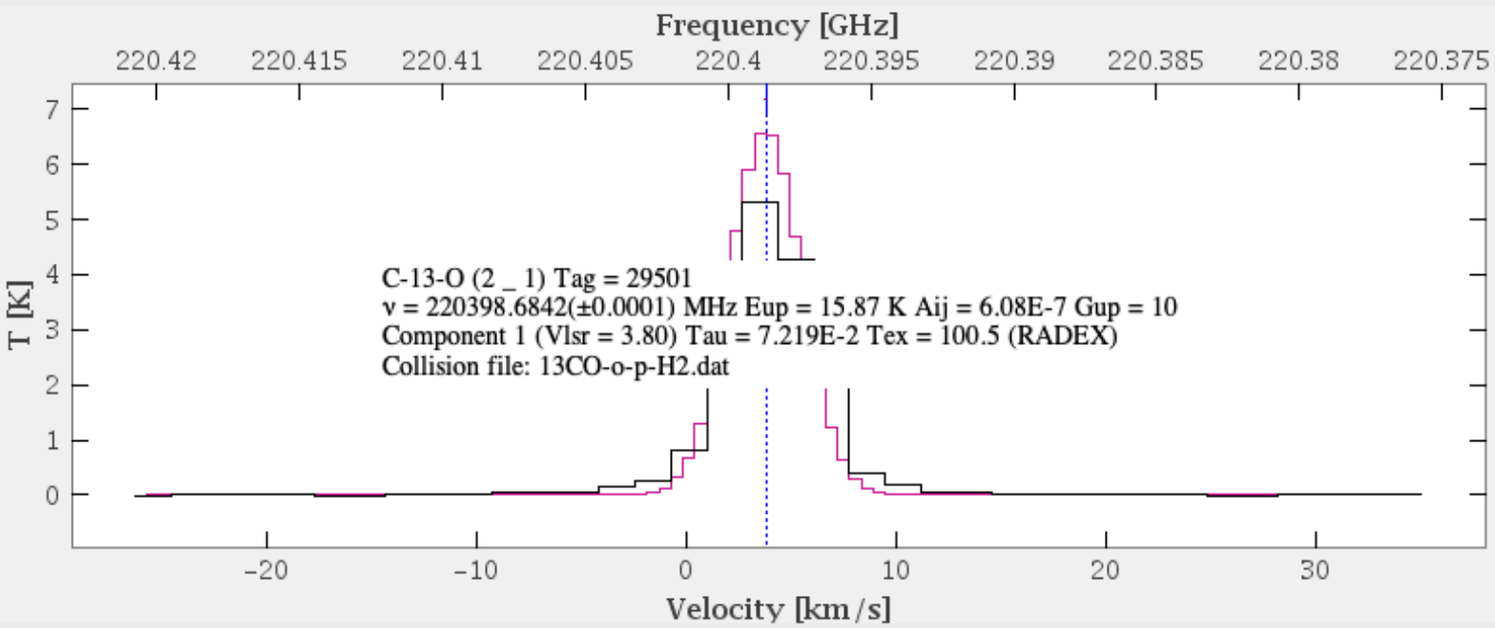
Mode: Full Radex | Interacting | $N(H_2)$ [cm^{-2}]: 7.5E22
Molecules: -- Operations -- | Geometry: Sphere | V_{lsr}: 3.8 km/s

Species	Tag	Database	Collision	Compute	N(Sp) (cm^{-2})	Abundance (/...	TKin (K)	FWHM (km/s)	Size (")
C-13-O	29501	CDMS	13CO-o-p-H...	✓	4.00E16	5.33E-7	100.00	4.00	3000.00

Cassis 6.0 - database from SQLITE (cassis20200513-FORCOM-HFS-IRAP.db)

File Edit Modules View Scripts Windows Database Preferences VO Help

Line Spectrum



Reference frequency: 220398.68

X Tools | Y Tools | Stack

Line sorting: Frequency
Plot number: < 2 [1,2] / 2 >
Step: < 22.19 MHz >

Fit | Advanced Fit | Tools
InfoPanel | Overlays | Species

Thresholds and Settings
eup min : * max : 150.0 K
Aij min : * max : *
Vlsr data : 3.8 plot : 3.8 km/s

Template: All Species

Species	Tag	Database	Sel.
(c-C3H2)CH2	52507	CDMS	
(O-18)2	36505	CDMS	
13C-CCH, v4=0,1mS	38504	CDMS	
13CH	14003	JPL	
13CH313CN	43005	JPL	
13CH3CH2OH	47094	IRAP	
13CH3D	18006	JPL	
15-NO	31009	JPL	

Display
Show signal
Show image
Display

```
!MOLECULE
HCN
!MOLECULAR WEIGHT
27.0
!NUMBER OF ENERGY LEVELS
4
!LEVEL + ENERGIES(cm^-1) + WEIGHT + J,F
   1          0.0000                3.0        0 1
   2          2.9564                1.0        1 0
   3          2.9564                3.0        1 1
   4          2.9564                5.0        1 2
!NUMBER OF RADIATIVE TRANSITIONS
33
!TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_u(K)
   1    2    1              2.4075e-05          88.6339360    4.25
   2    3    1              2.4075e-05          88.6304160    4.25
   3    4    1              2.4075e-05          88.6318470    4.25
```

```
!NUMBER OF COLL PARTNERS
1
!COLLISIONS BETWEEN
1 HCN-H2 scaled (*1.37) HCN-He from Green & Thaddeus (1974) + extrapolation
!NUMBER OF COLL TRANS
6
!NUMBER OF COLL TEMPS
4
!COLL TEMPS
                                5.0          10.0          20.0          30.0
!TRANS + UP + LOW + COLLRATES(cm^3 s^-1)
   1          2          1          1.3e-11       1.1e-11       9.2e-12       8.4e-12
   2          3          1          1.3e-11       1.1e-11       9.2e-12       8.4e-12
   3          3          2          0.0e+00       0.0e+00       0.0e+00       0.0e+00
   4          4          1          1.3e-11       1.1e-11       9.2e-12       8.4e-12
   5          4          2          0.0e+00       0.0e+00       0.0e+00       0.0e+00
   6          4          3          0.0e+00       0.0e+00       0.0e+00       0.0e+00
```

Spectroscopic parameters: matching needs to be done between the collision files and the spectroscopic parameters (JPL, CDMS) used in CASSIS.
For 1 molecule found in CDMS and JPL we need 2 collisional files (different quantum numbers, frequencies etc…)

Collisions

https://basecol.vamdc.eu/collisions.html

```
! Molecule
H2O - ortho
! MASS
18.01
! Number of Energy Level : jpl V6 PNov. 2005 -- http://spec.jpl.nasa.gov/ftp/pub/catalog/doc/d018003.cat
5
! LEVEL + ENERGY(CM-1) + WEIGHT + QUANTUM NOS.  Ka_Kc_tau_J
   1       23.794400       9     0_1_-1_1
   2       42.371700       9     1_0_1_2
   3       79.496400      15     1_2_-1_2
   4      134.901600      15     2_1_1_3
   5      136.761700      21     0_3_-3
! NUMBER OF RADIATIVE TRANSITIONS : jpl V6 PNov. 2005 -- http://spec.jpl.nasa.gov/ftp/pub/catalog/doc/d018003.cat
10
! TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_up(K)
   1    2    1      34.6009E-4      556.9360020     60.966475
   2    2    1      34.6009E-4      556.9360020     60.966576
   3    3    1      5.59938E-2     1669.9047750    114.383309
   4    3    1      5.59938E-2     1669.9047750    114.383273
   5    4    2      25.7413E-2     2773.9765880    194.103022
   6    4    2      25.7413E-2     2773.9765880    194.103127
   7    4    3      3.06509E-2     1661.0076370    194.103127
   8    4    3      3.06509E-2     1661.0076370    194.103022
   9    5    3      5.05947E-2     1716.7696330    196.779424
  10    5    3      5.05947E-2     1716.7696330    196.779452
! NUMBER OF COLLISION PARTNERS
1
! COLLISION PARTNER
1
! COLLISIONS BETWEEN, BASECOL V1 2017-10
2 para-H2-H2O-ortho
! NUMBER OF COLLISIONAL TRANSITIONS
10
! NUMBER OF COLLISION TEMPERATURES
7
! COLLISION TEMPERATURES
20.0       40.0       60.0       80.0       100.0      120.0      140.0
! TRANS + UP + LOW + RATE COEFFS(cm^3 s^-1)
   1    2    1    1.1700e-11    1.6000e-11    1.8900e-11    2.1600e-11    2.4400e-11    2.7200e-11    3.0300e-11
   2    3    1    2.0200e-11    2.1700e-11    2.2500e-11    2.3500e-11    2.4700e-11    2.6300e-11    2.7800e-11
   3    3    2    1.6800e-11    1.6800e-11    1.6100e-11    1.5600e-11    1.5200e-11    1.4900e-11    1.4800e-11
```

4

3

?

different quantum numbers compared to JPL

different frequencies and Einstein coef compared to JPL

References to the collisional database missing

JPL: 556935.9877 0.0003 -0.8189 3 23.7944 9 -180031404 1 1 0 0 1 0 1 0

Databases and interoperability

Our needs for radiative transfer: collisional databases based on LAMDA and/or BASECOL

The CASSIS software provides a database for the collision rates with a matching for the provided databases (~ 80 entries)

→ One species, multiple IDs. Exemple: SO 48501 (CDMS) and 48001 (JPL). Multiple collision files (ortho and para H_2, He scaled, multiple authors).

→ Matching of the frequencies, Aij, quantum numbers between the collision files and the spectroscopic databases to produce synthetic spectra.

To do for CASSIS: directly interrogate VAMDC to use the collision files (XSAMS): SAMP?

http://cassis.irap.omp.eu/?page=catalogs-collision

45506	HCS+	hcsp-h2.dat	H2	adopting HCO+ - H2 from Flower (1999) + extrapolation	from LAMDA, Aug 24, 2017	T=[10-2000] K
48001	SO	so-He-scaled.dat	He scaled (*1.363)	Lique et al (2006)	from LAMDA, Aug 23, 2017	T=[60-300] K
48001	SO	so-pH2.dat	para H2	Lique et al (2007)	constructed by CV from BASECOL, Aug 23, 2017	T=[5-50] K
48501	SO	so-He-scaled.dat	He scaled (*1.363)	Lique et al (2006)	from LAMDA, Aug 23, 2017	T=[60-300] K
48501	SO	so-pH2.dat	para H2	Lique et al (2007)	constructed by CV from BASECOL, Aug 23, 2017	T=[5-50] K
51501	HC3N	hc3n-oph2-cdms.dat	ortho and para H2	Faure et al. 2016 MNRAS 460 2103	Given by A. Faure	T=[10-300] K