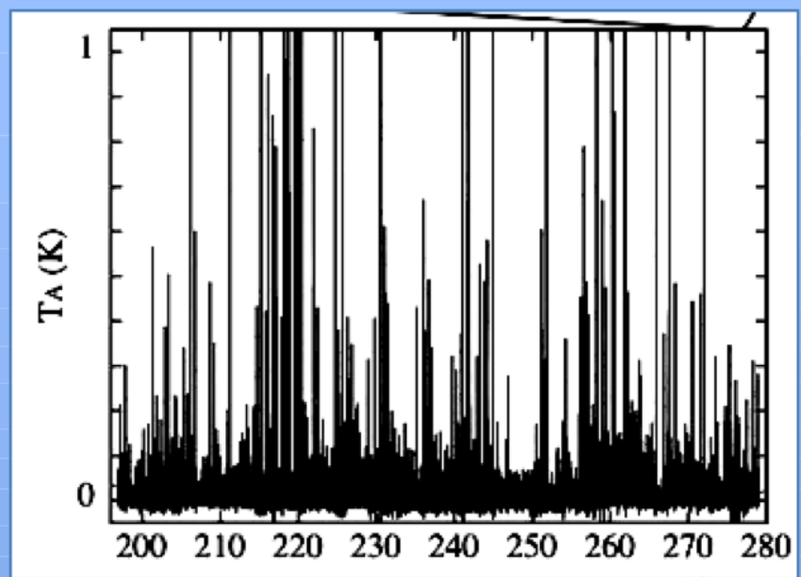
Radiative Transfer: link with the databases

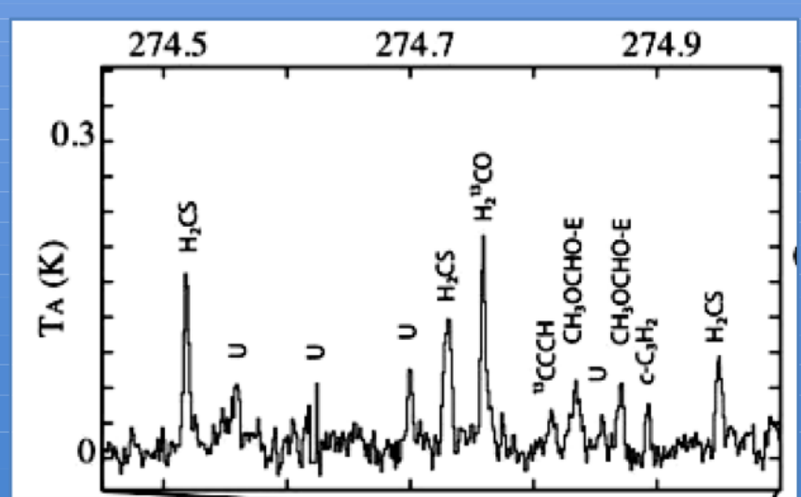
Charlotte Vastel

Workshop Pole Atomes et Molécules, 18-18 janvier 2018, Paris

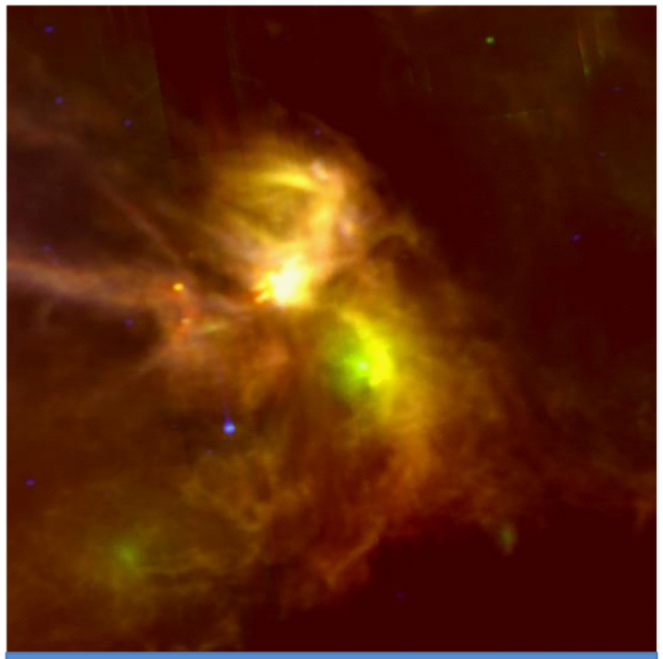
OBSERVATIONS



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

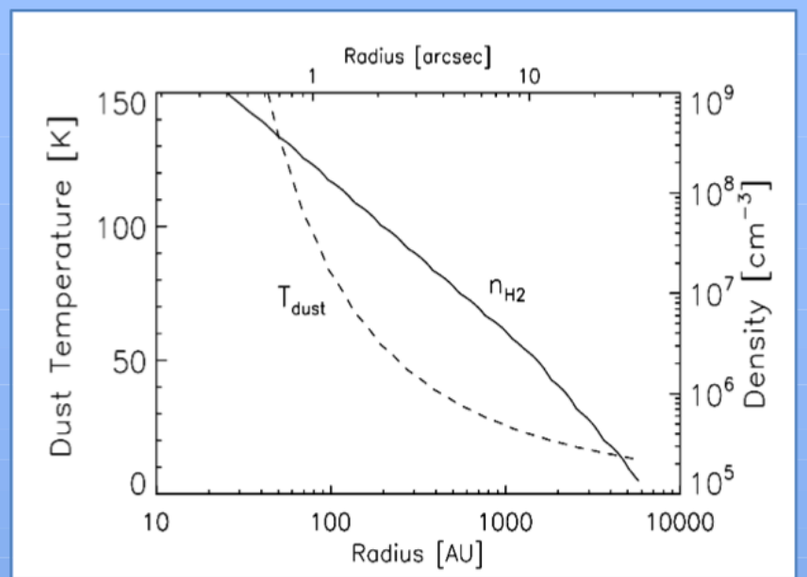


STEP2: Identify the lines and species.
Tool: spectroscopic data

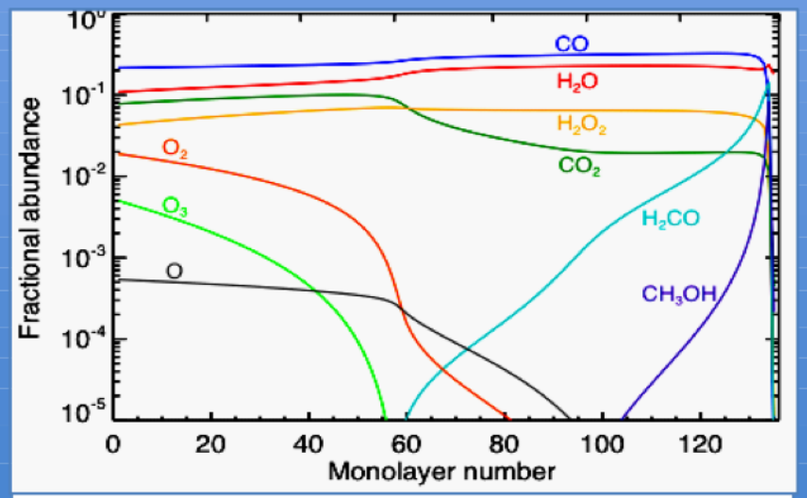


ASTROPHYSICAL OBJECT

TOOLS & MODELS

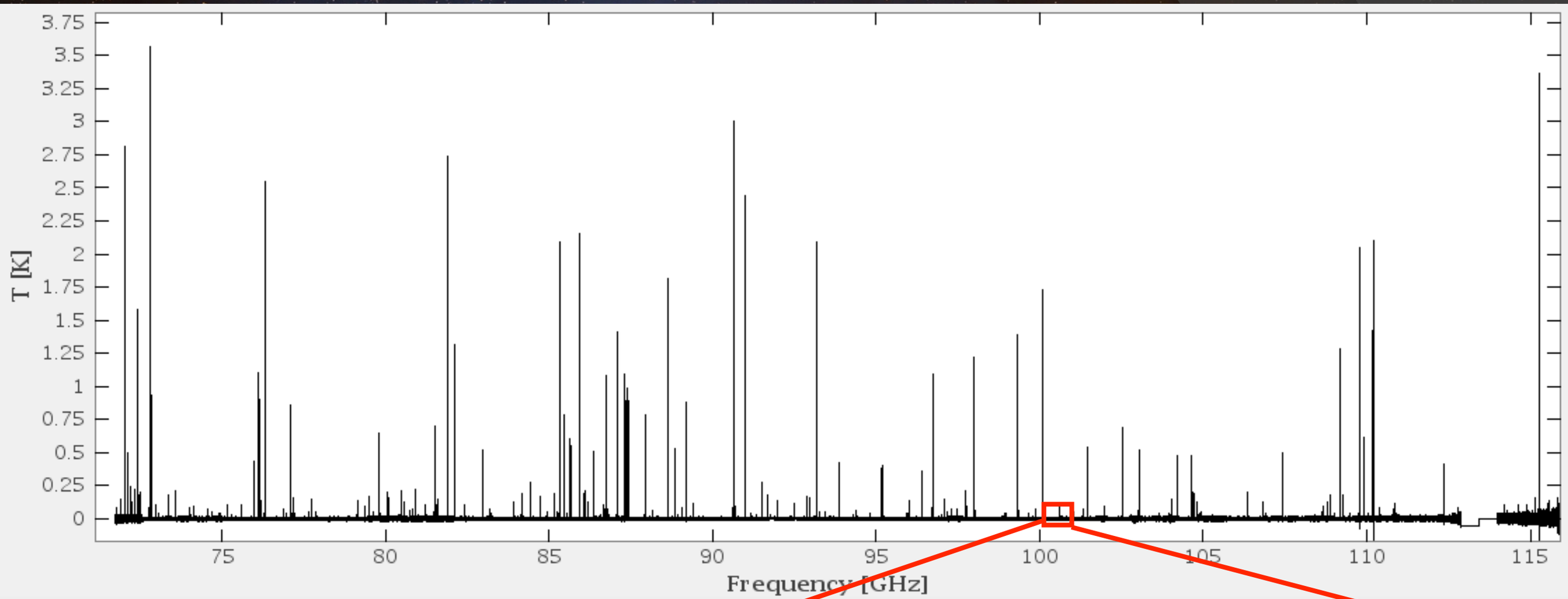


STEP3: Derive the physical and chemical structure.
Tool: radiative transfer models

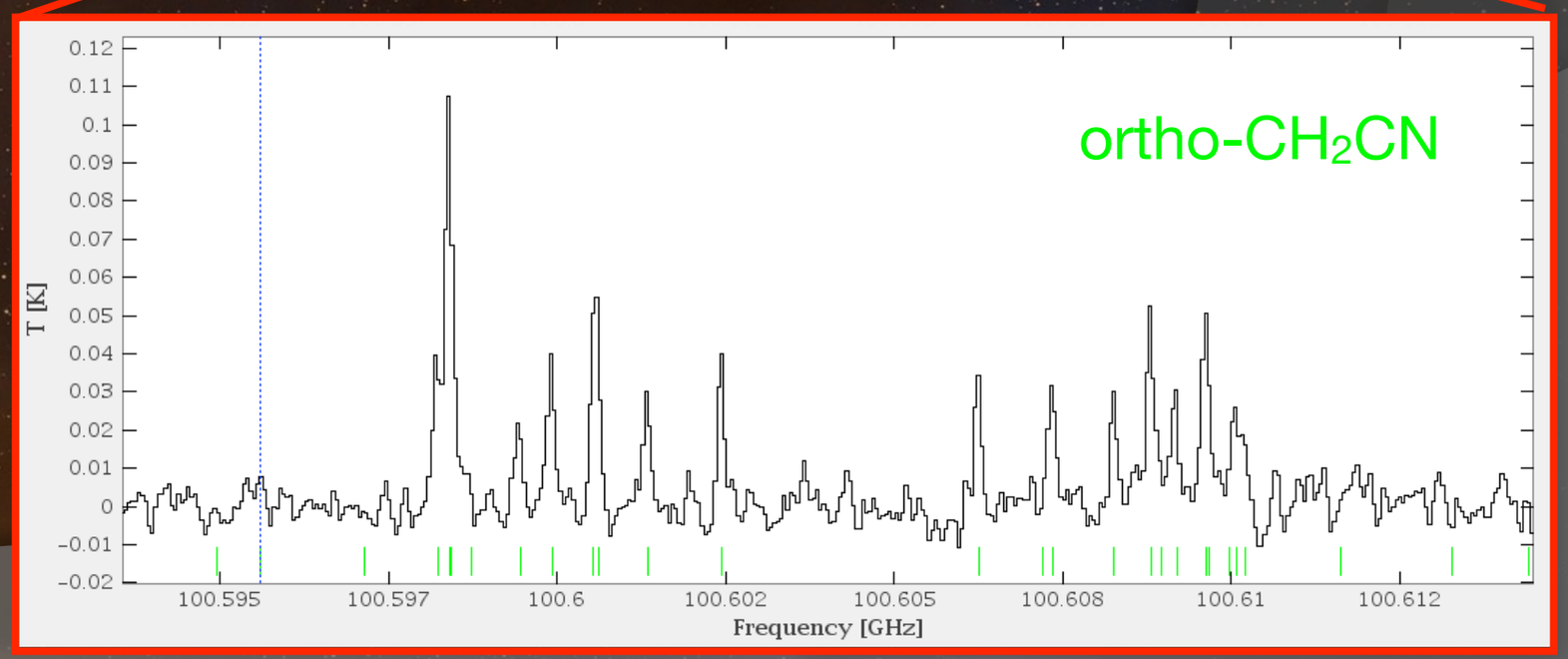


STEP4: Understand the chemical structure.
Tool: astrochemical models

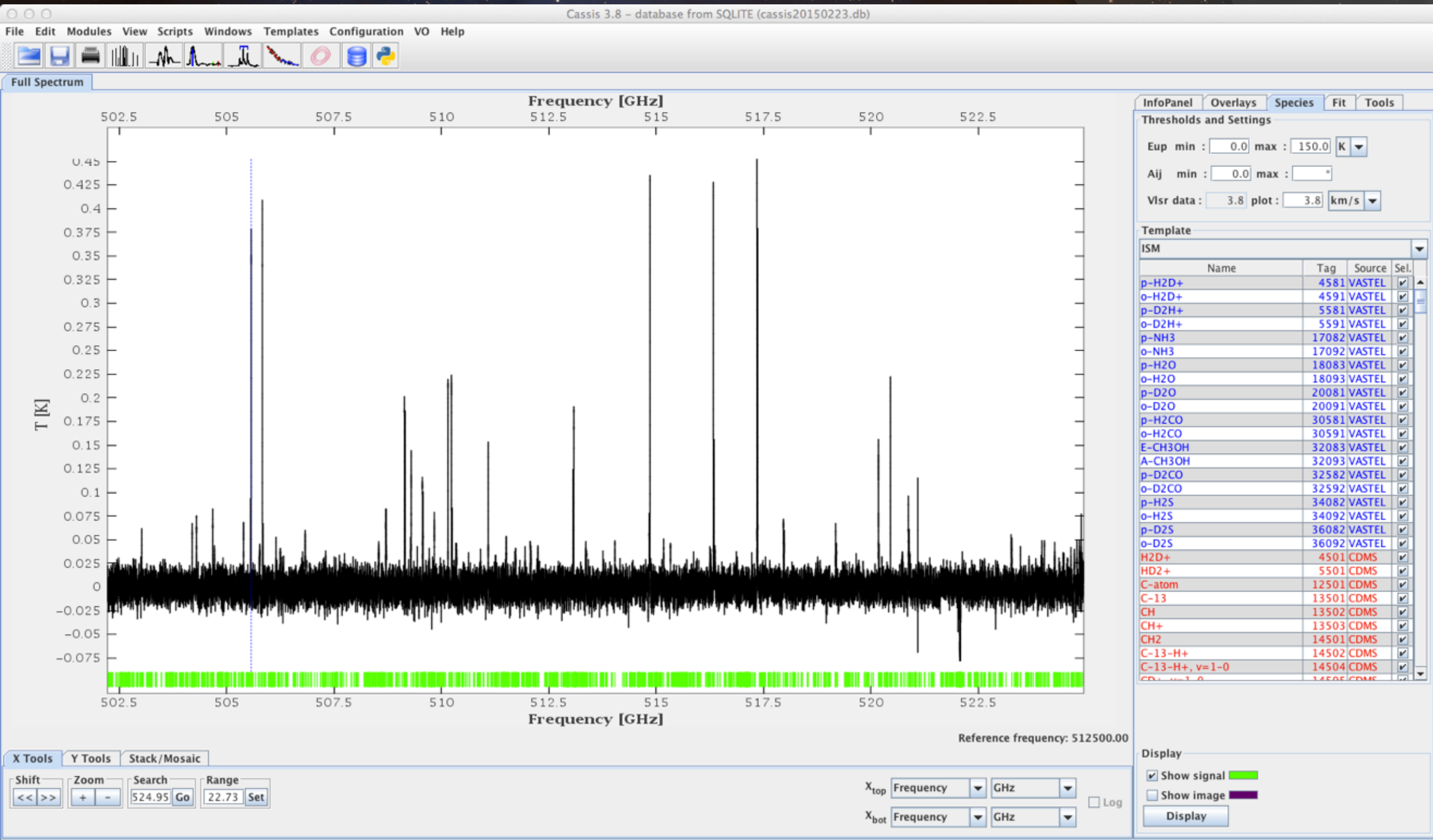
Line Identification



- JPL
- CDMS
- NIST/VALD
- Your own database
- VAMDC (CASSIS, MAGIX)



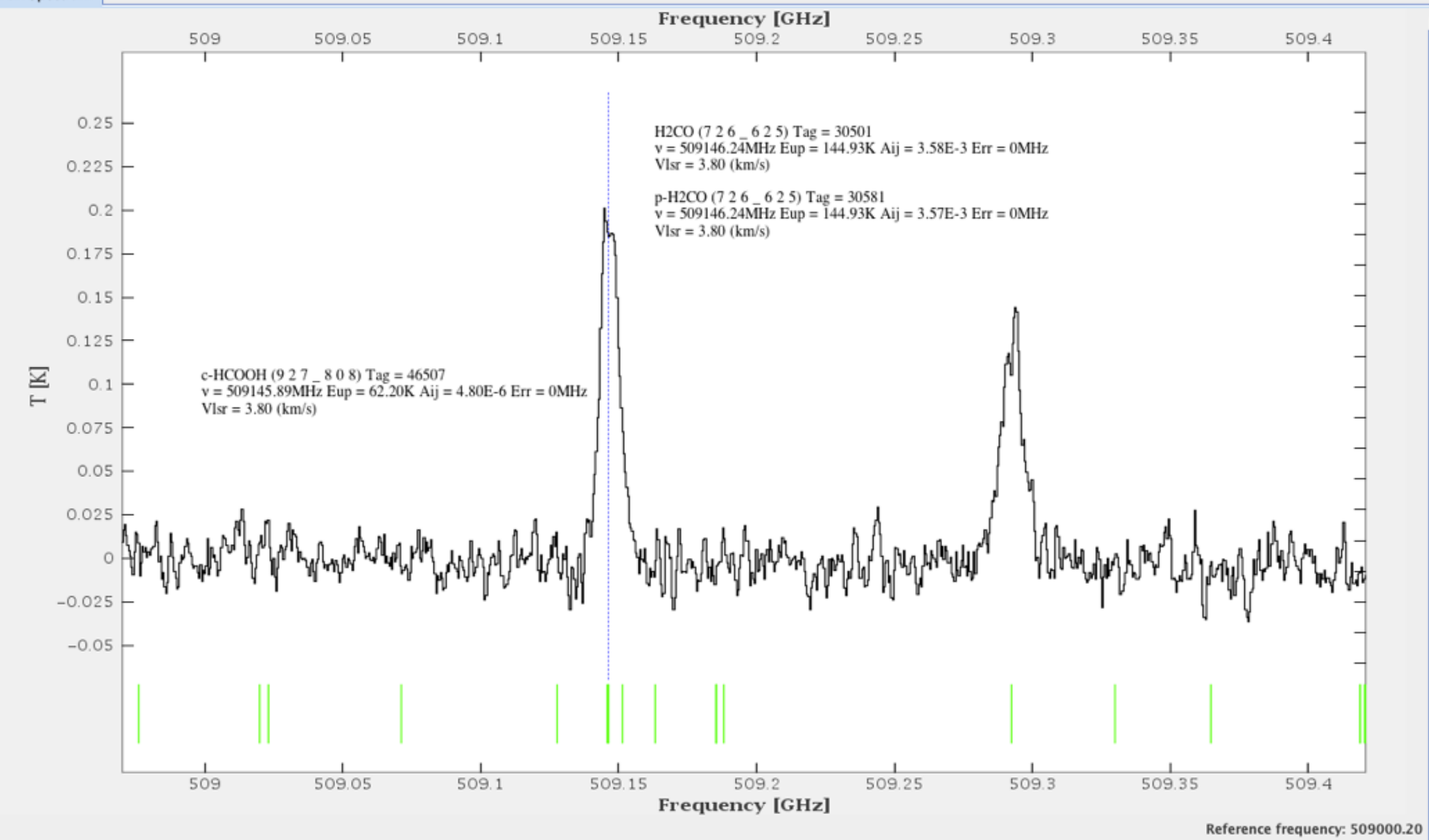
Line Identification



Cassis 3.8 – database from SQLITE (cassis20150223.db)

ile Edit Modules View Scripts Windows Templates Configuration VO Help

Full Spectrum



Reference frequency: 509000.20

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

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	✓

Display

✓ Show signal

Show image

Display

Databases and interoperability

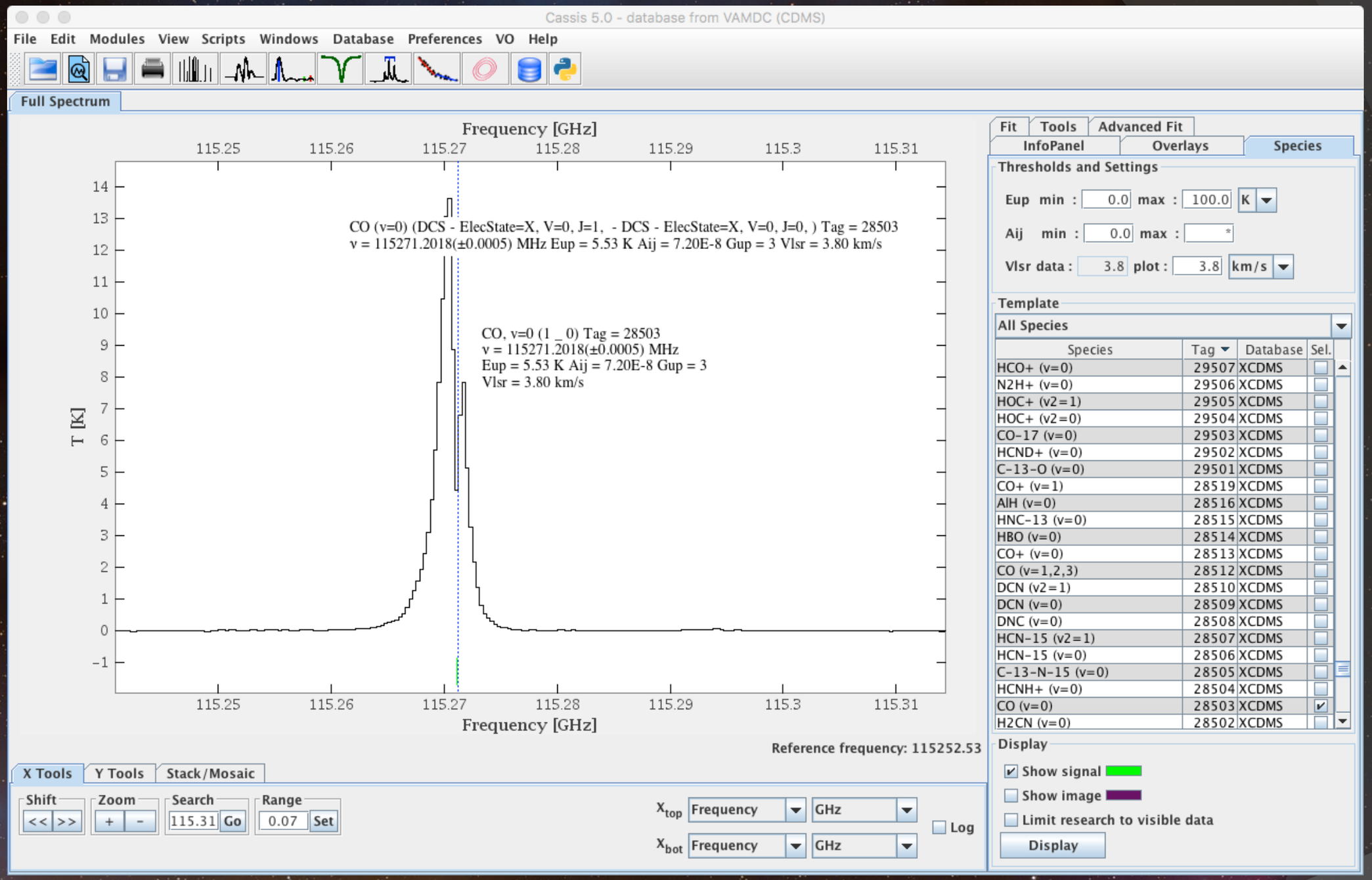
The astronomers need: atomic, molecular databases

Local database (SQLite), built on CDMS, JPL, NIST, and private databases (lab or computations), database with nuclear spin state (ortho, para, A and E)

Access to the CDMS, JPL and VALD databases linked through VAMDC

SSAP (Single Spectral Access Protocol) request through a CASSIS module allowing to access the IVOA services to retrieve and display any spectra (Hubble, Corot, Splatalogue, ISO, etc; http://registry.euro-vo.org)

VAMDC Access to CDMS

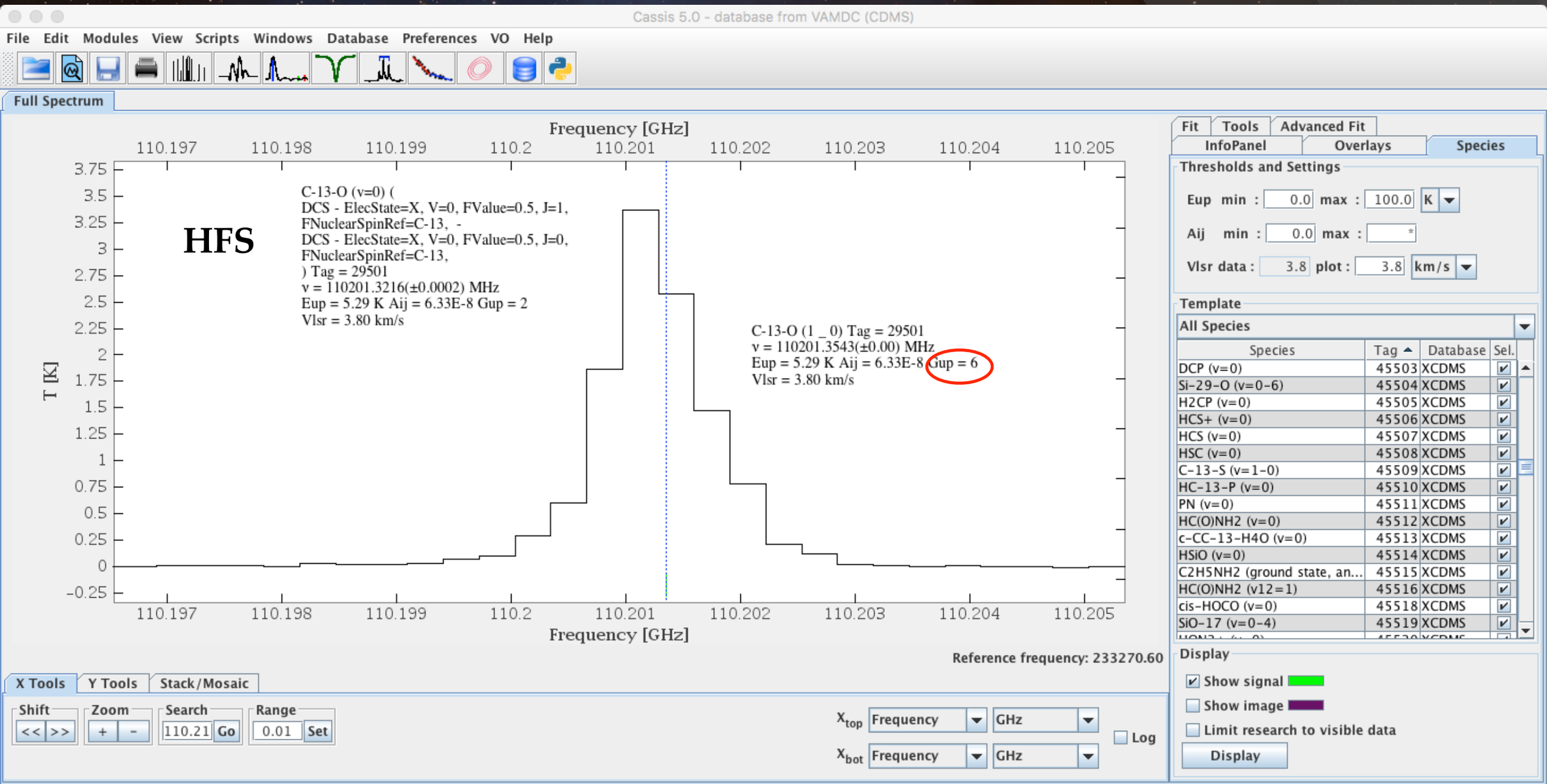


NH:

<hundb:ElecStateLabel>X</hundb:ElecStateLabel>
<hundb:S>1</hundb:S>
<hundb:v>0</hundb:v>
<hundb:J>2</hundb:J>
<hundb:N>1</hundb:N>
<hundb:F1 nuclearSpinRef="N">2.5</hundb:F1>
<hundb:F nuclearSpinRef="H">1.5</hundb:F>

4 quantum numbers in CDMS

VAMDC Access to CDMS

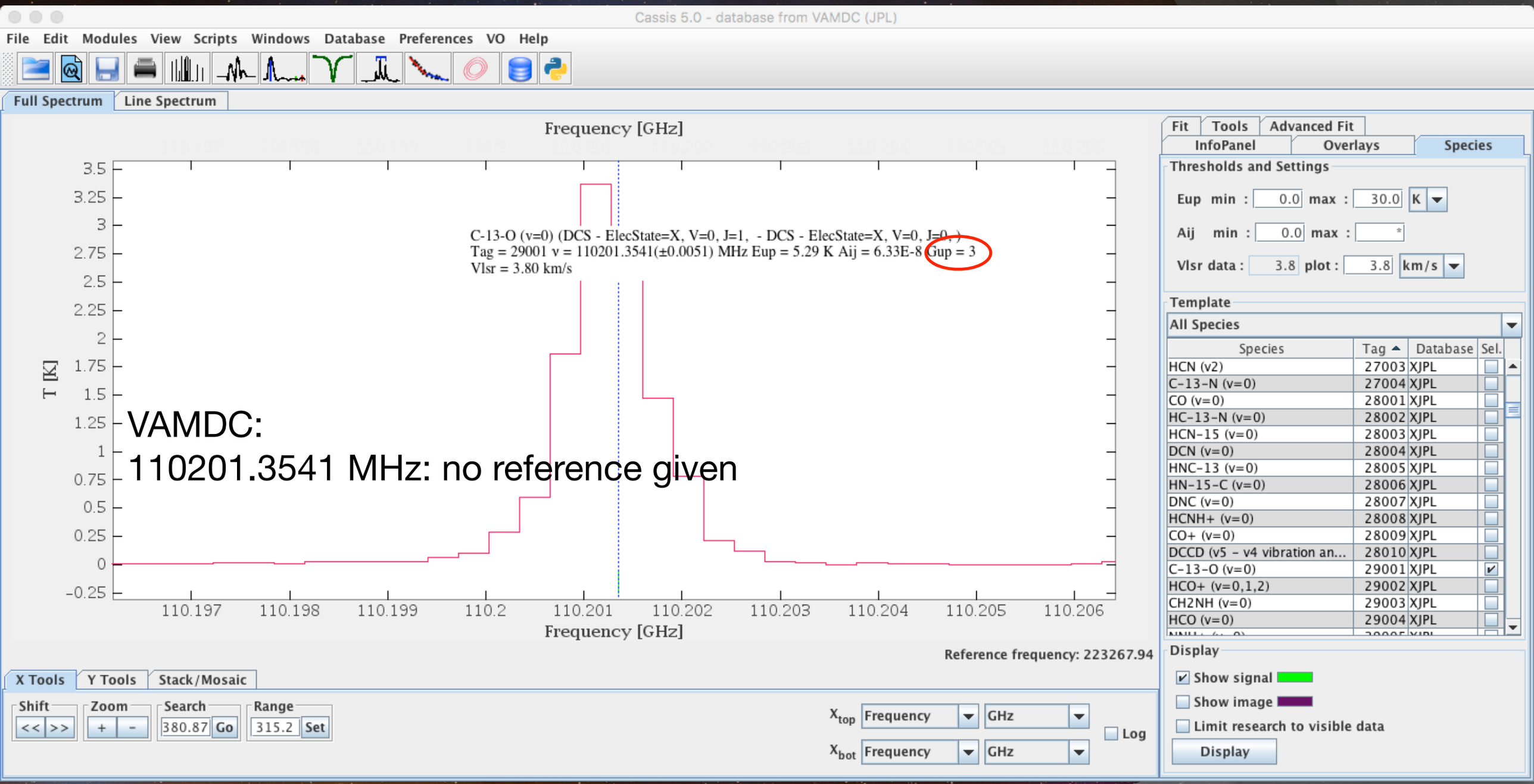


VAMDC:

110201.3216 MHz: derived with Herb Pickett's spfit / spcat fitting routines, based on experimental data: Predicted transition frequencies without experimental values with hyperfine structure

110201.3218 MHz: experimental transition frequencies

VAMDC Access to JPL



Atomic databases

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

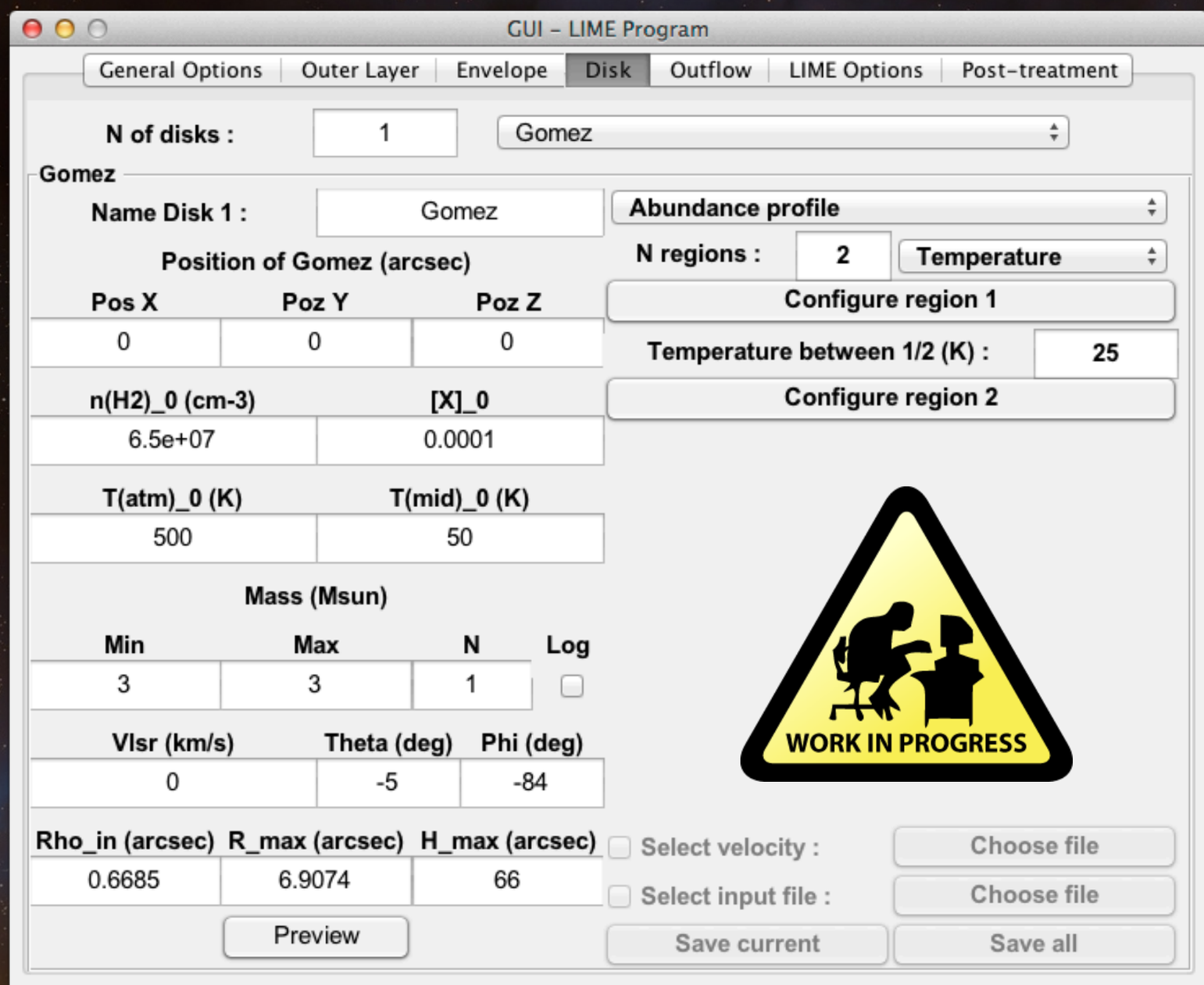
CHIANTI/VAMDC:
<SpeciesRef>Xchianti-1</SpeciesRef>
<Probability><TransitionProbabilityA><Value units="1/s">167000000.0</Value></TransitionProbabilityA><WeightedOscillatorStrength><Value units="unitless">0.0527</Value></WeightedOscillatorStrength></Probability>
<ProcessClass></ProcessClass></RadiativeTransition>
<RadiativeTransition id="Pchianti-R9"><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-4000001</UpperStateRef>
<LowerStateRef>Schianti-1000001</LowerStateRef>

With NIST (which is not in VAMDC):

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

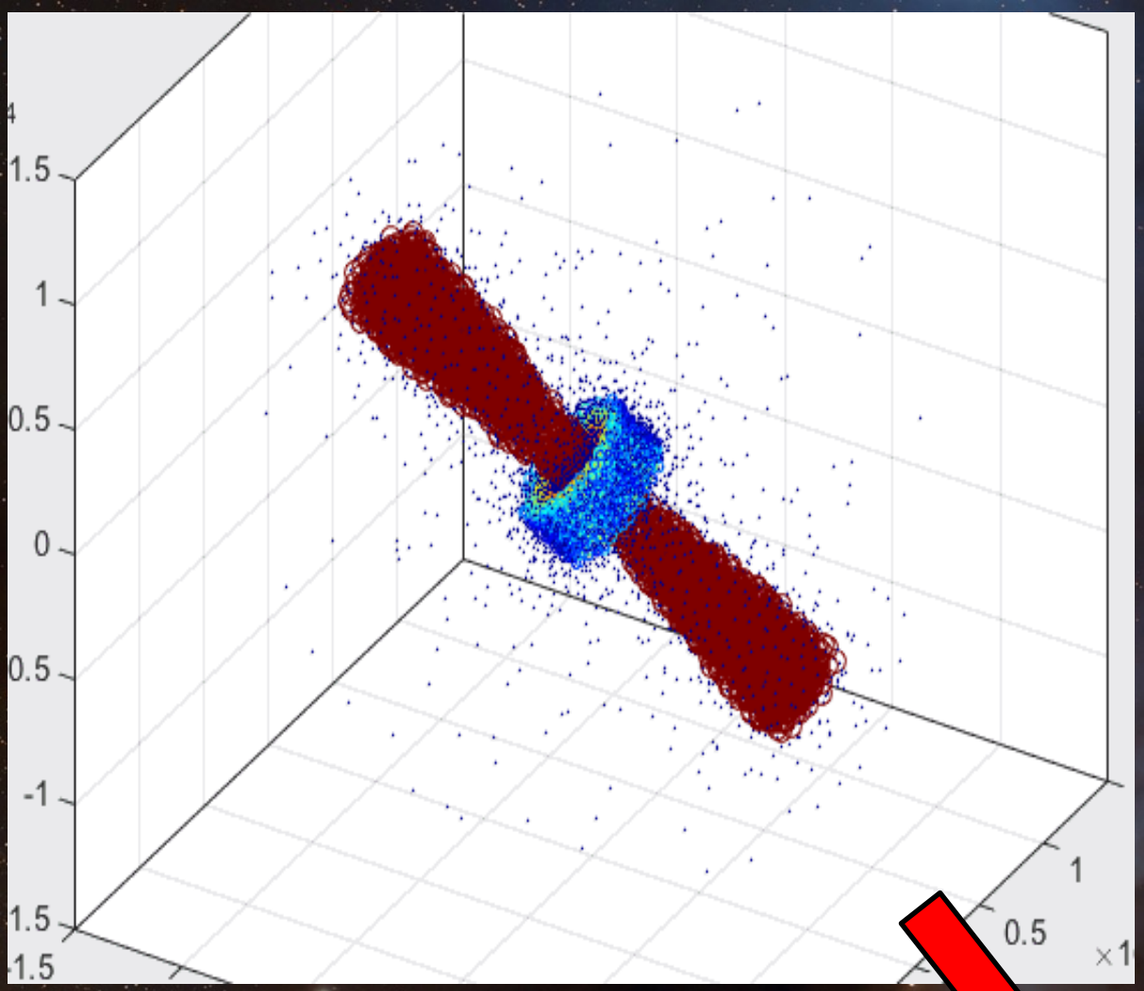
Avec VALD/VAMDC:
<SpeciesRef>Xvald-1</SpeciesRef>
<Probability><Log10WeightedOscillatorStrength><SourceRef>Bvald-CDROM18</SourceRef><Value units="unitless">-0.801</Value></Log10WeightedOscillatorStrength></Probability>
<ProcessClass></ProcessClass><Broadening name="natural" envRef="Evald-natural"><Comments>Natural 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>
<SpeciesRef>Xvald-1</SpeciesRef>

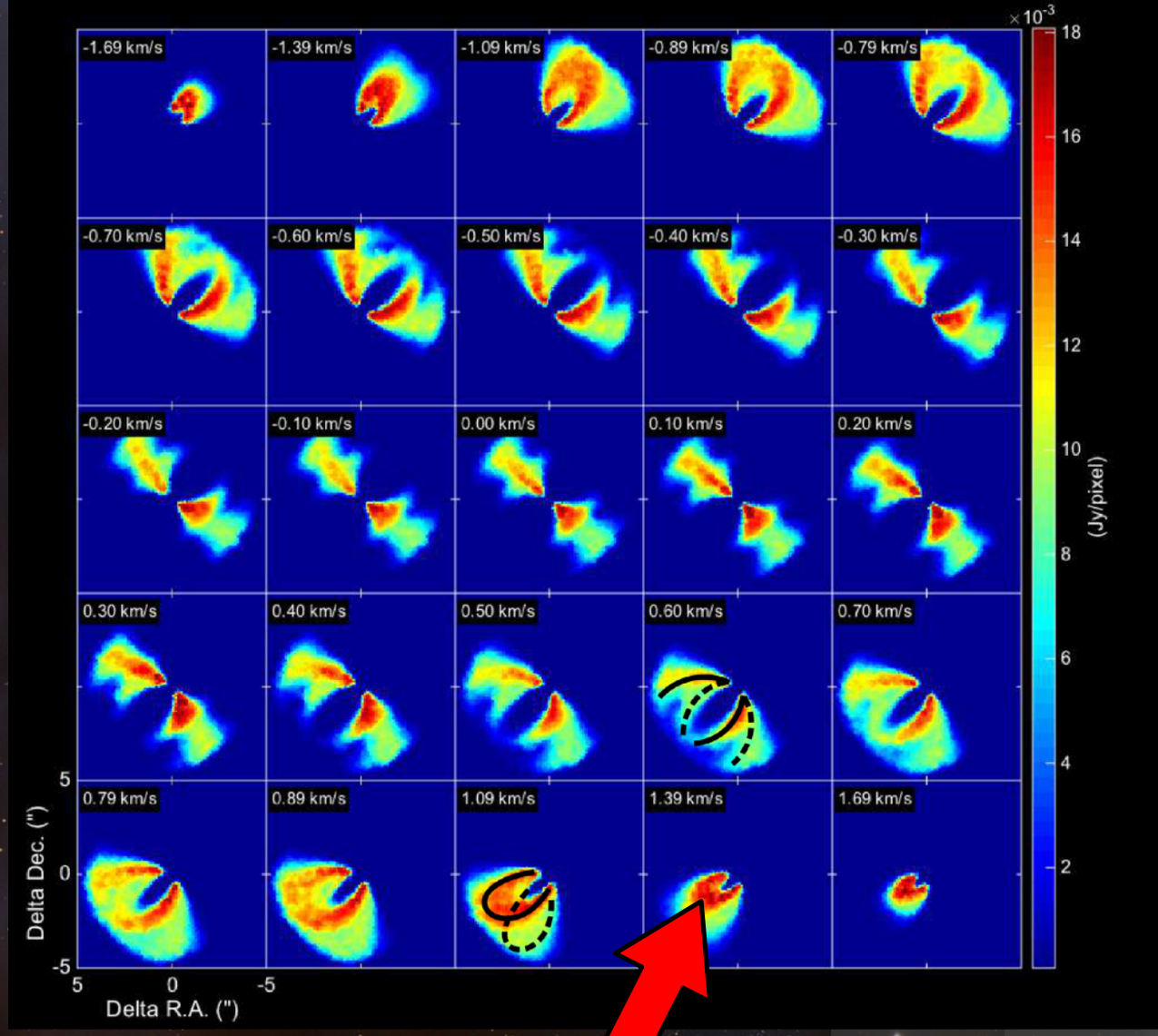
GASS Code
Generator of Astrophysical Sources Structures



- Description of GASS in Quénard et al. (2017a)
- d.quenard@qmul.ac.uk

- Publicly available
- Matlab-based software
- create, mix, manipulate and visualise 3D structures





GASS

Graphical User Interface (GUI)

Grid generation → Physical models → Post-treatment analysis → Line emission, continuum images, moment maps

LIME 3D code (generates fits files)

Brinch et al. (2010)

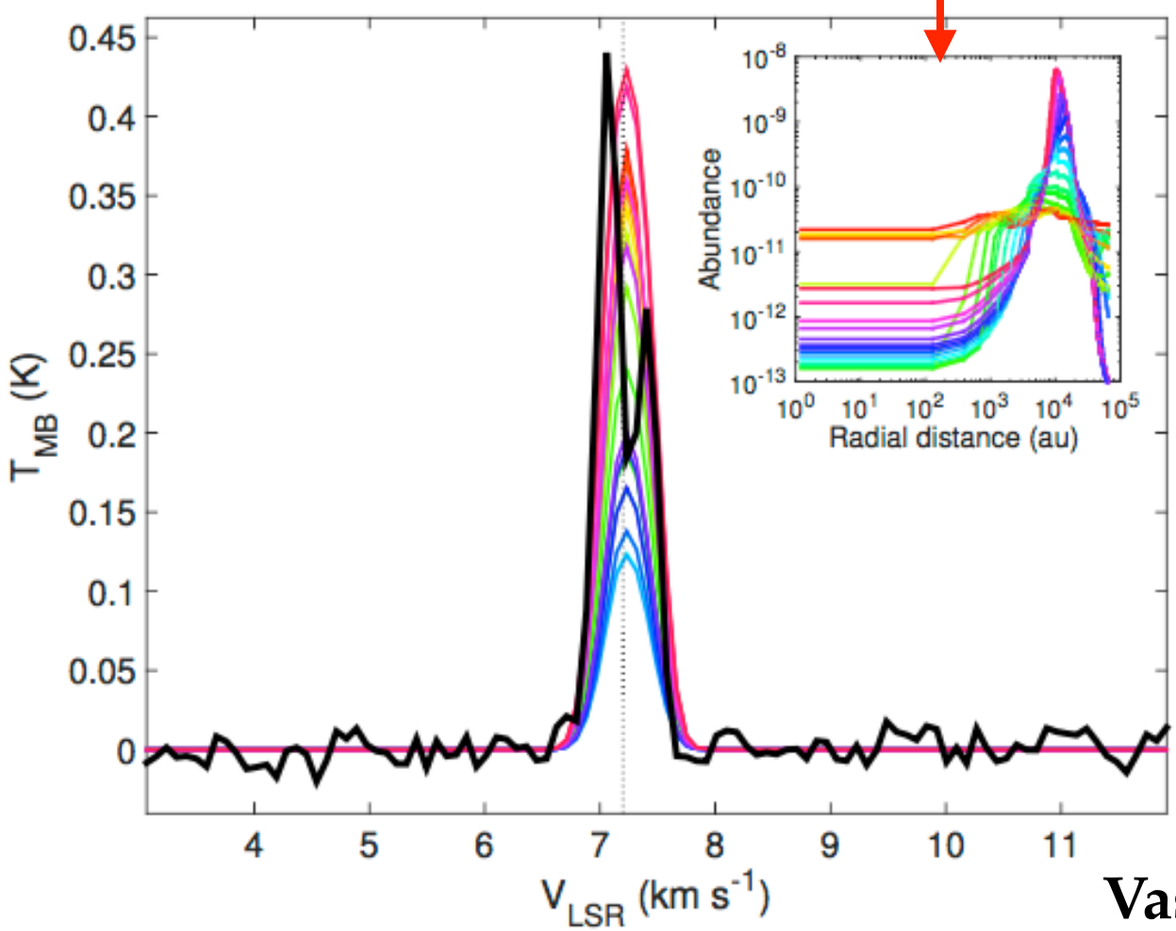
Quénard et al. (2017a)

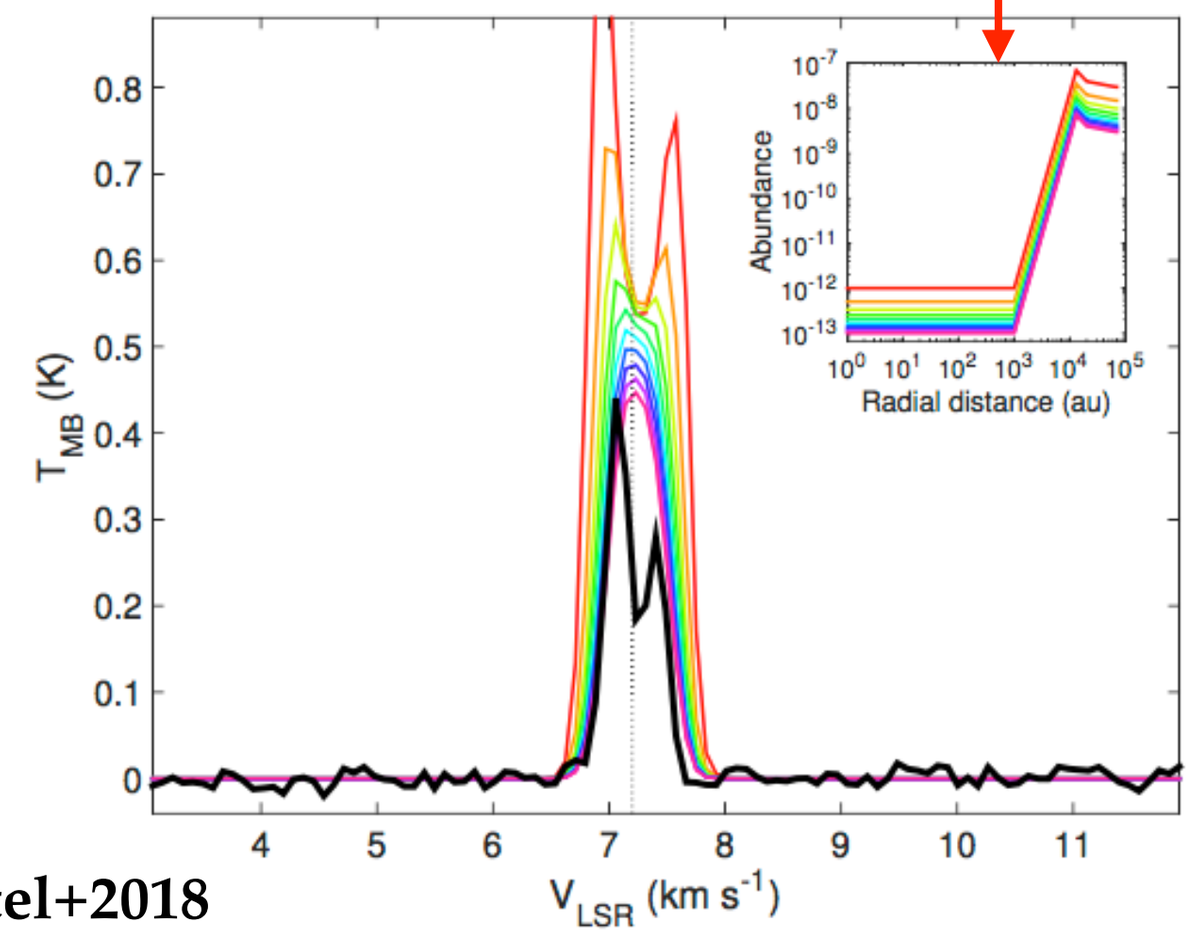
Example:

- Observed double-peak profile, known physical structure
- Try to reproduce the observations and constrain the abundance profile

Output from chemical modelling (Nautilus, UCL_CHEM)

Ad-hoc profiles





Vastel+2018

Need for the collision files

```
!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
```

Spectroscopic parameters

```
!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
```

Collisions

Spectcol tool

http://www.vamdc.org/activities/research/software/spectcol/

Group by specie inChiKey: UGFAIRIUMAVXCW-UHFFFAOYSA-N

Select a row from Transition table and either Collision table or Scaled Collision table

Transitions

	comment	source	structural formula	stoichiometric formula	spin	InChI key
2	28512- v1*:CO; $v=1,2,3$	CDMS 2018-01-12 08:24:33.242	CO	CO		UGFAIRIUMAVXCW-UHFFFAOYSA-N
7	28503- v 1:CO; $v=0$	CDMS 2018-01-12 08:24:33.242	CO	CO		UGFAIRIUMAVXCW-UHFFFAOYSA-N

Collisions

	comment	source	target...	...	t...	target InChI key	collider ...	collider stoichio...	collider spin	collider InChI key
1	Rotational de-excitation of CO by para-H$_2$ (j=0), 5K < T < 70K - 6 levels (Wernli et al., 2006)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	para	UFHFLCQGNIYNRP-UHFFFAOYSA-N
2	Rotational excitation of CO by ortho-H$_2$ (Flower, 2001)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	ortho	UFHFLCQGNIYNRP-UHFFFAOYSA-N
3	Rotational excitation of CO by para H$_2$ (Flower, 2001)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	para	UFHFLCQGNIYNRP-UHFFFAOYSA-N
4	Rotational de-excitation of CO by H for 5K < T< 100K (Balakrishnan & al, 2002)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H	H		YZCKVEUIGOORGS-UHFFFAOYSA-N
5	Vibrational de-excitation of CO by H (Balakrishnan & al, 2002)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H	H		YZCKVEUIGOORGS-UHFFFAOYSA-N
6	Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini & al, 2002)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	HE	HE		SWQJXJOGLNCZEY-UHFFFAOYSA-N
7	Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 2002)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	HE	HE		SWQJXJOGLNCZEY-UHFFFAOYSA-N
8	Rotational de-excitation of CO by H for 100K< T <3000K (Balakrishnan & al, 2002)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H	H		YZCKVEUIGOORGS-UHFFFAOYSA-N
9	Rotational de-excitation of CO by ortho-H$_2$ (j=1), 5K < T < 70K - 6 levels (Wernli et al., 2006)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	ortho	UFHFLCQGNIYNRP-UHFFFAOYSA-N
10	Rotational de-excitation of CO by para-H$_2$ (j=0), 1K < T < 3000K - 41 levels (Yang et al., 2010)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	para	UFHFLCQGNIYNRP-UHFFFAOYSA-N
11	Rotational de-excitation of CO by ortho-H$_2$ (j=1), 1K < T < 3000K - 41 levels (Yang et al., 2010)	BASECOL: VAMDC...	CO	...		UGFAIRIUMAVX...	H$_2$	H2	ortho	UFHFLCQGNIYNRP-UHFFFAOYSA-N

Scaled collisions

comment	source	target structural formula	target stoichiometric for...	target spin	target InChI key	collider structural formula	collider stoichiometric f...	collider spin	collider InChI key

Combine Spectroscopic data and collisional data

Show selection | Export as XSAMS

Ba Yaye-Awa <yaye-awa.ba@obspm.fr>

Quantum numbers selection

Select the relevant quantum numbers columns from one of the tables

Spectro DB – Energy Table

state	energy [1/c...	degeneracy	ElecStateLa...	J	v	F	F1	parity	AsSym
1	0	1	X	0	0				
2	3.845	3	X	1	0				
3	11.535	5	X	2	0				
4	23.069	7	X	3	0				
5	38.448	9	X	4	0				
6	57.67	11	X	5	0				
7	80.735	13	X	6	0				
8	107.642	15	X	7	0				
9	138.39	17	X	8	0				
10	172.978	19	X	9	0				
11	211.404	21	X	10	0				

BASECOL – Energy Table

state	energy [1/c...	degeneracy	ElecStateLa...	J ▲	v	F	F1	parity	AsSym
1	0		X	0					
2	3.845		X	1					
3	11.535		X	2					
4	23.07		X	3					
5	38.448		X	4					
6	57.67		X	5					
7	80.735		X	6					
8	107.642		X	7					
9	138.39		X	8					
10	172.978		X	9					
11	211.404		X	10					

Ok Cancel

Matching results then Save as Radex file or XSAMS file

http://basecol.obspm.fr/pages/data/matching/radex.php?id=41&idET=20&date=2007-10-09&tabl2=1

```
! Molecule
H2O
! 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. J_Ka_Kc_tau
   1       23.794400        9         1_0_1_-1
   2       42.371700        9         1_1_0_1
   3       79.496400       15         2_1_2_-1
   4      134.901600       15         2_2_1_1
   5      136.761700       21         3_0_3_-3
! NUMBER OF RADIATIVE TRANSITIONS : JPL V6 PNov. 2005 -- http://spec.jpl.nasa.gov/ftp/pub/catalog/doc/d018003.cat
5
! TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_up(K)
    1      2      1      3.46008659e-3        556.9360020       60.966475
    2      3      1      5.59938064e-2       1669.9047750      114.383309
    3      4      2      2.57413216e-1       2773.9765880      194.103022
    4      4      3      3.06508789e-2       1661.0076370      194.103022
    5      5      3      5.05947242e-2       1716.7696330      196.779424
! NUMBER OF COLLISION PARTNERS
1
! COLLISION PARTNER
1
! COLLISIONS BETWEEN, BASECOL V1 P2005-07
3 ortho-H2-H2O-ortho ,
! NUMBER OF COLLISIONAL TRANSITIONS
10
! NUMBER OF COLLISION TEMPERATURES
7
! COLLISION TEMPERATURES
      20       40       60       80      100      120      140
! TRANS + UP + LOW + RATE COEFFS(cm^3 s^-1)
    1      2      1      2.6800e-10      2.8600e-10      2.8900e-10      2.8900e-10      2.8800e-10      2.8900e-10      2.9100e-10
    2      3      1      9.7100e-11      1.1200e-10      1.2100e-10      1.2500e-10      1.2800e-10      1.3000e-10      1.3100e-10
    3      3      2      9.6700e-11      9.8300e-11      9.5000e-11      9.1300e-11      8.8100e-11      8.5600e-11      8.3500e-11
    4      4      1      2.1500e-11      2.3300e-11      2.5000e-11      2.6400e-11      2.7500e-11      2.8500e-11      2.9400e-11
```

different quantum numbers 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

<u>Our needs (LIME, RADEX etc…)</u>: collisional databases based on LAMDA and/or BASECOL

→ 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?

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

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