Bases de données pour l'astrochimie: past, present and futur

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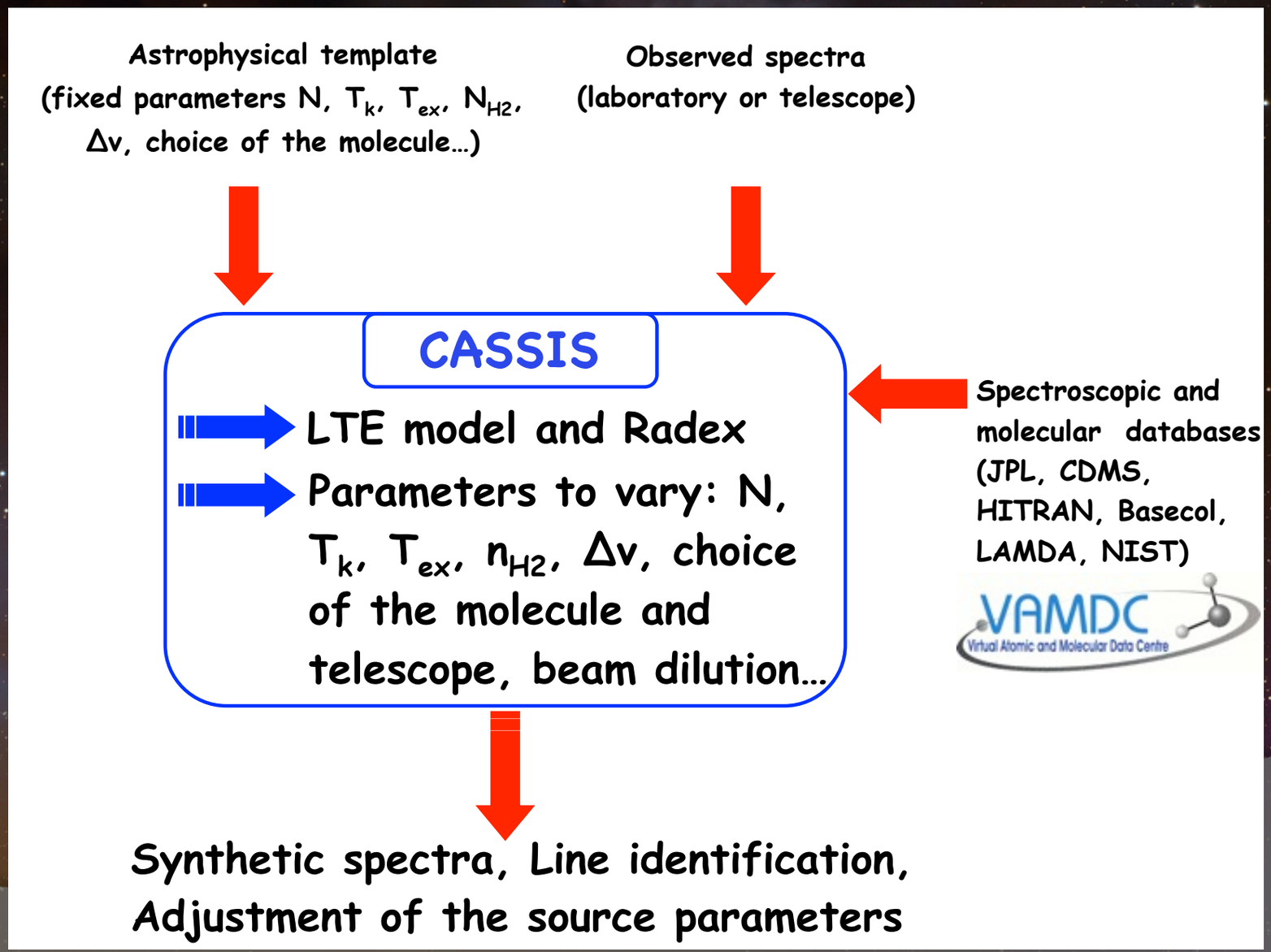
Atelier base de données pour l'astrochimie PCMI Marseille, 28 juin 2018

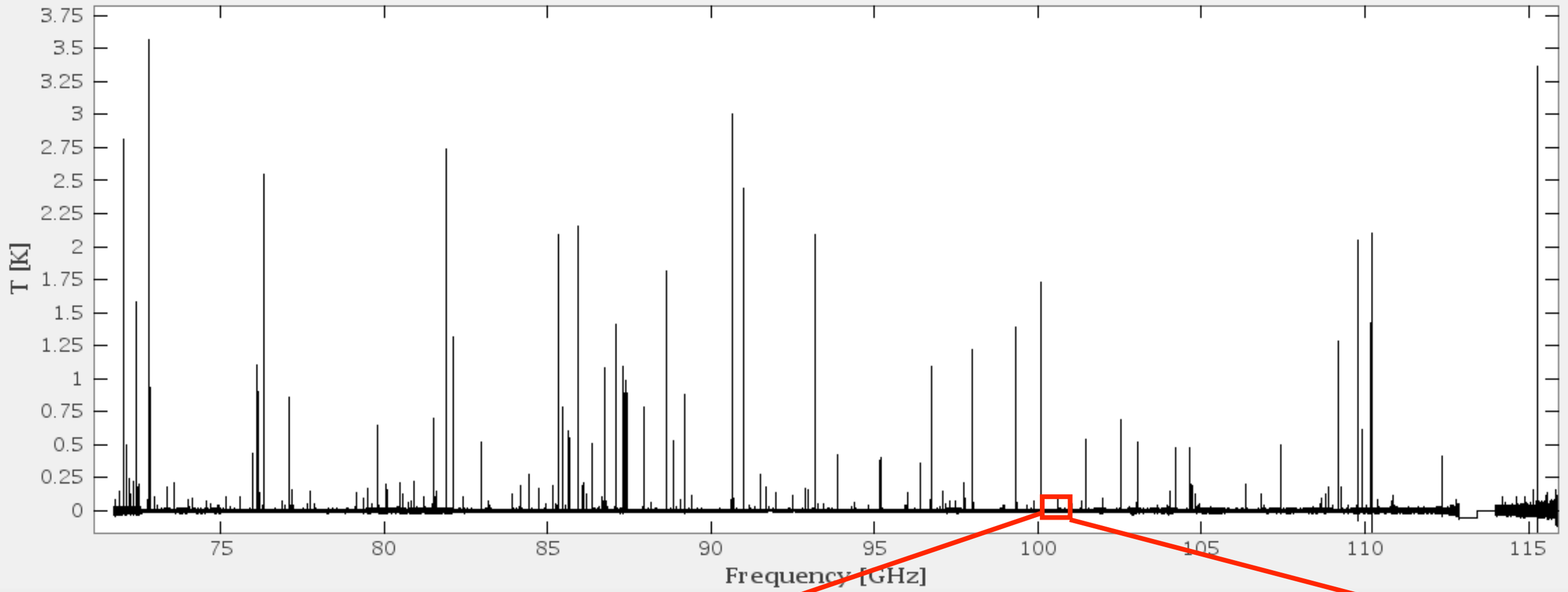
CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques):
http://cassis.irap.omp.eu/



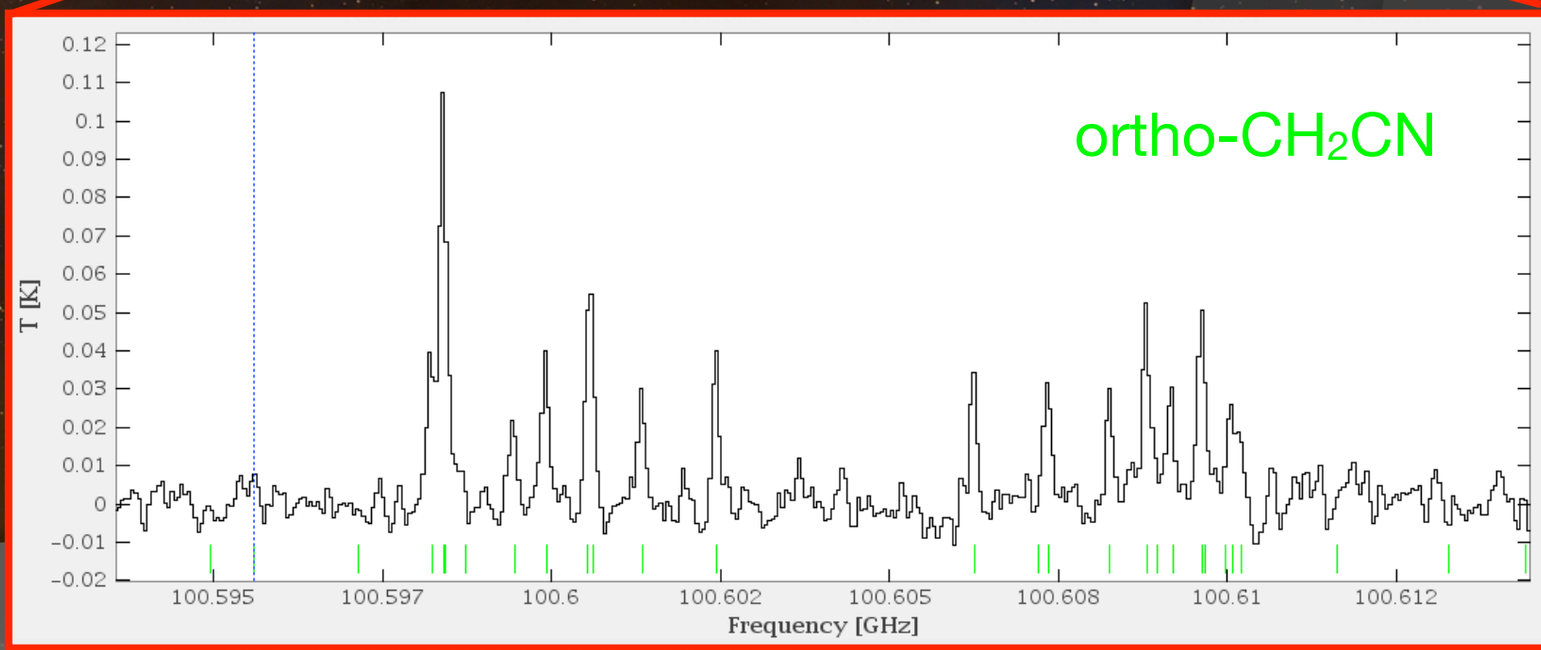
+CASSIS own databases with:

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

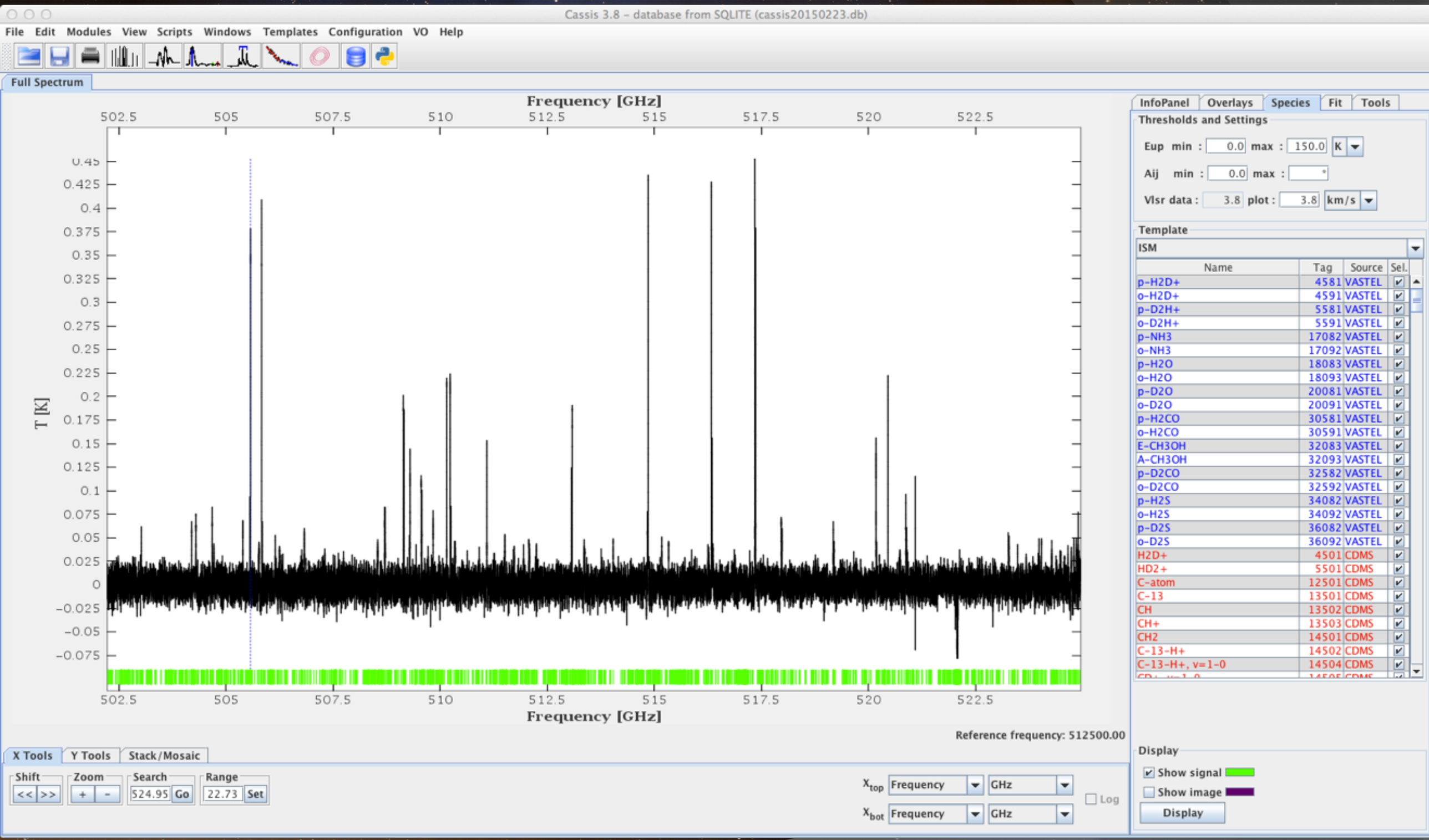
Line Identification



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



Line Identification



Databases and interoperability

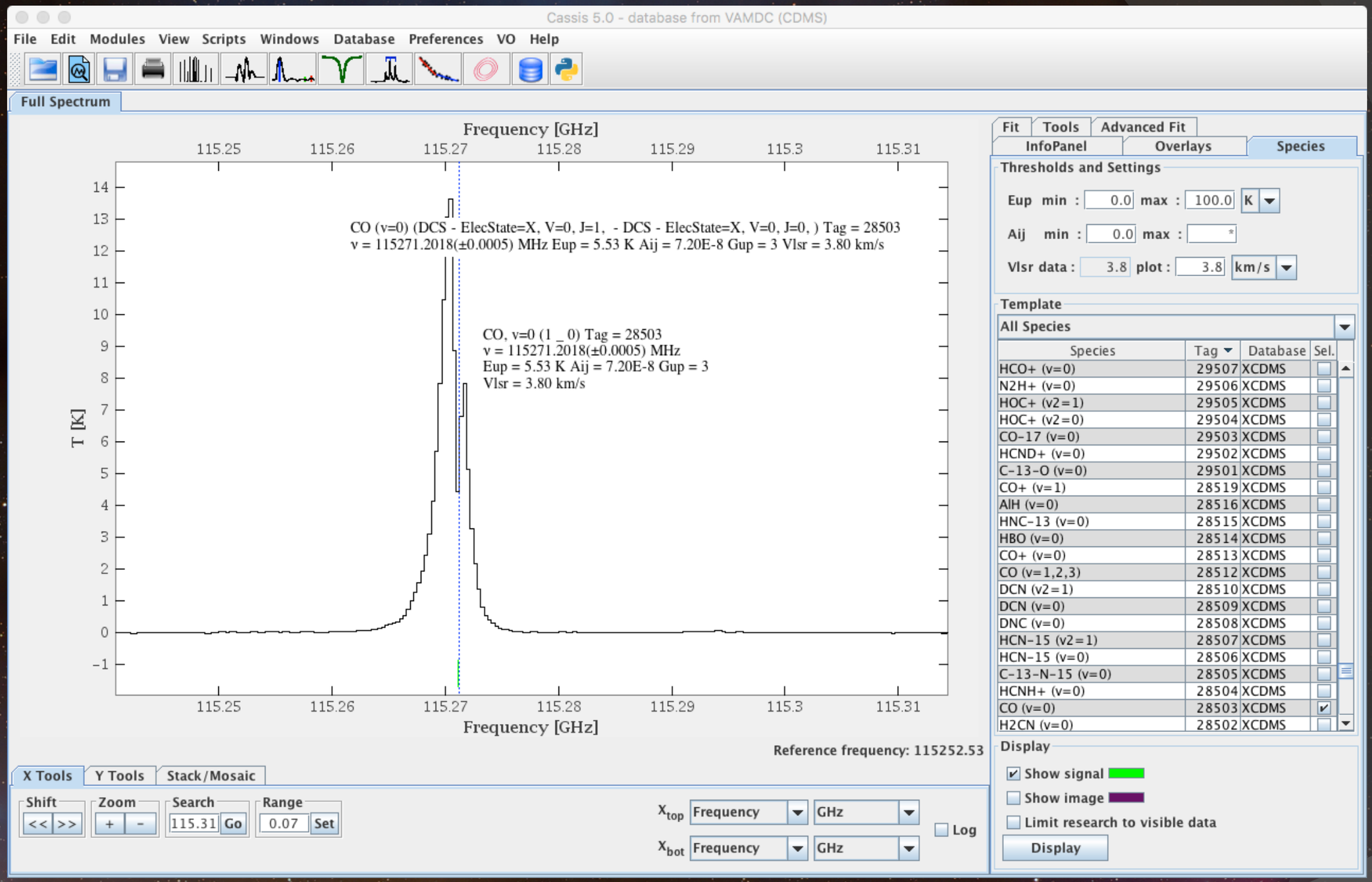
The astronomers need: atomic, molecular databases

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

→ 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

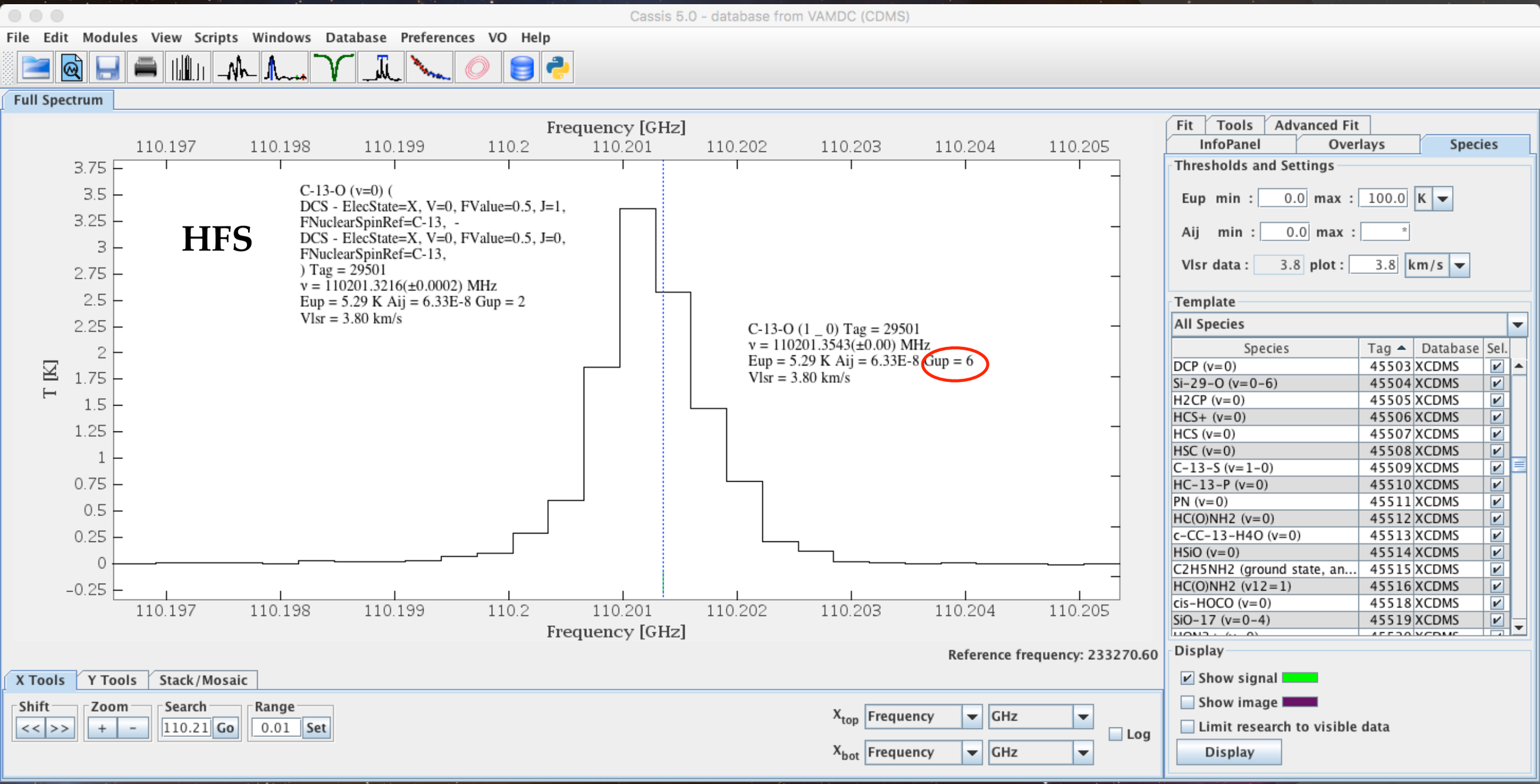


NH:

```
<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

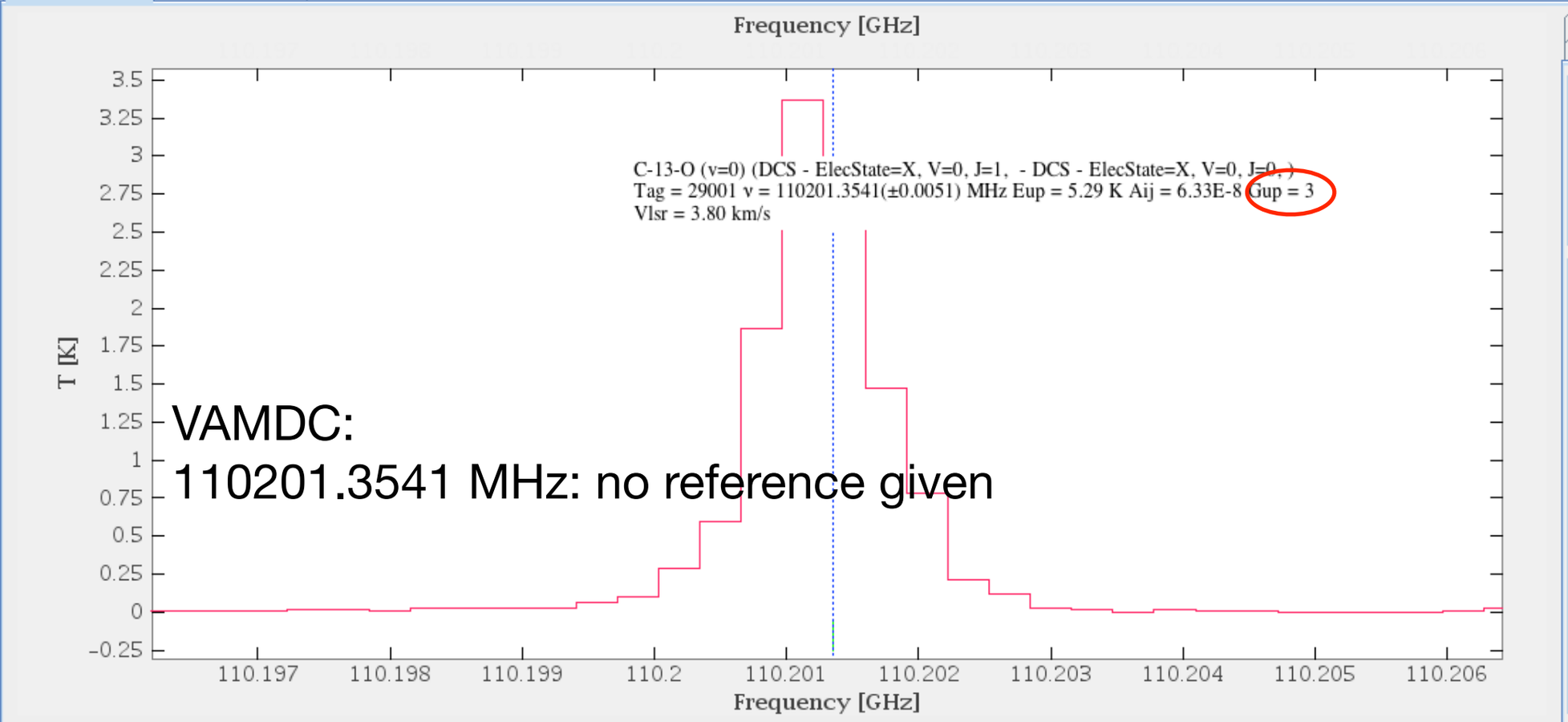
110201.3218 MHz: experimental transition frequencies

VAMDC Access to JPL

Cassis 5.0 - database from VAMDC (JPL)

File Edit Modules View Scripts Windows Database Preferences VO Help

Full Spectrum | Line Spectrum



Reference frequency: 223267.94

X Tools | Y Tools | Stack/Mosaic

Shift << >> Zoom + - Search 380.87 Go Range 315.2 Set

X_{top} Frequency GHz

X_{bot} Frequency GHz

Log

Fit | Tools | Advanced Fit

InfoPanel | Overlays | Species

Thresholds and Settings

Eup min : 0.0 max : 30.0 K

Aij min : 0.0 max : *

Vlsr data : 3.8 plot : 3.8 km/s

Template

All Species

Species	Tag	Database	Sel.
HCN (v2)	27003	XJPL	☐
C-13-N (v=0)	27004	XJPL	☐
CO (v=0)	28001	XJPL	☐
HC-13-N (v=0)	28002	XJPL	☐
HCN-15 (v=0)	28003	XJPL	☐
DCN (v=0)	28004	XJPL	☐
HNC-13 (v=0)	28005	XJPL	☐
HN-15-C (v=0)	28006	XJPL	☐
DNC (v=0)	28007	XJPL	☐
HCNH+ (v=0)	28008	XJPL	☐
CO+ (v=0)	28009	XJPL	☐
DCCD (v5 - v4 vibration an...	28010	XJPL	☐
C-13-O (v=0)	29001	XJPL	☑
HCO+ (v=0,1,2)	29002	XJPL	☐
CH2NH (v=0)	29003	XJPL	☐
HCO (v=0)	29004	XJPL	☐

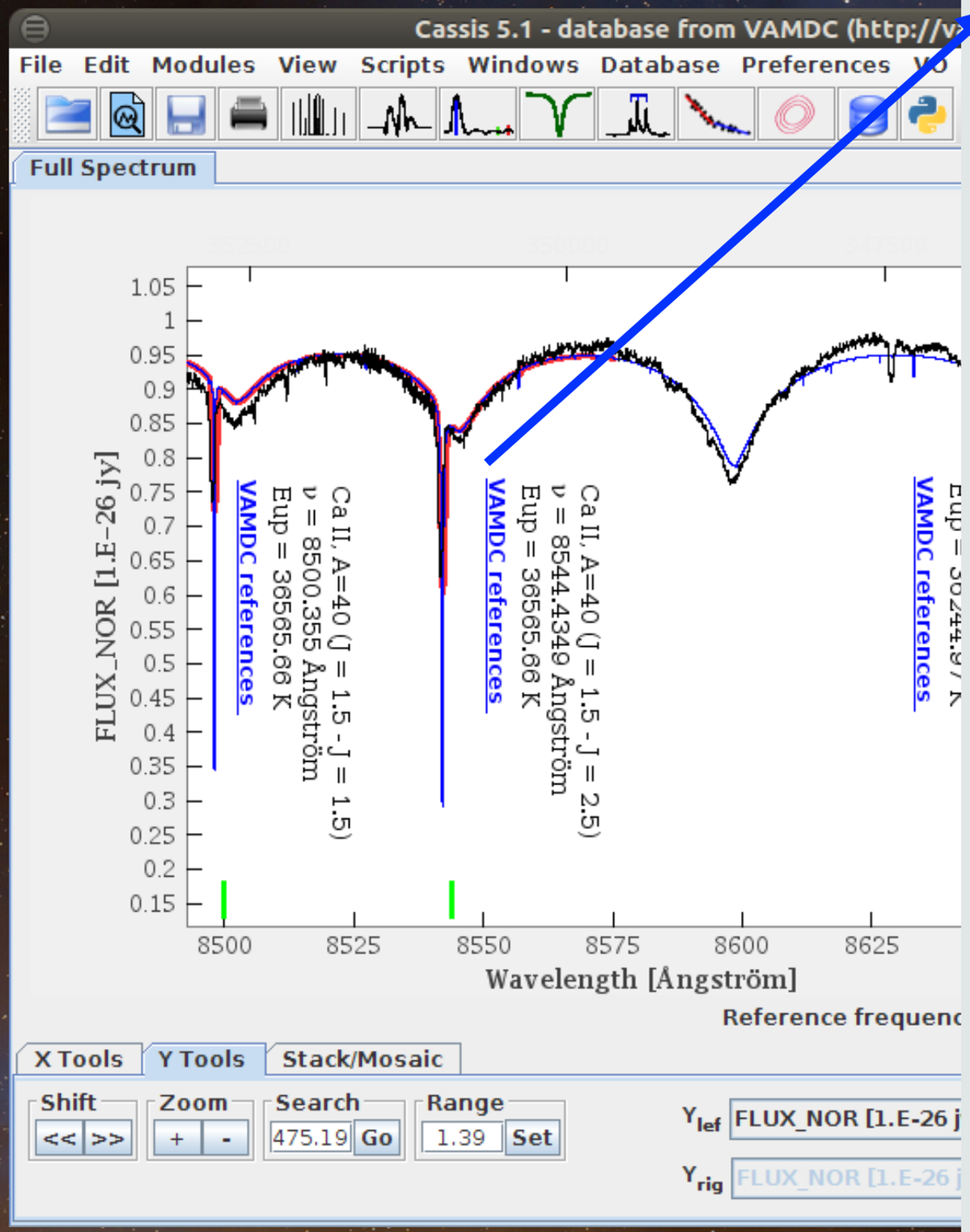
Display

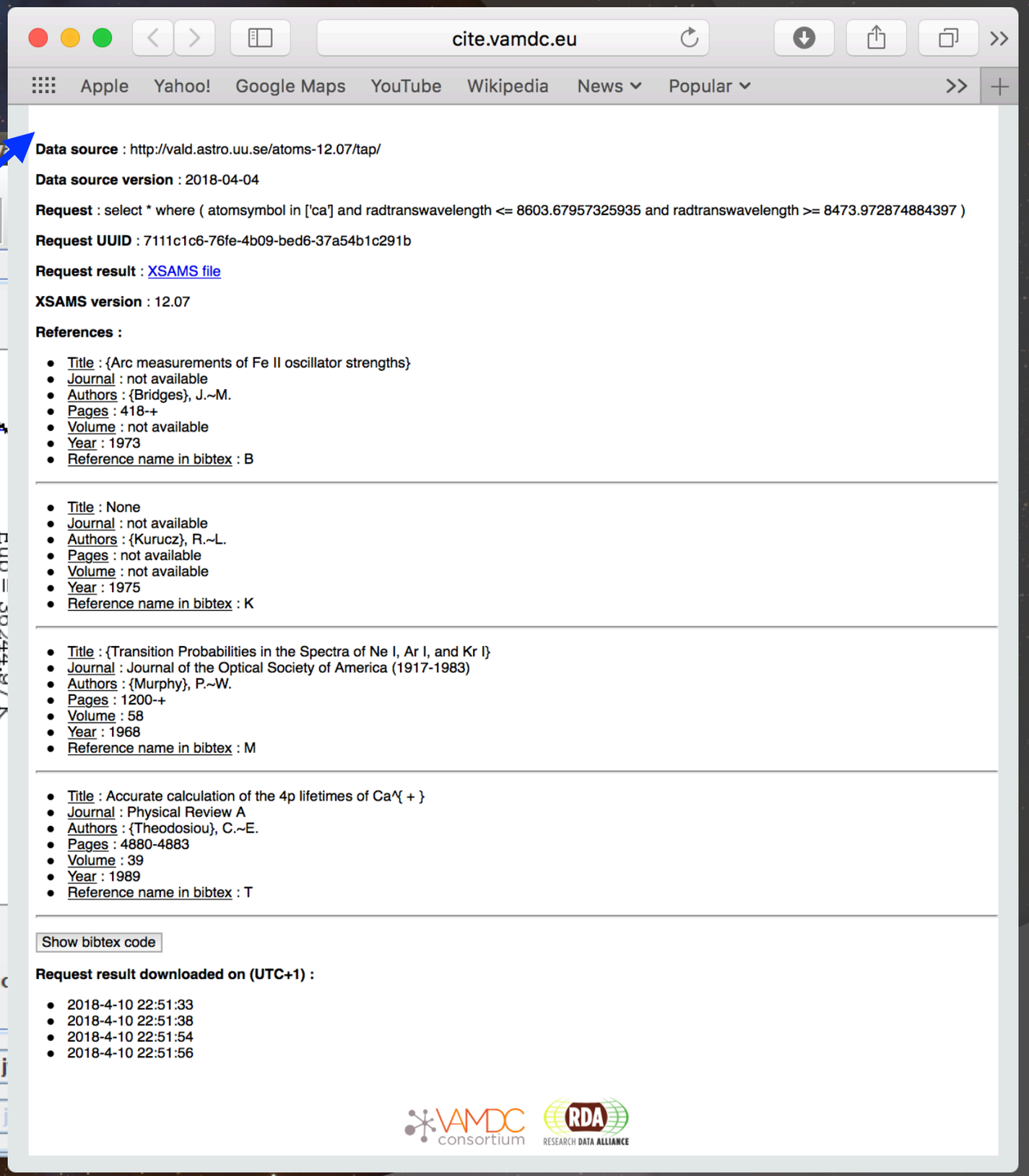
☑ Show signal

☐ Show image

☐ Limit research to visible data

Display





Interrogation de la base atomique VALD via VAMDC

Interrogation du query store de VAMDC → DOI et références des transitions

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>
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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>

!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

Databases and interoperability

Our needs (LIME, RADEX etc…): 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?

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

Link with astrochemical models

Nahoon/Nautilus

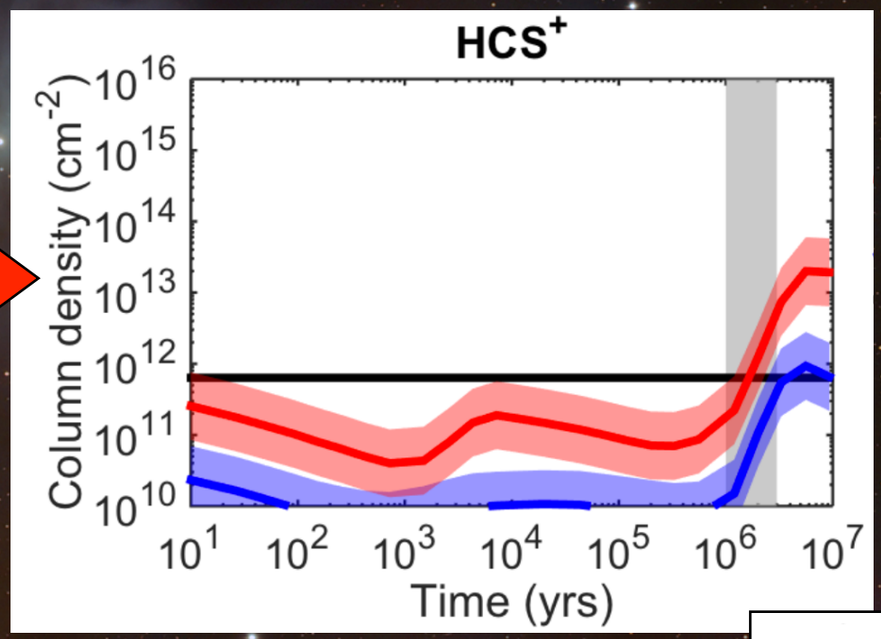
KIDA

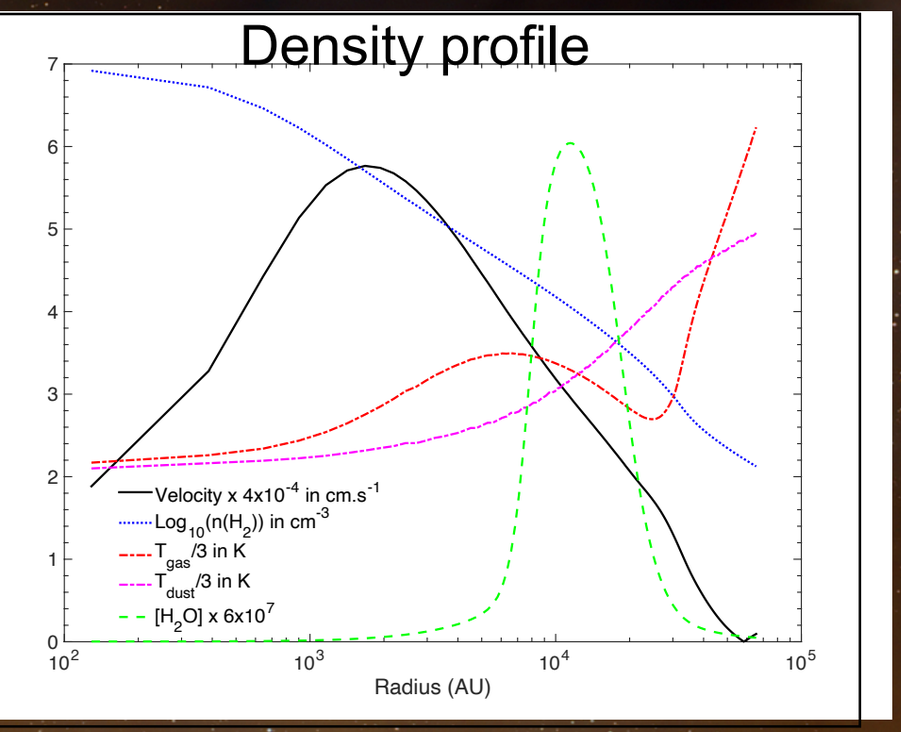
abundance vs time

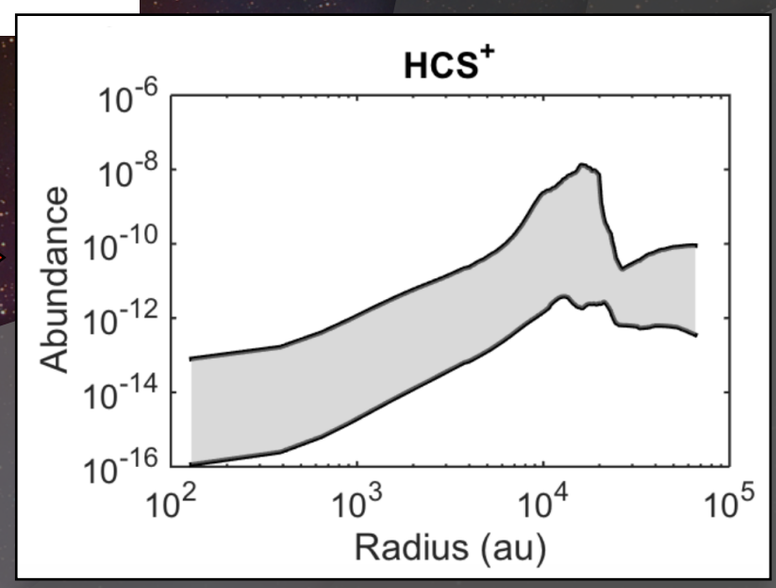
density profile

CASSIS

column densities







Évolutions : du radio aux UV/X!

- A l'origine, CASSIS prévu pour les spectres FIR-(sub)mm en K
  → ouverture vers d'autres longueurs d'ondes demande des outils supplémentaires

- UV/FUV
  - largeur équivalente, "curve of growth"
  - "profile fitting" : intégration de l'utilisation du module Owens pour la modélisation de ces spectres (collaboration avec C. Gry)

→ Owens database, based on Morton 1999's and other data files

Évolutions : du radio aux UV/X!

- ***SPEX***: software package SPEctral X-ray and UV modelling and analysis. Developed by SRON-Utrecht. A synthetic spectra program that convolves the calculated input spectra with representative instrumental response functions and a subroutine for Differential Emission Measure (DEM) modelling is available.
- ***SPEX*** includes more than a million lines from 30 chemical elements (from H to Zn) in the far UV and X-ray band.
- Lines produced by excitation from electron impact, radiative and dielectronic recombination and by innershell excitation and ionization. Also, the code calculates the contributions from continuum radiation due to free-free, freebound, and two-photon emission and includes several absorption models.

Already used by XMM-Newton, Chandra, Suzaku, and Hitomi.
Athena: high sensitivity and spectral resolution

An alternate solution is XSPEC

Évolutions : du radio aux UV/X!