



Feedbacks from user-oriented tools: CASSIS

Charlotte Vastel

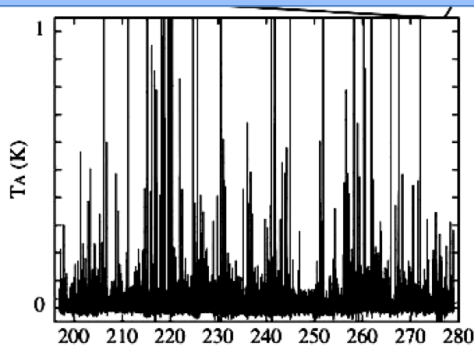
for the CASSIS team:

Jean-Michel Glorian & Mickael Boiziot

Emmanuel Caux, Sandrine Bottinelli

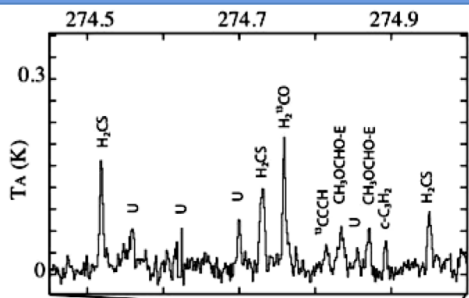
& Audrey Coutens

OBSERVATIONS



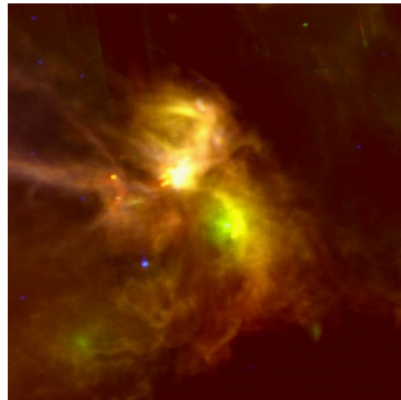
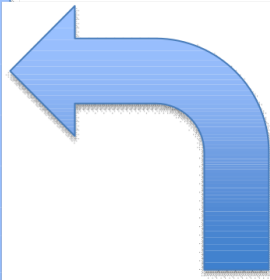
STEP1: Observe the spectrum of the source.

Tool: telescope

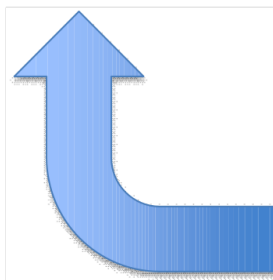


STEP2: Identify the lines and species.

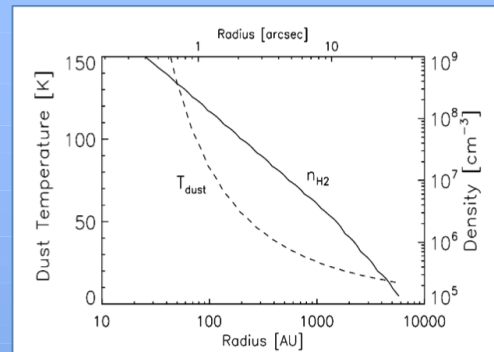
Tool: spectroscopic data



ASTROPHYSICAL OBJECT

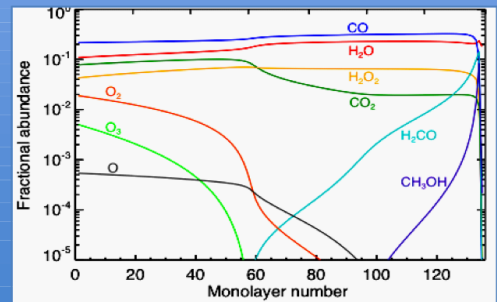


TOOLS & MODELS



STEP3: Derive the physical and chemical structure.

Tool: radiative transfer models

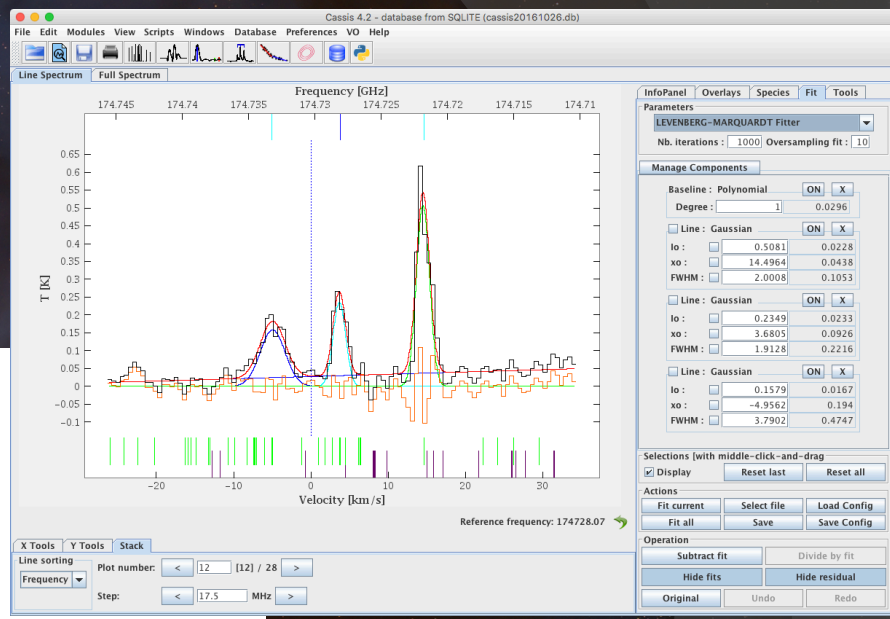


STEP4: Understand the chemical structure.

Tool: astrochemical models

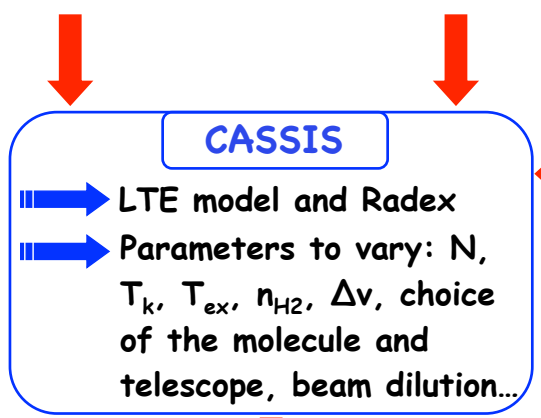
CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques):

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



Astrophysical template
(fixed parameters N , T_k , T_{ex} , N_{H_2} , Δv , choice of the molecule...)

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



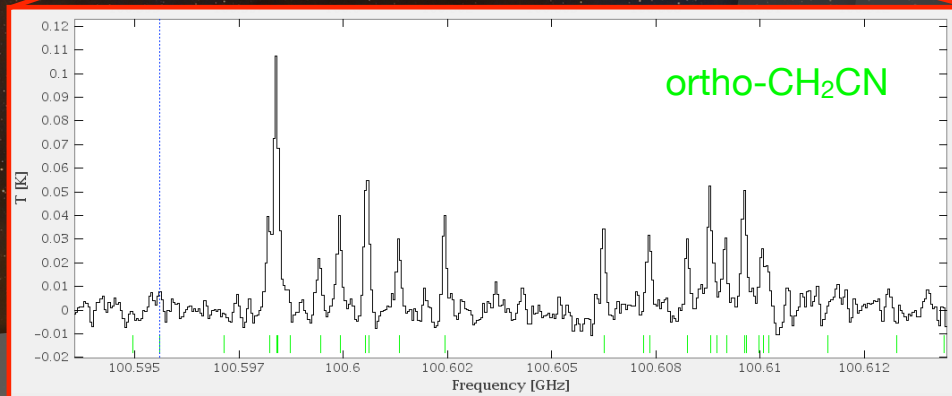
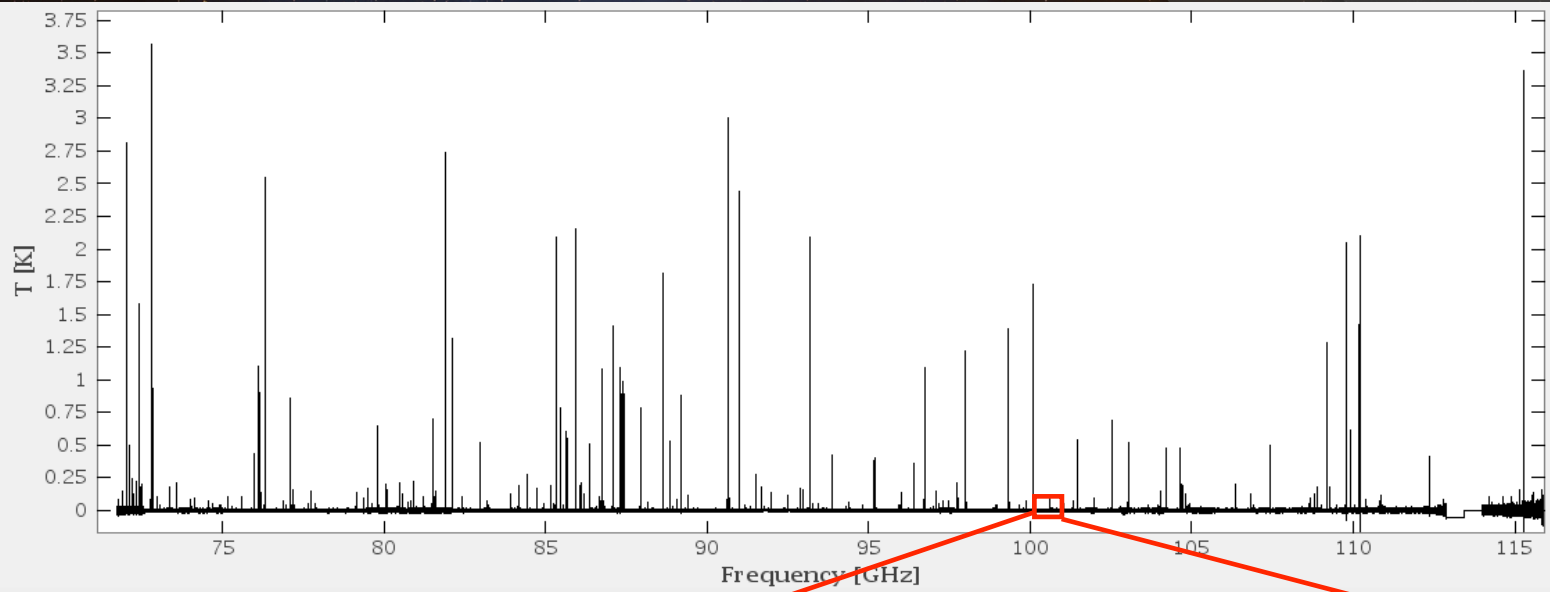
Spectroscopic and molecular databases
(JPL, CDMS, NIST)

TAP protocol (IVOA)

- + CASSIS own databases with:
- 1) ortho / para / A / E separation
 - 2) HFS
 - 3) ~80 entries for Radex compatible collisional files

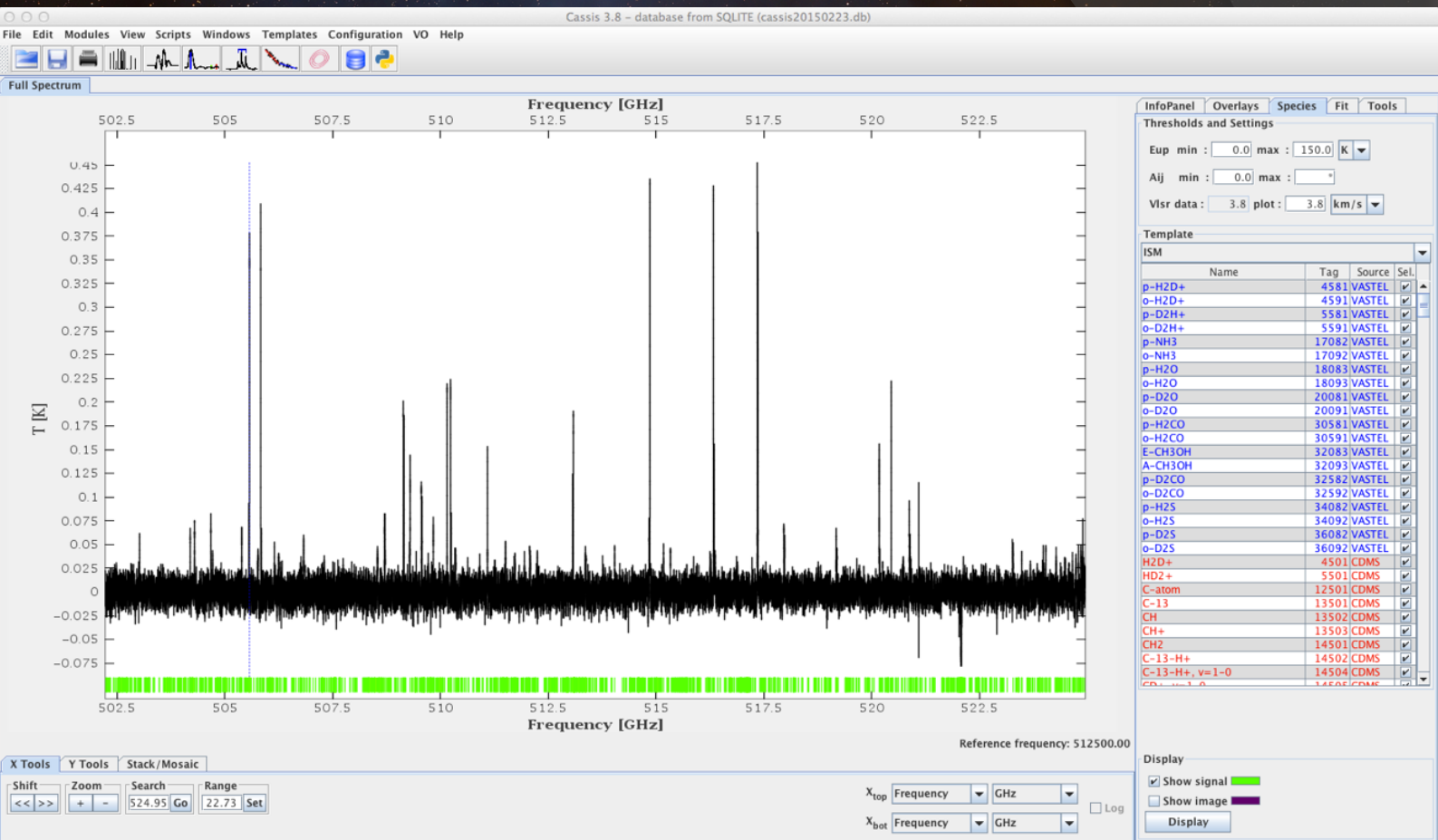
Synthetic spectra, Line identification, Automatic adjustment (MCMC, χ^2), Rotational diagram

I. Line Identification



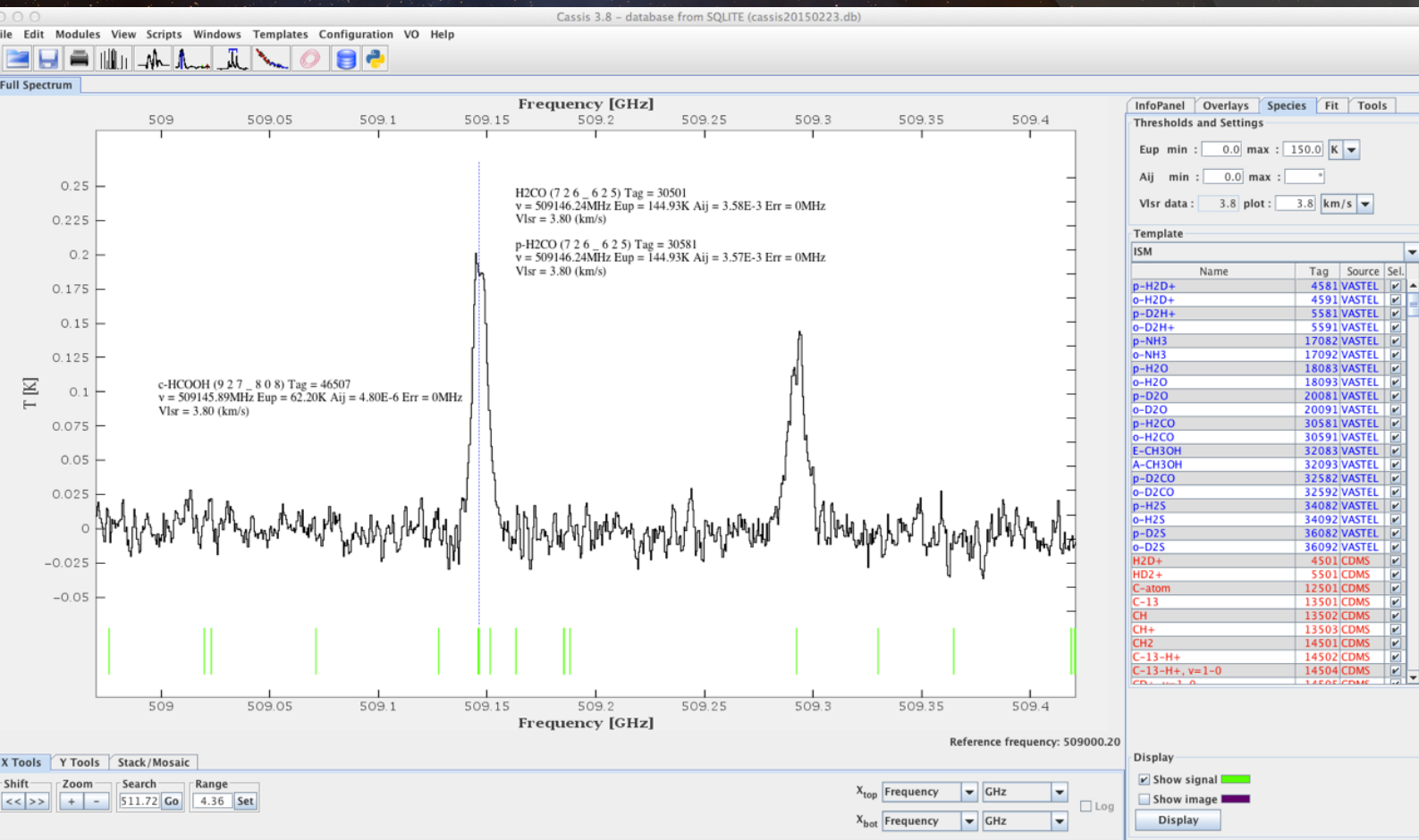
- * JPL standalone
- * CDMS standalone
- * Your own database
- * VAMDC: NIST, JPL, VALD, CDMS etc...

I. Line Identification



SQLite database

I. Line Identification



SQLite database

I. 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

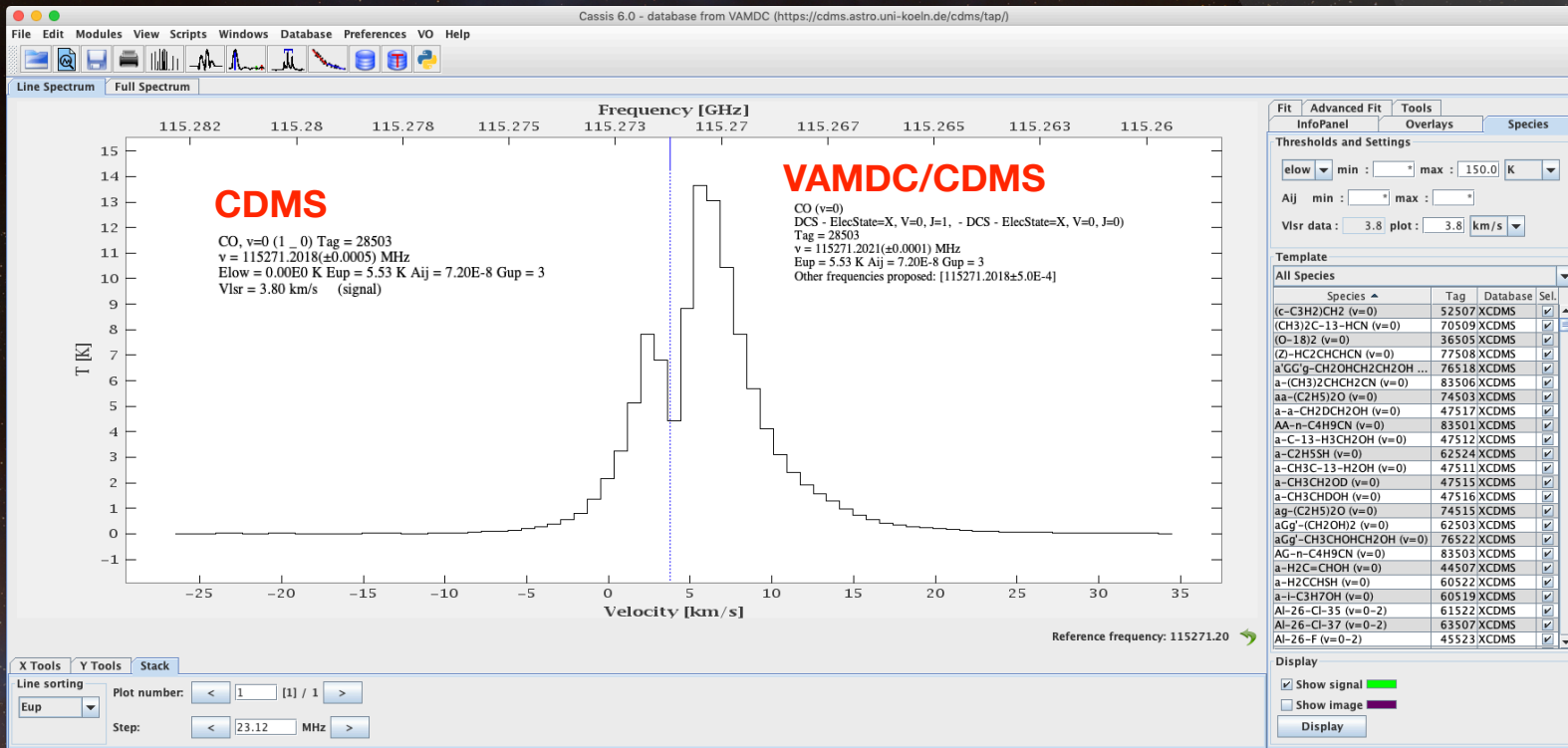


Access to the CDMS, JPL, NIST and VALD databases linked through VAMDC: *very slow*

Questions:

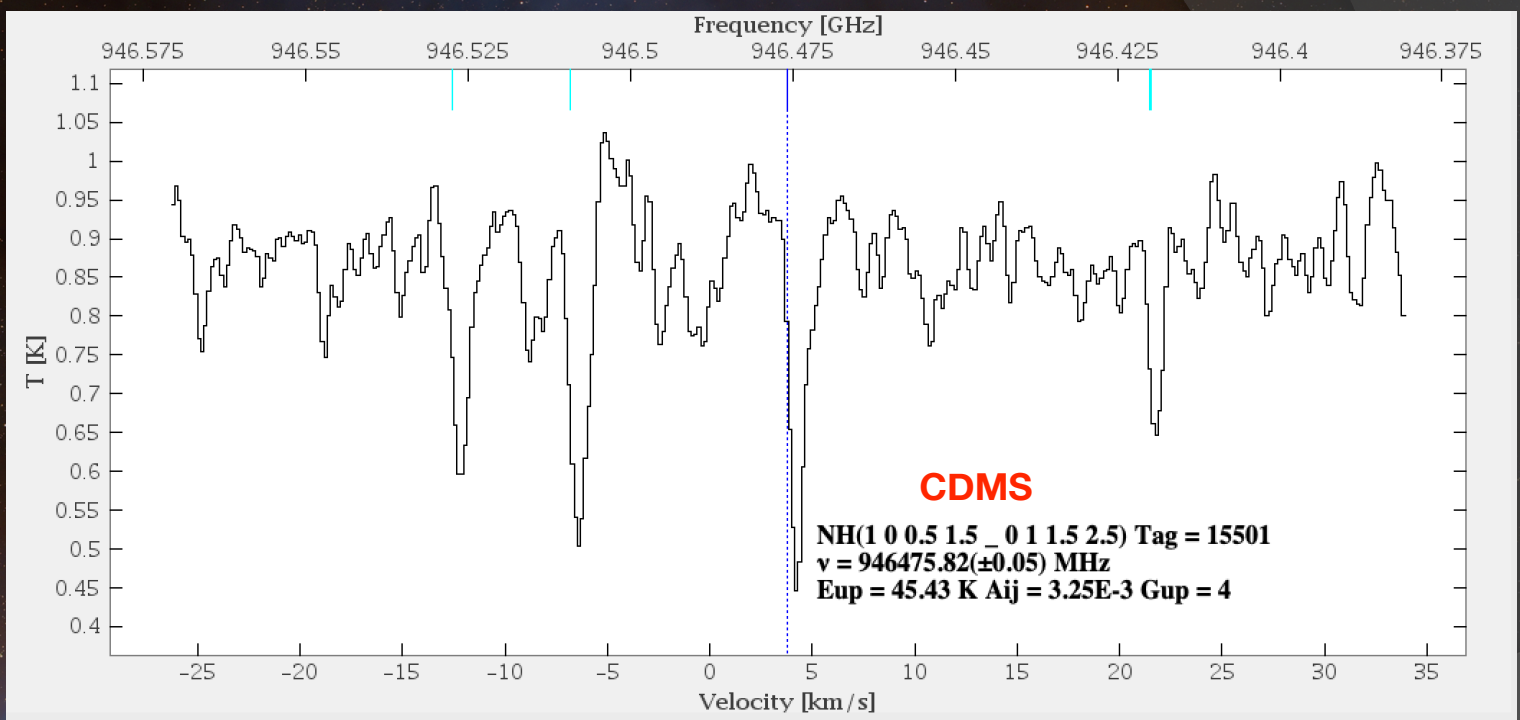
- 1) Define the best value for the frequency: EXP, THEO...
- 2) Within CASSIS, we must retrieve everything, references included: not "useful" for a quick line identification! Too time consuming. Solution: json?
- 3) Through the portal, is it possible to select a database only? And define criteria?
- 4) Retrieve a whole SQLite database from VAMDC with regular updates? How big?

I. Line Identification: VAMDC Access to CDMS



VAMDC: not limited for example for the 3 digit limit on the statistical weigh
 When many frequencies available, we choose the one with the lowest uncertainty.

I. Line Identification: VAMDC Access to CDMS



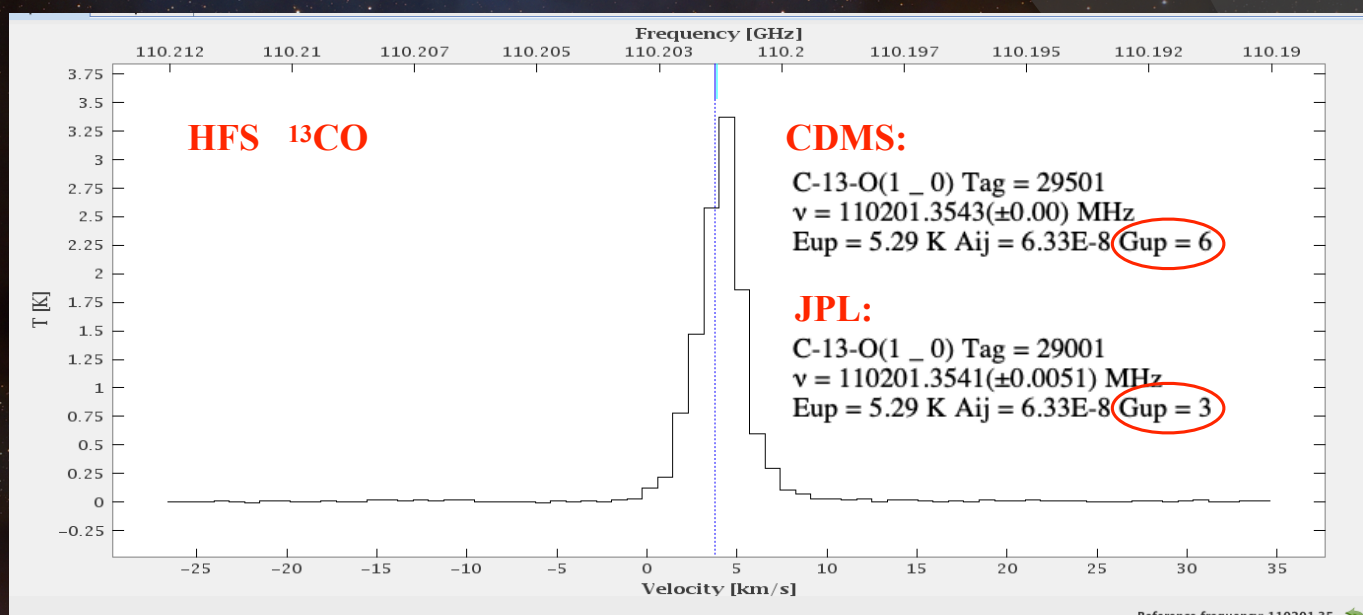
NH from VAMDC decoded in CASSIS:

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
 $\nu = 946475.8538(\pm 0.033)$ MHz
 Eup = 45.43 K Aij = 3.25E-3 Gup = 4
 Other frequencies proposed: [946475.82±0.05]



9 versus 4 quantum numbers

I. 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
 $\nu = 110201.3707(\pm 0.0001)$ 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,
 $\nu = 110201.3543(\pm 0.00)$ 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
 $\nu = 110201.3216(\pm 0.0002)$ MHz, Eup = 5.29 K Aij = 6.33E-8 Gup = 2
 Other frequencies proposed: [110201.3218±7.0E-4]

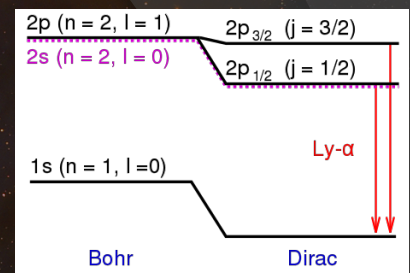
VAMDC/JPL:

- DCS - ElecState=X, V=0, J=1, - DCS - ElecState=X, V=0, J=0,
 $\nu = 110201.3541(\pm 0.0051)$ MHz
 Eup = 5.29 K Aij = 6.33E-8 Gup = 3

Factor 2 for the partition function

II. Line Identification: atomic databases

1 simple species, (Lyman-alpha), 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>
```

Kentucky database (Not in VAMDC):

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

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>
```

Some quantum numbers in VALD but not for everything. Also need some decoding to get the QN listed in the above figure. Not very useful...

II. Line Identification: atomic databases

NIST VAMDC:

```
<RadiativeTransition id="PASD-R275805"><Comments>Wavelength is for vacuum.</
Comments><EnergyWavelength><Wavelength><Value units="A">1215.6699</Value></Wavelength></
EnergyWavelength><UpperStateRef>SASD-001001.001.000002</UpperStateRef>
<LowerStateRef>SASD-001001.001.000001</LowerStateRef>
<Probability><TransitionProbabilityA><Value units="1/s">6.2648e+08</Value></
TransitionProbabilityA><Log10WeightedOscillatorStrength><Value units="unitless">-0.55657</Value></
Log10WeightedOscillatorStrength></Probability>
<ProcessClass></ProcessClass></RadiativeTransition>
```

```
<RadiativeTransition id="PASD-R275807"><Comments>Wavelength is for vacuum.</
Comments><EnergyWavelength><Wavelength><Value units="A">1215.6699</Value></Wavelength></
EnergyWavelength><UpperStateRef>SASD-001001.001.000004</UpperStateRef>
<LowerStateRef>SASD-001001.001.000001</LowerStateRef>
<Probability><TransitionProbabilityA><Value units="1/s">6.2647e+08</Value></
TransitionProbabilityA><Log10WeightedOscillatorStrength><Value units="unitless">-0.25555</Value></
Log10WeightedOscillatorStrength></Probability>
<ProcessClass></ProcessClass></RadiativeTransition>
```



No quantum numbers in NIST/VAMDC!! Not very useful...

NIST:

Observed	Ritz Wavelength	A_{ij}							
1215.6699	1215.668237310	6.2647e+08	1s	2S	1/2	2p	2P°	3/2	
1215.6699	1215.673644608	6.2648e+08	1s	2S	1/2	2p	2P°	1/2	

II. Stellar spectra (with CASSIS NIST database)

Registry & Services selection

Registry: <http://reg-vv.org/taq> Query

All Registry Favorite Manual

Polarisbase SSAP service for ESPaDOns/Naval spectra

POLLUX Database

POPSTAR with Chabrier IMF

POPSTAR with Ferrini IMF

POPSTAR with Kroupa IMF

POPSTAR with Salpeter (1955) IMF with m=(0.15-100)Msun

Deselect all Select all Add service Find

Results

Polarisbase SSAP

Index	Title	DataLength	TargetPos	SpectralAxisName	SpectralAxisUnit	spectralsi	FluxAxisName	FluxAxisUnit	f
19990	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_107	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19991	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_108	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19992	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_112	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19993	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_114	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19994	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_116	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19995	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_117	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19996	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_119	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19997	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_123	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19998	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_125	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
19999	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_129	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1
20000	harval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_130	213803	279.235 38.7817	AWAV	nanometer	1E-9 L	FLUX	dimensionless	1

Deselect all Download selected Download all Display selected Display all Open Clear results

Simple Spectral Access (SSA)

Request

Global Parameters

Object name: vega Resolve

RA: 18:36:56.336 DEC: +38:47:01.28

SEARCH RADIUS: 10 arcsec

BAND: Spectral range, can be empty

TIME: Time coverage, can be empty

FORMAT: none

Query

queryData&POS=279.234734787,38.783688956482E=0.0027777777777777778 Advanced Query

Frequency [GHz]

457000 456750 456500 456250

Flux [1E-26 J]

4 3.75 3.5 3.25 3 2.75 2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5

Wavelength [Ångström]

6557.5 6560 6562.5 6565 6567.5 6570

H I (112_3/2) Tag = 1101
 $\lambda = 6564.5226 (\pm 0.00)$ Ångström
 Elow = 118352.27 K Eup = 82258.92 K Aij = 6.90E-1 Gap = 2
 Vlsr = 20.60 km/s

X Tools Tools Stack/Mosaic

Shift Zoom Search Range

<< >> + - 564.28 Go 14.58 Set

Plot min/max

6556.991 | 6571.574 Set

X_top Frequency GHz

X_bot Wavelength Ångström

Log

Fit Tools Advanced Fit

InfoPanel Overlays Species

Plot Info

Spectrum Analysis 1

21aug13_Nnorm_vega_117_2

in: SKY

Spectrum Analysis 2

M_p8000g3.5x2.25x1.0_a_0_...

in: SKY

Tools Results

Result AtV 1

in: SKY

Result VA 1

in: SKY

Result AV 2

in: SKY

Result AV 3

in: SKY

Other Species

Remove All

Full Spectrum

Frequency [GHz]

800000 700000 600000 500000 400000 300000

flux [erg/cm^2/s/Å]

100 90 80 70 60 50 40 30 20 10 0 -10

Wavelength [Ångström]

4000 5000 6000 7000 8000 9000 10000

X Tools Y Tools Stack/Mosaic

Shift Zoom Search Range

<< >> + - 993.84 Go 458.77 Set

Plot min/max

3364.457 | 10823.229 Set

X_top Frequency GHz

X_bot Wavelength Ångström

Log

Fit Tools Advanced Fit

InfoPanel Overlays Species

Plot Info

Spectrum Analysis 2

21aug13_Nnorm_vega_117_2

in: SKY vlsr: 0

Remove All

II. Stellar spectra (with VAMDC CHIANTI database)

Simple Spectral Access (SSA)

Registry: <http://reg-g-vo.org/tap>

Object name: Resolve

RA: 18.36.56.336 DEC: +38.47.01.28

SEARCH RADIUS: 10 arcsec

BAND: Spectral range, can be empty

TIME: Time coverage, can be empty

FORMAT: none

Query: queryData&POS=279.234734787,38.783688956650E=0.0027777777777777778

Results

Index	Title	DataLength	TargetPos	SpectralAxisName	SpectralAxisUnit	spectrals1	FluxAxisName	FluxAxisUnit
19990	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_107	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19991	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_108	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19992	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_112	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19993	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_114	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19994	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_116	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19995	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_117	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19996	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_119	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19997	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_123	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19998	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_125	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
19999	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_129	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1
20000	narval_2013_21aug13_Nnorm_21aug13_Nnorm_vega_130	213803	279.235 38.7837	AWAV	nanometer	IE-9 L FLUX	dimensionless	1

Frequency [GHz]

H I (J = 1.5 - J = 0.5) Tag = Xchianti-1
 $\lambda = 6564.52 (\pm 0.00)$ Angstrom
 Elow = 118352.24 K Eup = 140269.72 K
 Aij = 5.39E7 Gup = 4
[VAMDC references](#)

Full Spectrum

flux [erg/cm²/s/A]

Frequency [GHz]

Wavelength [Angstrom]

Fit Tools Advanced Fit

InfoPanel Overlays Species

Thresholds and Settings

eup min: 0.0 max: 1.112E K

elow min: 0.0 max: 150.0

A min: 0.0 max: 1

visr data: 0.0 plot: 20.6 km

Template

All Species

Name	Id	Database	Set
Al II	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al III	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al IX	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al V	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al VI	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al VII	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al VIII	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al X	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al XI	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al XII	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Al XIII	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Ar III	Xchia...	Xchianti	<input checked="" type="checkbox"/>
Ar IV	Xchia...	Xchianti	<input checked="" type="checkbox"/>

Display Show Limit research to visible data Display

Plot Info

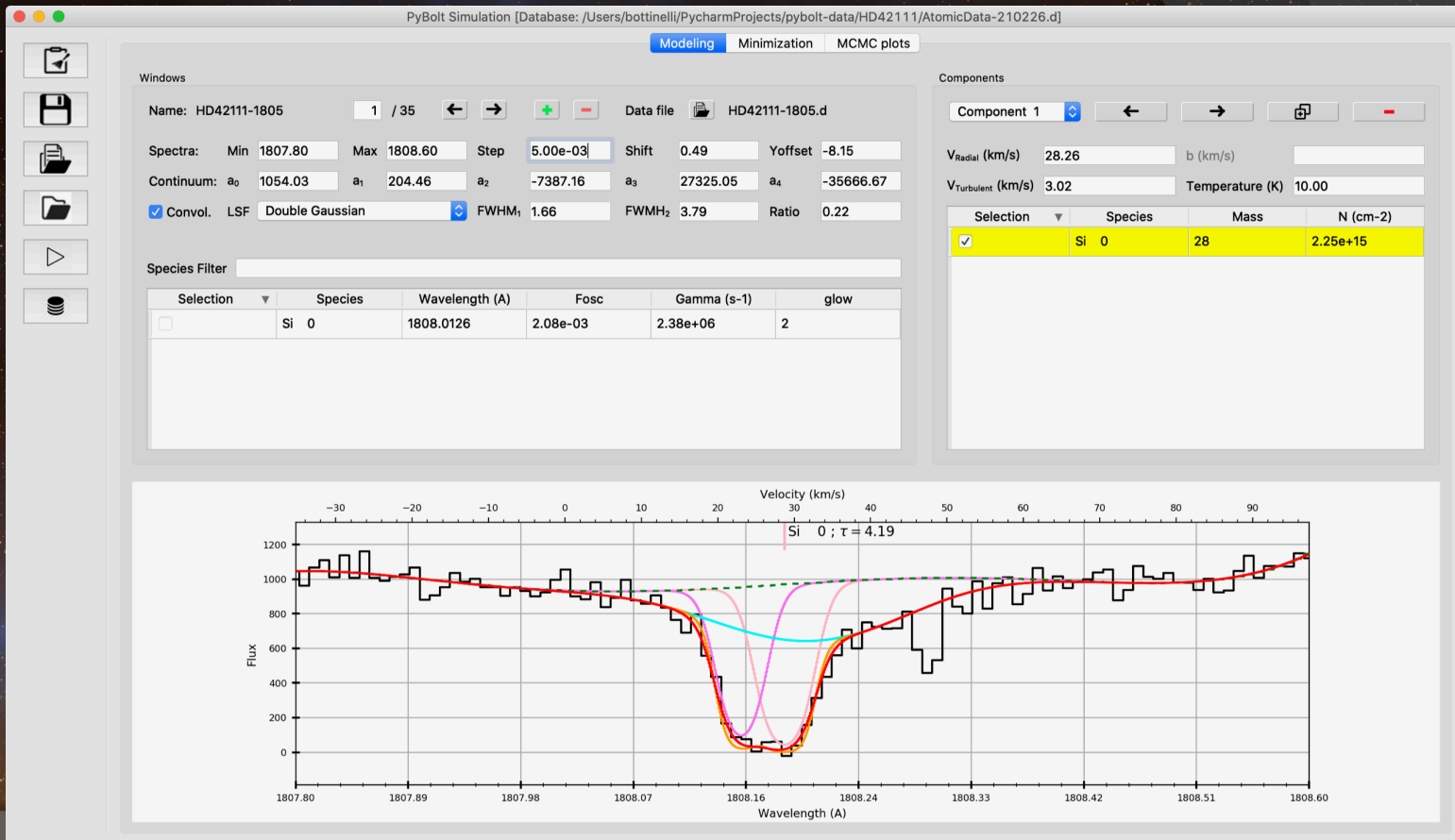
Spectrum Analysis 2

21aug13_Nnorm_vega_117_2

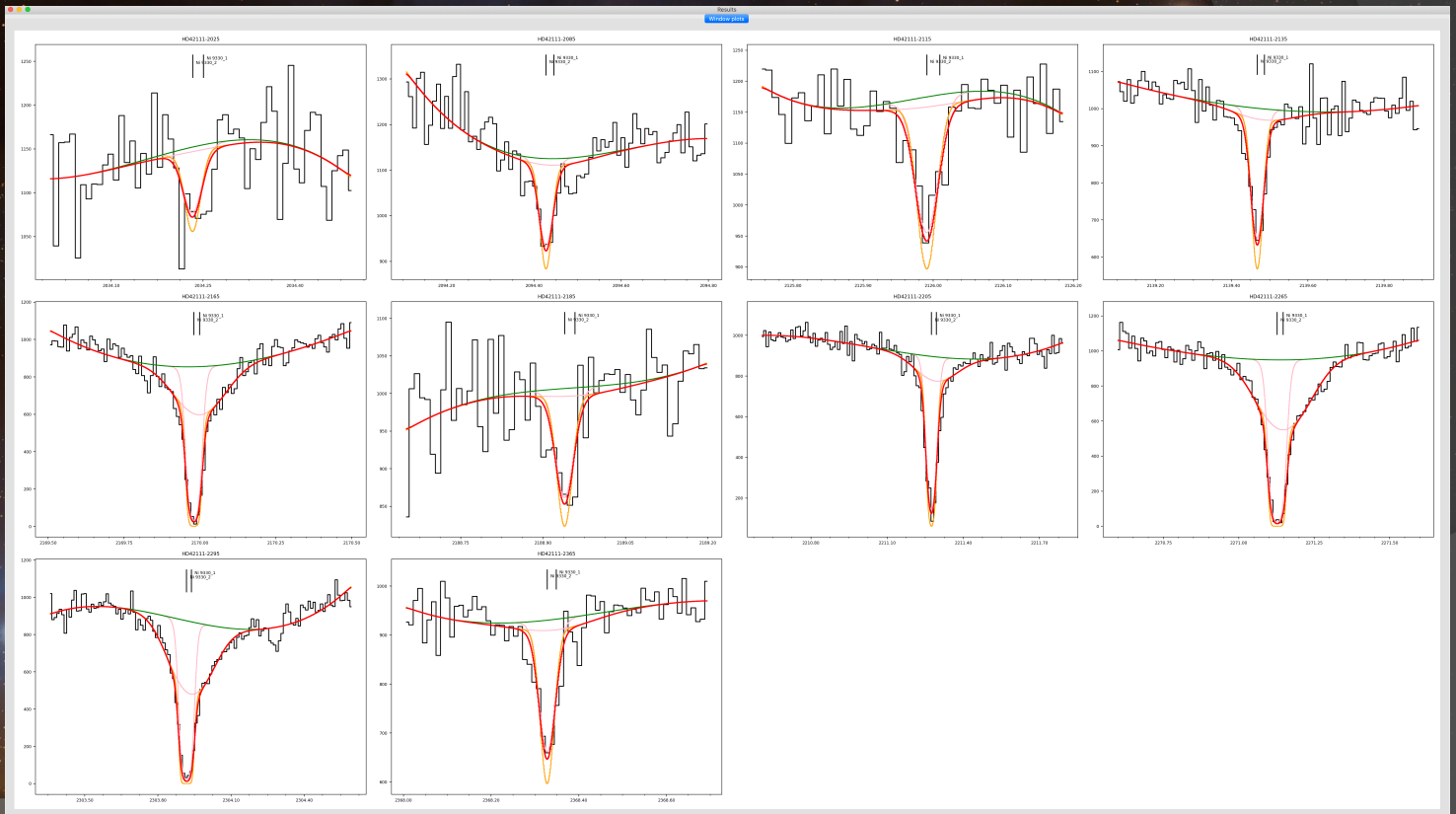
in: SKY visr: 0

Remove All

Absorption spectra (with Ad'Hoc database) PyBolt module (in progress)



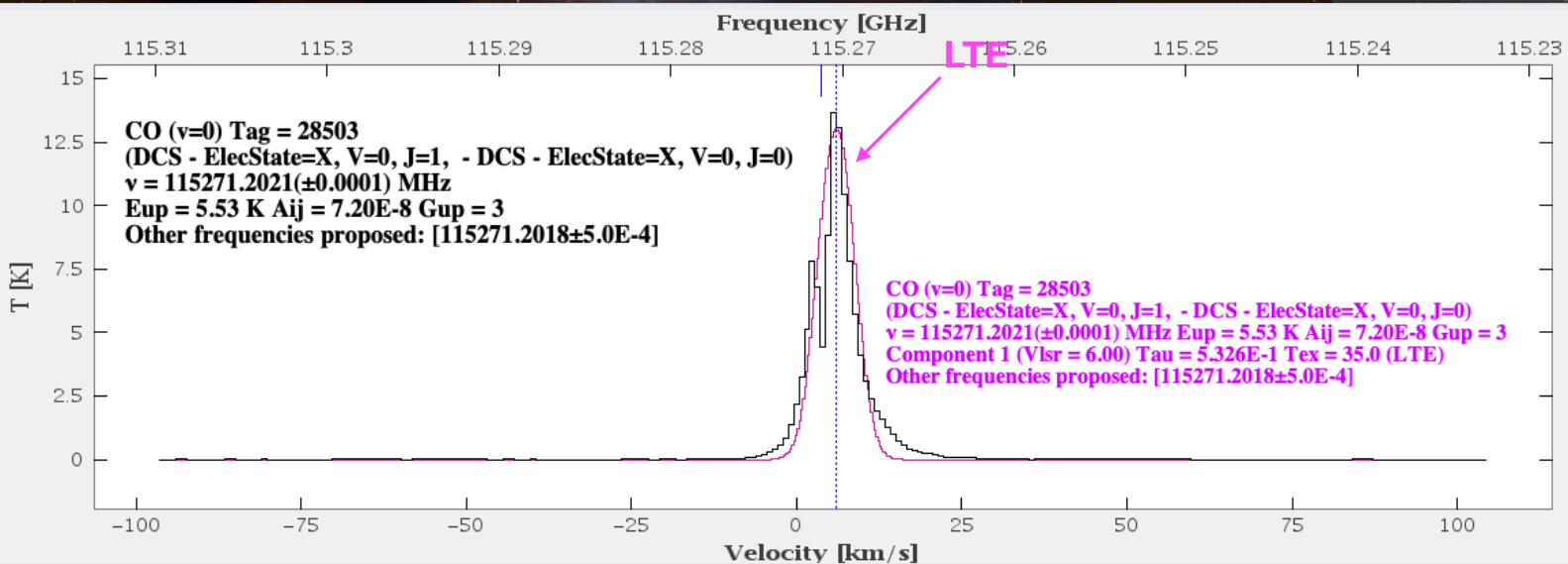
Absorption spectra (with Ad'Hoc database) PyBolt module (in progress)



III. Radiative transfer: LTE

- 1) Line identification through VAMDC
- 2) LTE modelling using the partition function, A_{ij} , g_u , frequencies given by VAMDC

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



Radiative transfer:
non-LTE (Radex)

Collisional databases
present : lambda + local
futur : VAMDC + EMAA

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: Kup min: Lup min: Mup min:

LTE-RADEX

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

Continuum: Component 1

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

Species	Tag	Database	Collision	Compute	N(Sp) [cm ⁻²]	Abundance (J...)	TKin (K)	FWHM (km/s)	Size (")
C-13-O	29501	CDMS	13CO-o-p-H...	<input checked="" type="checkbox"/>	4.00E16	3.33E-7	100.00	4.00	3000.00

Cassini 6.0 - database from SQLITE (cassisi20200513-FORCOM-HFS-IRAP.db)

File Edit Modules View Scripts Windows Database Preferences VO Help

Line Spectrum

Frequency [GHz]: 220.42, 220.415, 220.41, 220.405, 220.4, 220.395, 220.39, 220.385, 220.38, 220.375

T [K]: 7, 6, 5, 4, 3, 2, 1, 0

Velocity [km/s]: -20, -10, 0, 10, 20, 30

Reference frequency: 220398.68

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	<input type="checkbox"/>
(O-18)2	36505	CDMS	<input type="checkbox"/>
13C-CCH, v4=0,1mS	38504	CDMS	<input type="checkbox"/>
13CH	14003	JPL	<input type="checkbox"/>
13CH3 13CN	43005	JPL	<input type="checkbox"/>
13CH3CH2OH	47094	IRAP	<input type="checkbox"/>
13CH3D	18006	JPL	<input type="checkbox"/>
15-NO	31009	JPL	<input type="checkbox"/>

Display

Show signal █

Show image █

Display

X Tools Y Tools Stack

Line sorting: Frequency

Plot number: 2 [1,2] / 2

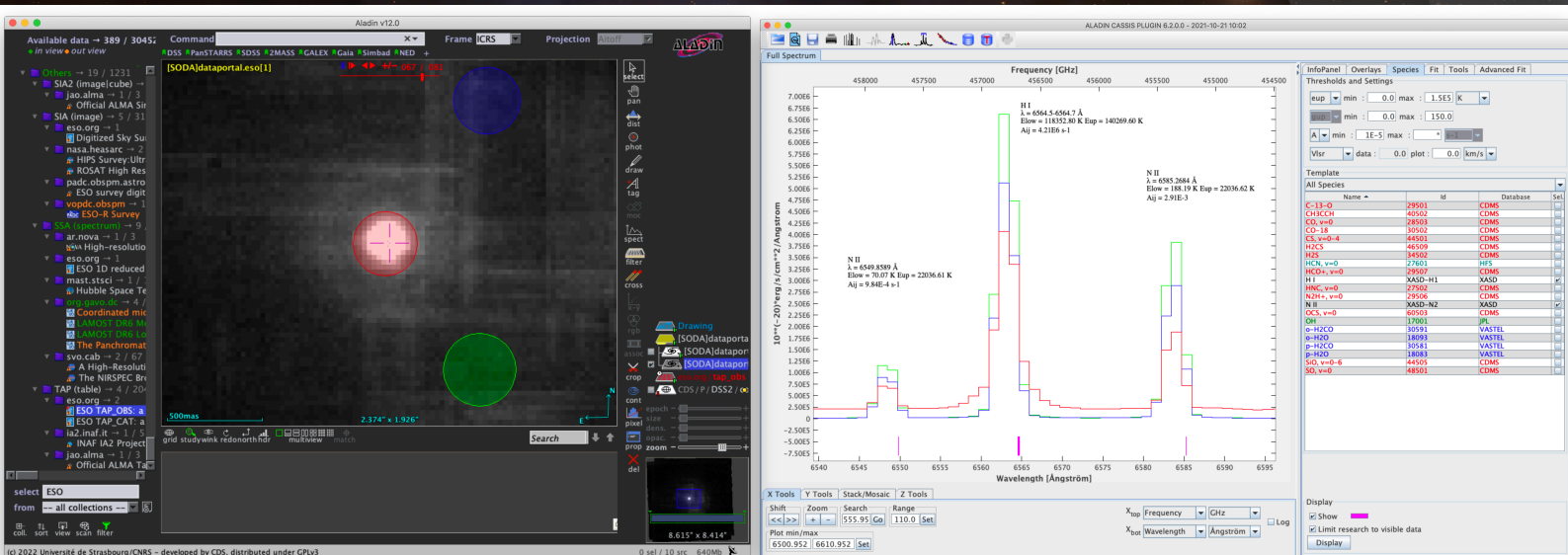
Step: 22.19 MHz

To do: retrieve some collision files from VAMDC, through Spectcol

IV. The Aladin connection: VO

<https://aladin.u-strasbg.fr/> developed by CDS Aladin team (Centre de Données Astronomiques de Strasbourg)

Select database for the cube (E.g. MUSE with ESO ObsTAP) and extract a data sub-cube (ESO SODA: datalink): define a polygon, extract the spectrum from the polygon and send to CASSIS (cursors and spectral profiles are synchronised between the two applications)



<http://cassis.irap.omp.eu/?page=publicationsandtalks>

<https://wiki.ivoa.net/internal/IVOA/InterOpNov2021Apps/2021-IVOA-Northern-Fall-interop-CASSIS-Aladin-Plugin-final.mp4>

<http://cassis.irap.omp.eu/download/presentations/Cassis Adass 2021 D3-001.pdf>

III. The Aladin connection: VO

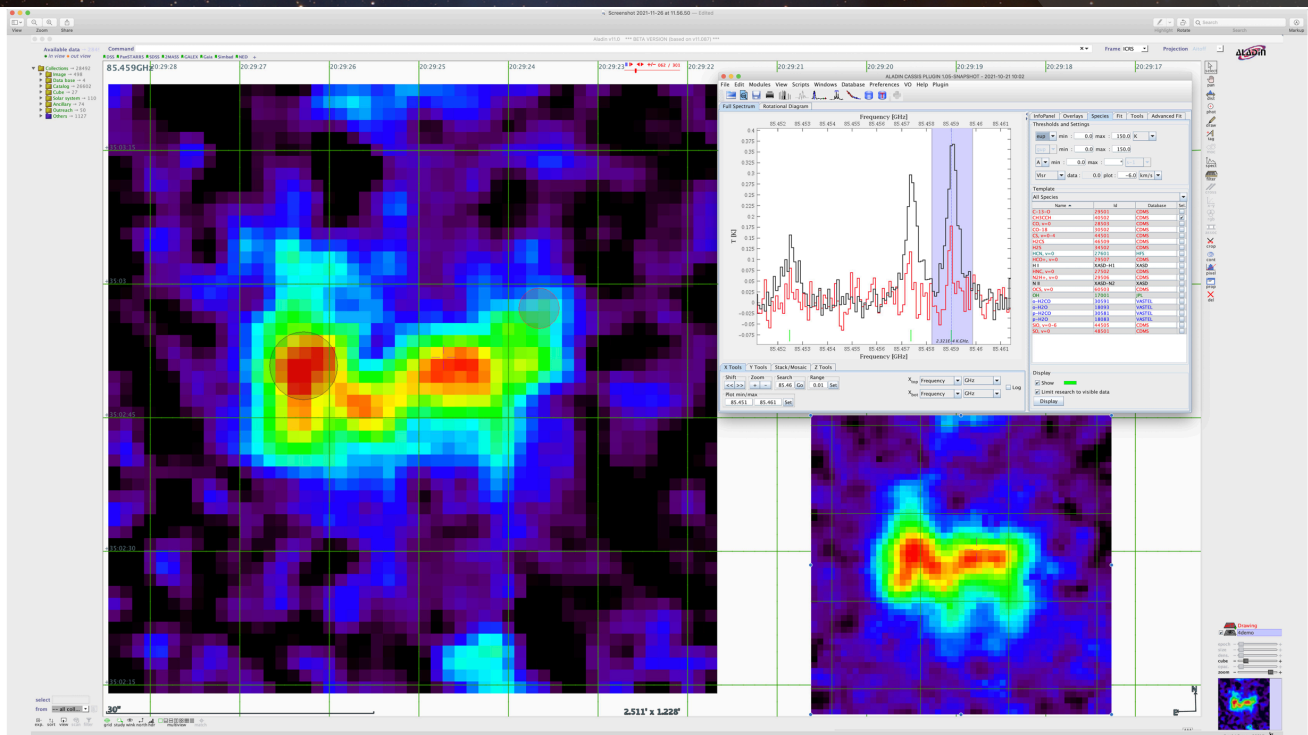


Figure 2. Selected areas on the cube field in Aladin (left) with the corresponding spectra in CASSIS (top right) and integrated spectral plane in Aladin driven by the blue limits set on the spectrum into the CASSIS window (bottom right).