

CASSIS

Centre d'Analyse Scientifique de Spectres Infrarouges
et Submillimétriques

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

Développement à l'IRAP

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Spectroscopic and molecular databases
(JPL, CDMS, NIST, HITRAN, Basecol, LAMDA)



CASSIS



LTE model and Radex



Parameters to vary: N ,
 T_k , T_{ex} , n_{H_2} , Δv , choice
of the molecule and
telescope, beam dilution...

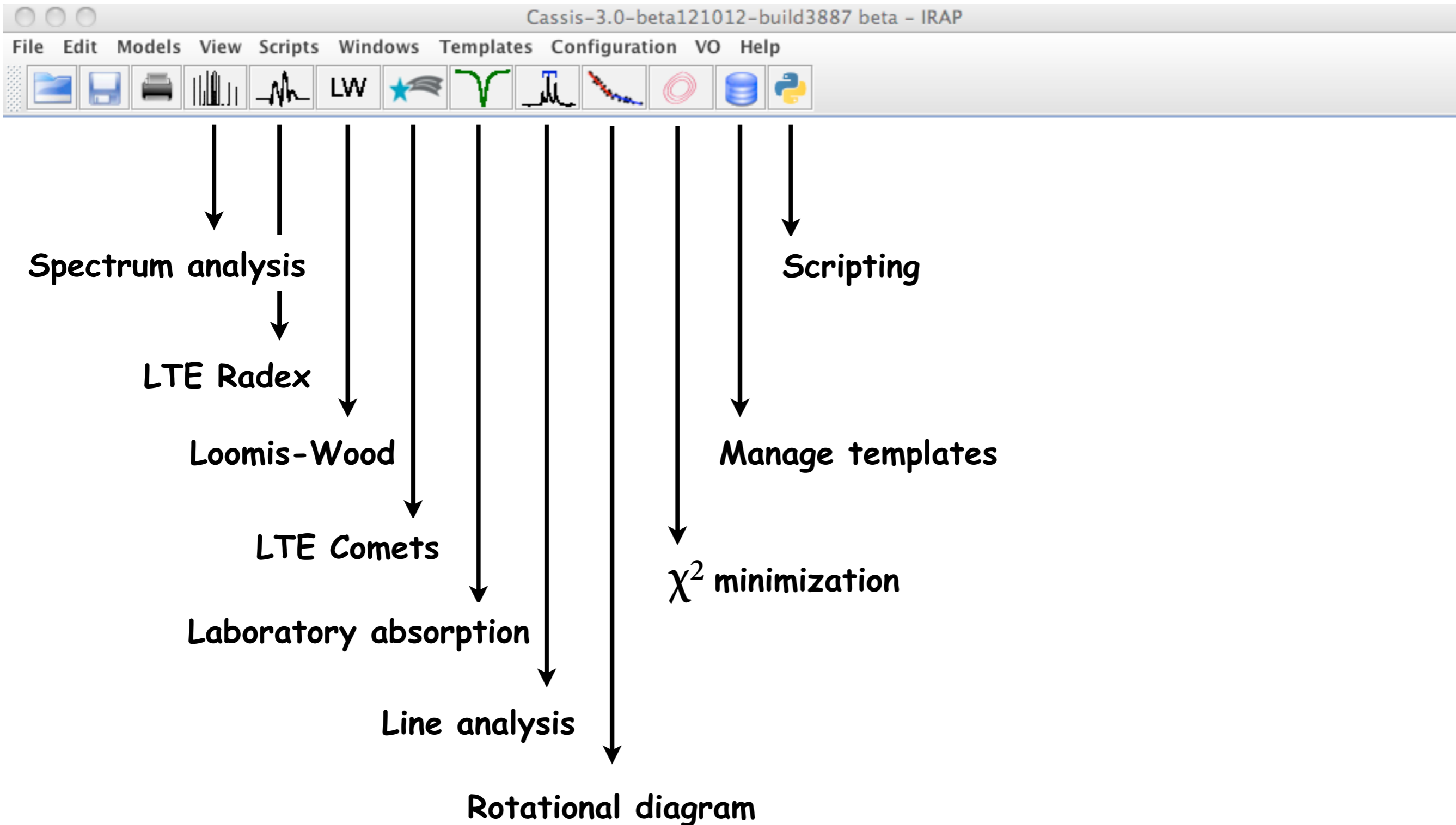


Observed spectra
(laboratory or
telescope)



Synthetic spectra, Line identification, Adjustment of the source parameters

CASSIS Tools



Spectral analysis

Line Analysis

Data
 Load Vlsr: Telescope

Tuning
 Range min: max: Band:

Threshold
 Eup min: max: Aij min: max:
 Jup min: max: Kup min: max: Lup min: max: Mup min: max:

Template
 Full CDMS

Name	Tag	Sel.
PH	32501	<input type="checkbox"/>
D2CO	32502	<input type="checkbox"/>
H2CO-18	32503	<input type="checkbox"/>
*CH3OH, vt=0,1	32504	<input checked="" type="checkbox"/>
DCO-18+	32505	<input type="checkbox"/>
H2C-13-OH+	32506	<input type="checkbox"/>
HDC-13-O	32507	<input type="checkbox"/>
O2-X, v=0	32508	<input type="checkbox"/>
C-13-F+, v=0,1	32509	<input type="checkbox"/>
O2-a	32510	<input type="checkbox"/>
S-atom	32511	<input type="checkbox"/>
LiCCN	32512	<input type="checkbox"/>

LTE-RADEX

Parameters
 Telescope: Tmb->Ta conv
 Imin:
 Noise: rms:
 Oversampling:

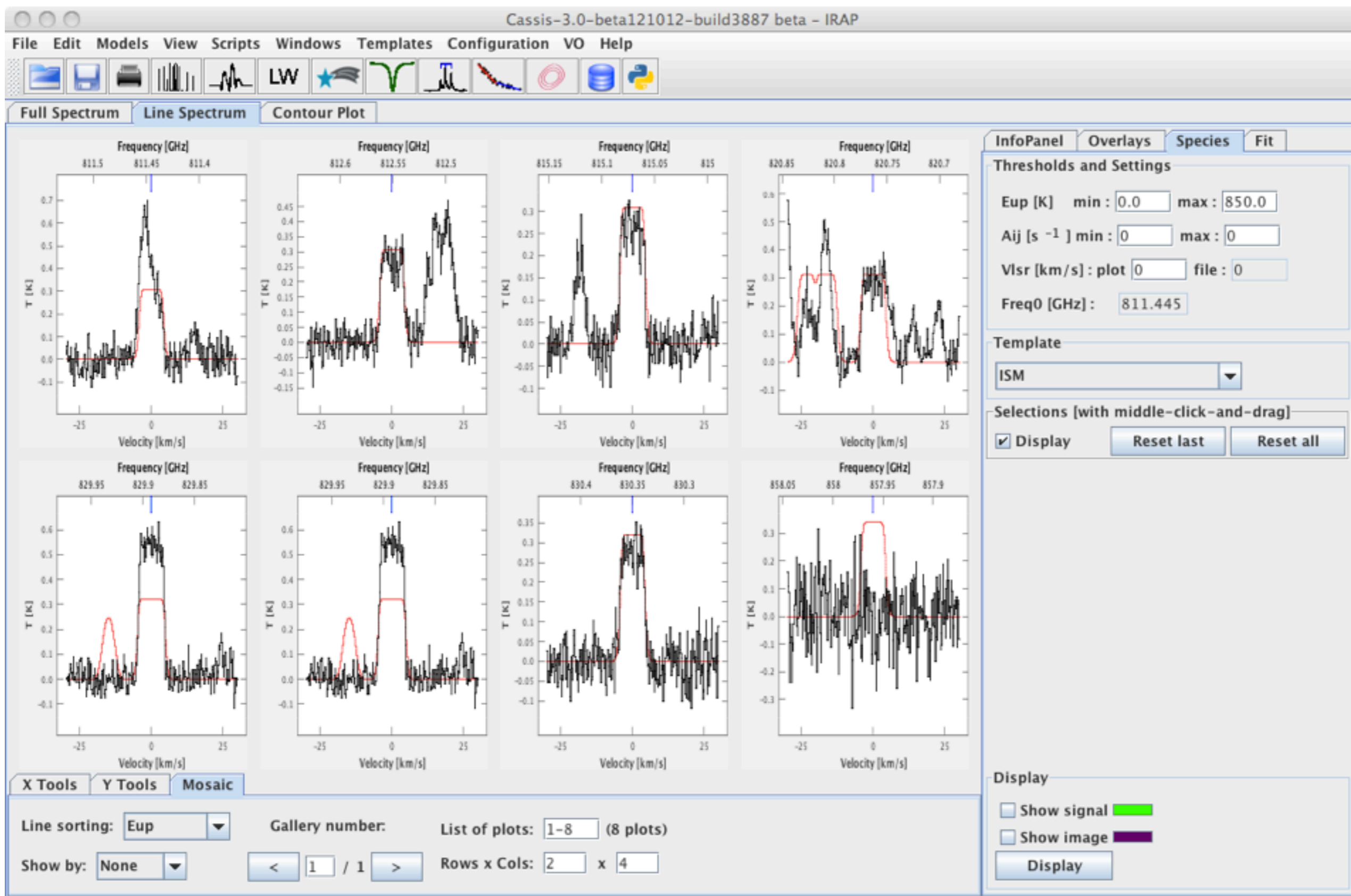
Component 1

Mode: Interacting
 Molecules: Geometry:
 Tbg [K]: N(H₂) [cm⁻²]:
 V_{lsr}:
 Continuum:

Species	Tag	Database	Compute	N(Sp) (cm ⁻²)	Abundance (/H ₂)	Tex (K)	FWHM (km/s)	Size (")
E-CH3OH	32083	VASTEL	<input type="checkbox"/>	7.00E16	9.33E-7	100.00	4.00	2.00
A-CH3OH	32093	VASTEL	<input type="checkbox"/>	7.00E16	9.33E-7	100.00	4.00	2.00
CH3OH	32003	JPL	<input type="checkbox"/>	3.00E16	4.00E-7	100.00	4.00	3.00
*CH3OH, vt=0,1	32504	CDMS	<input checked="" type="checkbox"/>	1.00E19	0.00	265.00	3.75	1.00

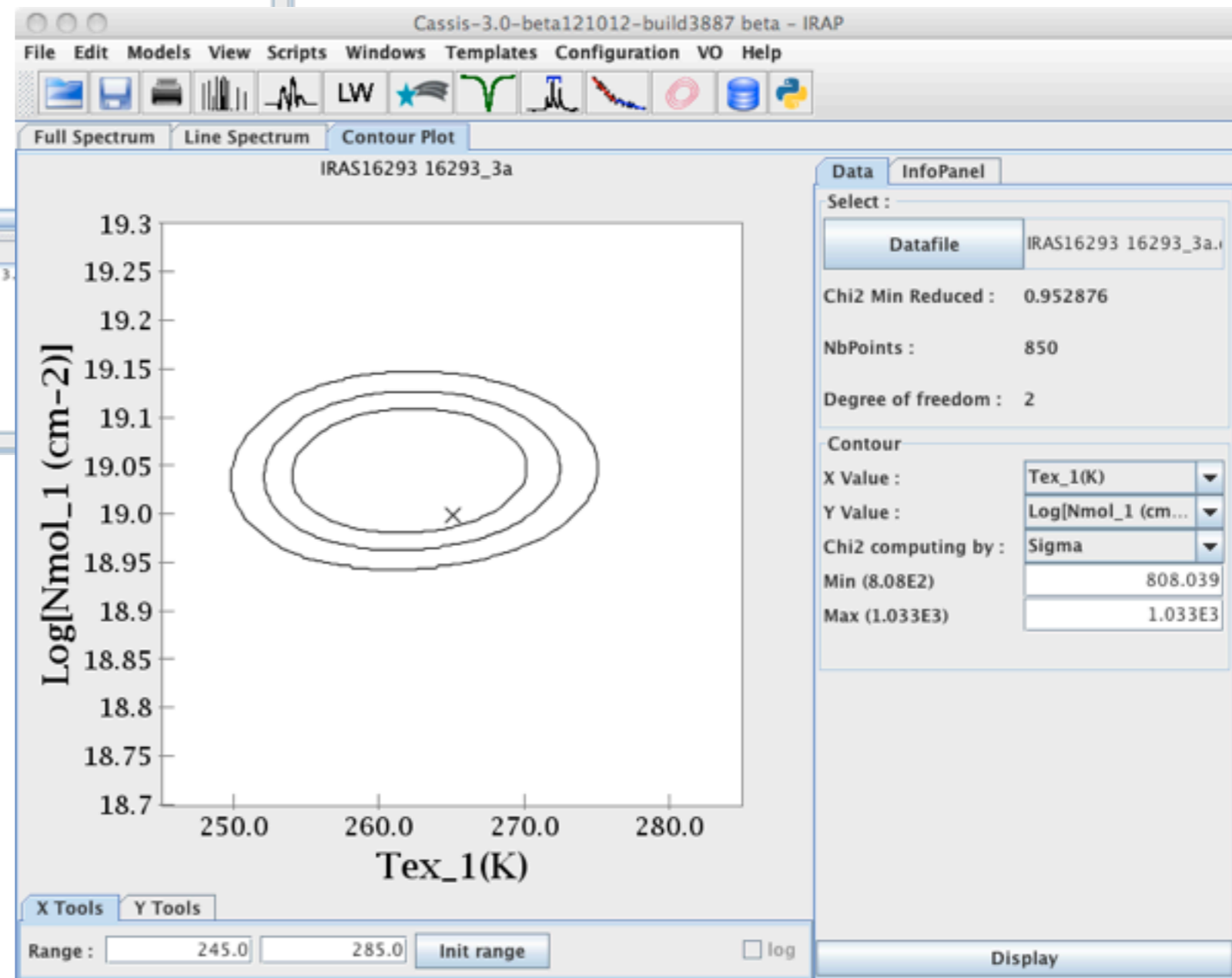
Buttons: Load config, Display, Save config

Spectral analysis



Spectral analysis

```
Jython Script - /Users/vastel/TALK/VAMDC/CH3OH_RG_LTE.py
Run Run Block Stop Load Save Save As... Save All Clear Comment Options
ScriptRadexLA.py CO_RG.py CH3OH_RG_LTE.py
# Line 13
f13 = [857.94, 857.98]
apex = CASSIS_DIR + "/delivery/telescope/apex"
hifi = CASSIS_DIR + "/delivery/telescope/hifi"
alma_400m = CASSIS_DIR + "/delivery/telescope/alma_400m"
iram_ABCD = CASSIS_DIR + "/delivery/telescope/iram_ABCD"
userInputs = UserInputs(
telescope = "hifi",
tuningRange = [799.024, 859.6065],
tuningBand = 25.0,
aijMin = 1.0e-3,
eup = [0.0, 202.0],
#kup = [0,0],
template = "Full COMS",
moltags = [32504],
fileName = "16293_3a",
#suffixName = [".peak_cont"],
extensionName = ".fus",
sourceName = "IRAS16293 ",
workingDir = "/Users/vastel/TALK/VAMDC/",
reducingFactor = 1.5,
tmb2ta = False,
isoUnique = False,
warning = True,
outputConcatFile = "",
# Enter here the lines not to be excluded of the computation
notExcludedLines = [0,1,2,3,4,5,6,7,8,9,10,11],
# Lines data
Console
Best parameters 1: PhysicalModel(vlsr = 0, tex = 265, n_H2 = 1e+08, nmol = 1e+19, size = 1, fwhm = 3.
Total nb of points used in the computation = 850
Computing the best model... OK
OverSampling: 5
Telescope: hifi
Computing the chi2 contour... OK
$$$
```



Spectral analysis

Line Analysis

Data: Load Vlsr: 0 km/s Telescope: ???

Tuning: Range min: 799.0245 max: 859.6065 GHz Signal Band: 60.0 Km/s

Threshold: Eup min: 0.0 max: 150.0 K Aij min: 1.0E-4 max: *
Jup min: * max: * Kup min: * max: * Lup min: * max: * Mup min: * max: *

LTE-RADEX

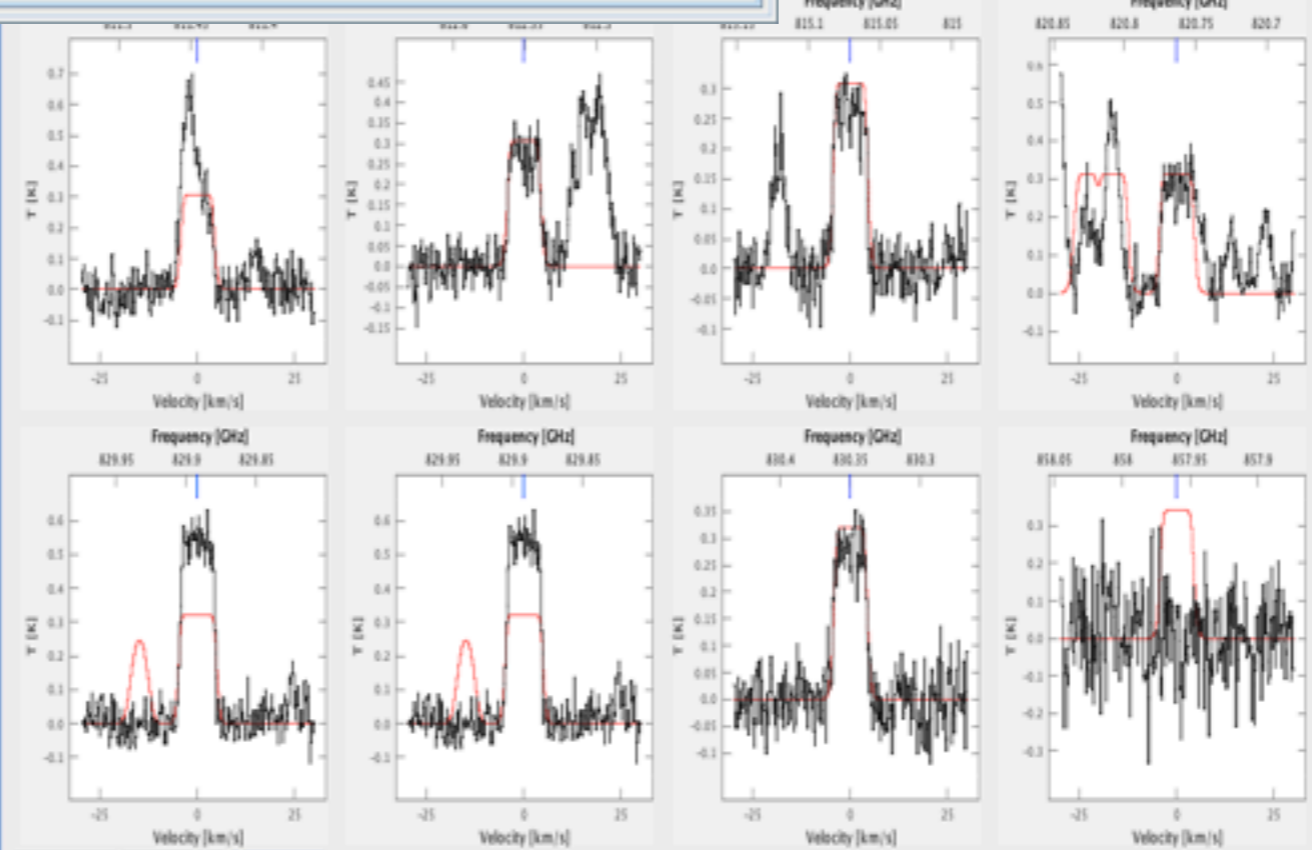
Parameters: Telescope: hifi Tmb->Ta conv: hifi Imin: 0.0 mK Noise: rms: 0.0 mK Oversampling: 3.0

Component 1 X +

Mode: Full LTE Interacting Tbg [K]: 2.73 N(H₂) [cm⁻²]: 7.5E22 Continuum: Continuum 0 [K]
Molecules: -- Operations -- Geometry: Sphere V_{lsr}: 0.0 Km/s

Species	Tag	Database	Compute	N(Sp) (cm ⁻²)	Abundance (/H ₂)	Tex (K)	FWHM (km/s)	Size (")
E-CH ₃ OH	32083	VASTEL	<input type="checkbox"/>	7.00E16	9.33E-7	100.00	4.00	2.00
A-CH ₃ OH	32093	VASTEL	<input type="checkbox"/>	7.00E16	9.33E-7	100.00	4.00	2.00
CH ₃ OH	32003	JPL	<input type="checkbox"/>	3.00E16	4.00E-7	100.00	4.00	3.00
*CH ₃ OH, vt=0,1	32504	CDMS	<input checked="" type="checkbox"/>	1.00E19	0.00	265.00	3.75	1.00

D-beta121012-build3887 beta - IRAP



InfoPanel Overlays Species Fit

Thresholds and Settings

Eup [K] min: 0.0 max: 850.0
Aij [s⁻¹] min: 0 max: 0
Vlsr [km/s]: plot 0 file: 0
Freq0 [GHz]: 811.445

Template: ISM

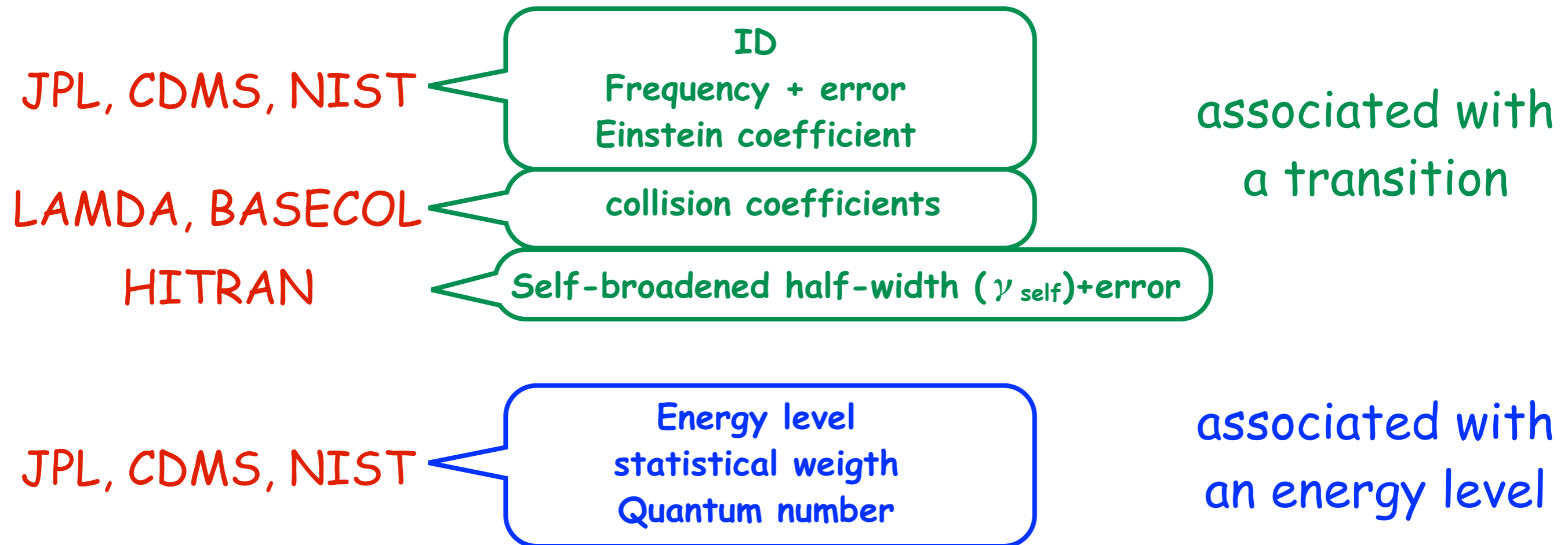
Selections [with middle-click-and-drag]:
 Display

Display:
 Show signal
 Show image

X Tools Y Tools Mosaic

Line sorting: Eup Gallery number: List of plots: 1-8 (8 plots)
Show by: None / 1 Rows x Cols: 2 x 4

CASSIS database: link through VAMDC



All of these can be retrieved through VAMDC in a unified way (perfect for the matching of the quantum numbers in the case of the collision coefficients)

VAMDC libraries as used by CASSIS

Elaboration of a simple software (use of the spectcol libraries) that retrieves the data needed for CASSIS through the VAMDC protocols (XSAMS deciphering).

Provider

Get VAMDC PROVIDER

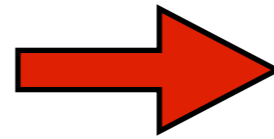
no provider

Species

Tag = ?
Name = ?
Molecular weight = ?
Part. Function Temp = partition ?
Part. Function Q = partition ?

Transitions

ID	Gup	elow	frequency	error	aint	Quantum N...
?	?	?	?	?	?	?



Provider

Get VAMDC PROVIDER

ivo://vamdc/smpo-sample
ivo://vamdc/reims-ethylene
ivo://vamdc/ghosst
ivo://vamdc/chianti/django
ivo://vamdc/CDMS/Django
ivo://vamdc/vald/uu/django
ivo://vamdc/VamdcSpeciesDB-TapService
ivo://vamdc/OACatania/LASP

Species

Tag = ?
Name = ?
Molecular weight = ?
Part. Function Temp = partition ?
Part. Function Q = partition ?

Transitions

ID	Gup	elow	frequency	error	aint	Quantum N...
?	?	?	?	?	?	?

Spectcol as used by CASSIS

Provider

Get VAMDC PROVIDER

- ivo://vamdc/smpo-sample
- ivo://vamdc/reims-ethylene
- ivo://vamdc/ghosst
- ivo://vamdc/chianti/django
- ivo://vamdc/CDMS/Django
- ivo://vamdc/vald/uu/django
- ivo://vamdc/VamdcSpeciesDB-TapService
- ivo://vamdc/OACatania/LASP

Species

XCDMS-83 (UGFAIRIUMAVXCW-UHF	Tag =	?
XCDMS-96 (UGFAIRIUMAVXCW-OUB	Name =	?
XCDMS-98 (UGFAIRIUMAVXCW-VQE	Molecular weight =	?
XCDMS-117 (UGFAIRIUMAVXCW-HQ	Part. Function Temp =	partition ?
XCDMS-118 (UGFAIRIUMAVXCW-ZD	Part. Function Q =	partition ?

Transitions

ID	Gup	elow	frequency	error	aint	Quantum N...
?	?	?	?	?	?	?

Species ID

InChIKey

Provider

Get VAMDC PROVIDER

- ivo://vamdc/smpo-sample
- ivo://vamdc/reims-ethylene
- ivo://vamdc/ghosst
- ivo://vamdc/chianti/django
- ivo://vamdc/CDMS/Django
- ivo://vamdc/vald/uu/django
- ivo://vamdc/VamdcSpeciesDB-TapService
- ivo://vamdc/OACatania/LASP

Species

XCDMS-83 (UGFAIRIUMAVXCW-UHFFF	Tag =	28503
XCDMS-96 (UGFAIRIUMAVXCW-OUBTZ	Name =	Carbon Monoxide
XCDMS-98 (UGFAIRIUMAVXCW-VQEHI	Molecular weight =	28.0
XCDMS-117 (UGFAIRIUMAVXCW-HQMP	Part. Function Temp =	[2.725, 5.0, 9.375, ...
XCDMS-118 (UGFAIRIUMAVXCW-ZDOI	Part. Function Q =	[1.4053, 2.1824, 3.7...

Transitions

ID	gup	elow	frequency	error	aint	Quantum Numbers
SCDMS-90...	3	0.0	115271.2021	1.0E-4	7.2036033...	J=1, vi=0-j=0, vi=0
SCDMS-90...	5	3.845033	230538.0	1.0E-4	6.9106122...	J=2, vi=0-j=1, vi=0
SCDMS-90...	7	11.534953	345795.9899	2.0E-4	2.4966366...	J=3, vi=0-j=2, vi=0
SCDMS-90...	9	23.069466	461040.7681	2.0E-4	6.1265235...	J=4, vi=0-j=3, vi=0
SCDMS-90...	11	38.448131	576267.931	3.0E-4	1.2213113...	J=5, vi=0-j=4, vi=0
SCDMS-90...	13	57.67036	691473.076	3.0E-4	2.1374519...	J=6, vi=0-j=5, vi=0
SCDMS-90...	15	80.735419	806651.8008	4.0E-4	3.4223102...	J=7, vi=0-j=6, vi=0
SCDMS-90...	17	107.642427	921799.7039	5.0E-4	5.1340598...	J=8, vi=0-j=7, vi=0
SCDMS-90...	19	138.390355	1036912.3...	7.0E-4	7.3298815...	J=9, vi=0-j=8, vi=0
SCDMS-90...	21	172.978029	1151985.4...	9.0E-4	1.0063633...	J=10, vi=0-j=9, vi=0
SCDMS-90...	23	211.404127	1267014.4...	0.0012	1.3389996...	J=11, vi=0-j=10, v...
SCDMS-90...	25	253.667181	1381995.1...	0.0015	1.7352838...	J=12, vi=0-j=11, v...
SCDMS-90...	27	299.765576	1496922.9...	0.0018	2.2008533...	J=13, vi=0-j=12, v...
SCDMS-90...	29	349.69755	1611793.5...	0.0021	2.7389771...	J=14, vi=0-j=13, v...
SCDMS-90...	31	403.461194	1726602.5...	0.0024	3.3542527...	J=15, vi=0-j=14, v...
SCDMS-90...	33	461.054454	1841345.5...	0.0028	4.0498262...	J=16, vi=0-j=15, v...
SCDMS-90...	35	522.475129	1956018.1...	0.0030	4.8286611...	J=17, vi=0-j=16, v...
SCDMS-90...	37	587.720871	2070615.9...	0.0033	5.6948070...	J=18, vi=0-j=17, v...
SCDMS-90...	39	656.789186	2185134.6...	0.0035	6.6496799...	J=19, vi=0-j=18, v...
SCDMS-90...	41	729.677434	2299569.8...	0.0037	7.6947944...	J=20, vi=0-j=19, v...
SCDMS-90...	43	806.382828	2413917.1...	0.0038	8.8342715...	J=21, vi=0-j=20, v...
SCDMS-90...	45	886.902435	2528172.0...	0.0039	0.0010065...	J=22, vi=0-j=21, v...
SCDMS-90...	47	971.233178	2642330.3...	0.0039	0.0011390...	J=23, vi=0-j=22, v...
SCDMS-90...	49	1059.371...	2756387.585	0.0040	0.0012807...	J=24, vi=0-j=23, v...
SCDMS-90...	51	1151.315	2870339.4	0.0041	0.0014319	J=25, vi=0-j=24, v...

CASSIS Engine

- Full java (requires java 1.6 or above) - multi platform
 - Tested on MacOSX, Linux and Windows
- GUI based, but scripting available
- Use of simple configuration files
- User-friendly automatic installer
- Frequent updates reflecting bugs correction
- Automatic and tunable update
- Bugs reporting system

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

CASSIS Database

- The complete database is resident on the laptop (< 1 Gb)
- Sqlite Format (no need of any extra software)
 - Use of JPL, CDMS and NIST databases
 - ortho-para-A-E separation for a few species (H_2O , H_2S , D_2O , D_2S , H_2CO , D_2CO , CH_3OH , $c\text{-C}_3\text{H}_2$, CH_3CCH , H_2D^+ , D_2H^+)
- Allows a quick access with various sorting
- Regular updates to reflect new entries in the databases
- Can be populated separately by each user (expert mode)

Atrochemistry and Physics of the Interstellar Medium: gas-grain coupling

