VIOMASS: making MADCUBA VO-compliant

Ricardo Rizzo

Spanish Virtual Observatory

Centro de Astrobiología

IVOA Interop Meeting

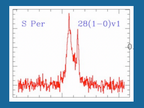
October 2022

➡ Short overview of MADCUBA software and SLIM task

➡ VIOMASS: concept and objectives

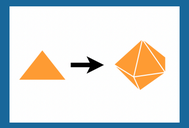
➡ Data model, physical parameters and tables

➡ Interoperability



➡ First science case

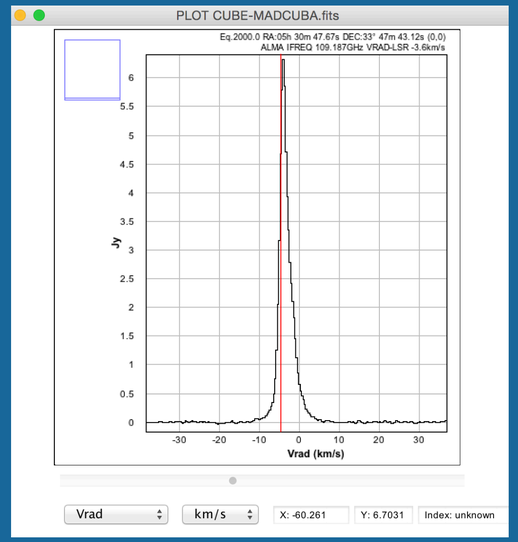
➡ To Do list: provenance and UCD

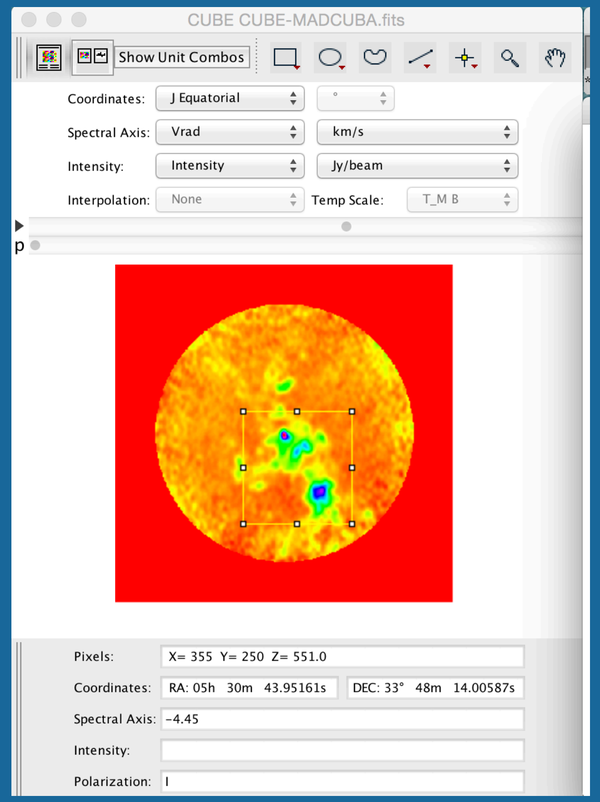


➡ Current status and prospects.

Overview of MADCUBA

- Suite able to deal with large data cubes (although data should be on disk)
- Java-based using imageJ infrastructure
- Able to read several formats (FITS, GILDAS, CASA) and data models (IRAM, ALMA, Herschel, VLA, GBT, …)
- Built-in molecular line databases (CDMS, JPL, others)
- Visualize and manipulate data cubes (baselines, smoothing, moments, …)

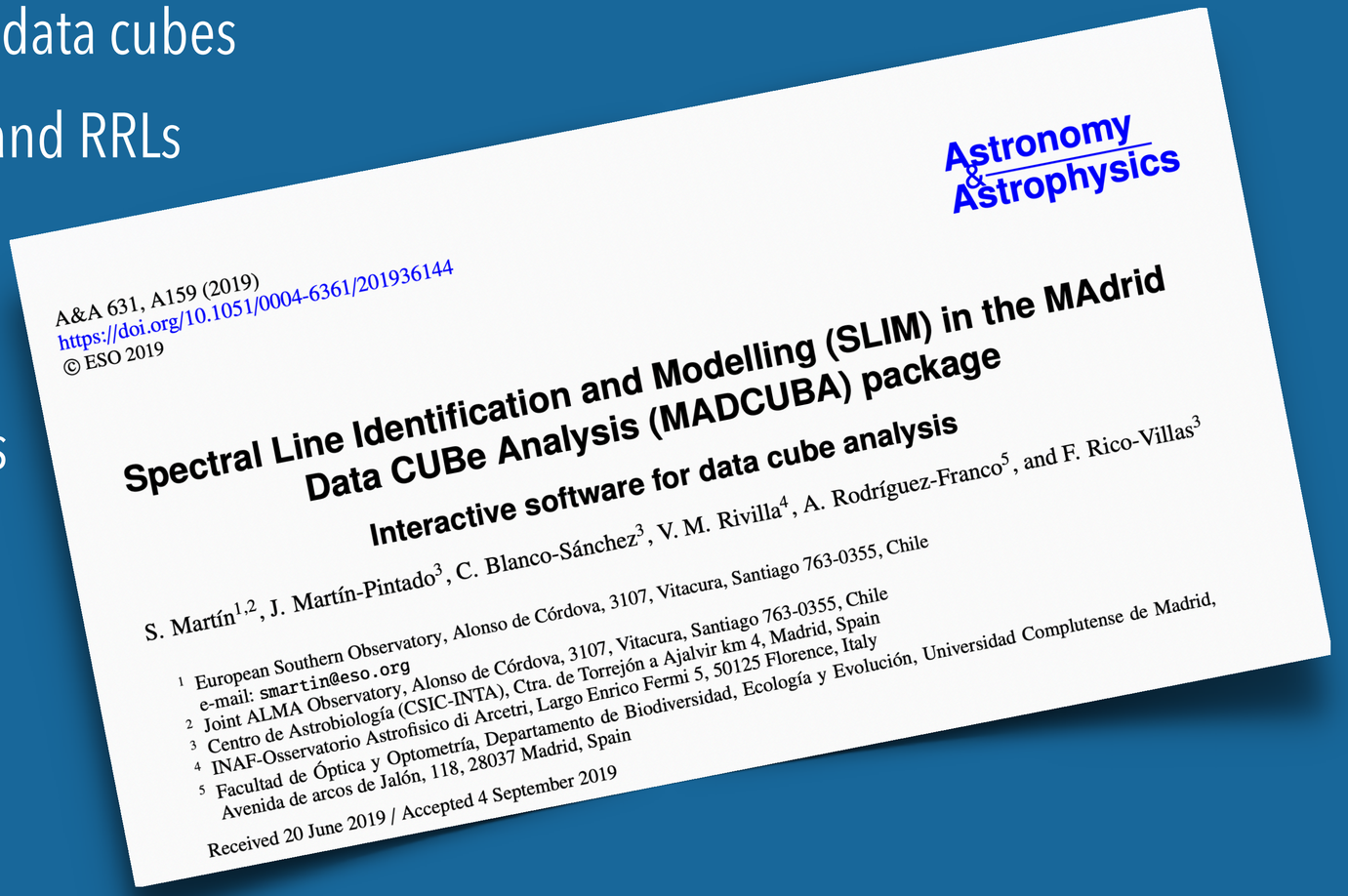




SLIM / AutoFit task

- Visualize, analyze, and model spectroscopic data cubes
- Automatic identification of molecular lines and RRLs
- Derive line parameters. LTE fitting
- Autofitting of one or many molecular lines
- Highly interactive. Fast and reliable graphics
- Hosted and supported by CAB
- Available at:

  https://cab.inta-csic.es/madcuba/



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https://doi.org/10.1051/0004-6361/201936144

Astronomy & Astrophysics

Spectral Line Identification and Modelling (SLIM) in the MAdrid Data CUBe Analysis (MADCUBA) package

Interactive software for data cube analysis

S. Martín[1,2], J. Martín-Pintado[3], C. Blanco-Sánchez[3], V. M. Rivilla[4], A. Rodríguez-Franco[5], and F. Rico-Villas[3]

[1] European Southern Observatory, Alonso de Córdova, 3107, Vitacura, Santiago 763-0355, Chile
e-mail: smartin@eso.org
[2] Joint ALMA Observatory, Alonso de Córdova, 3107, Vitacura, Santiago 763-0355, Chile
[3] Centro de Astrobiología (CSIC-INTA), Ctra. de Torrejón a Ajalvir km 4, Madrid, Spain
[4] INAF-Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, 50125 Florence, Italy
[5] Facultad de Óptica y Optometría, Departamento de Biodiversidad, Ecología y Evolución, Universidad Complutense de Madrid, Avenida de arcos de Jalón, 118, 28037 Madrid, Spain

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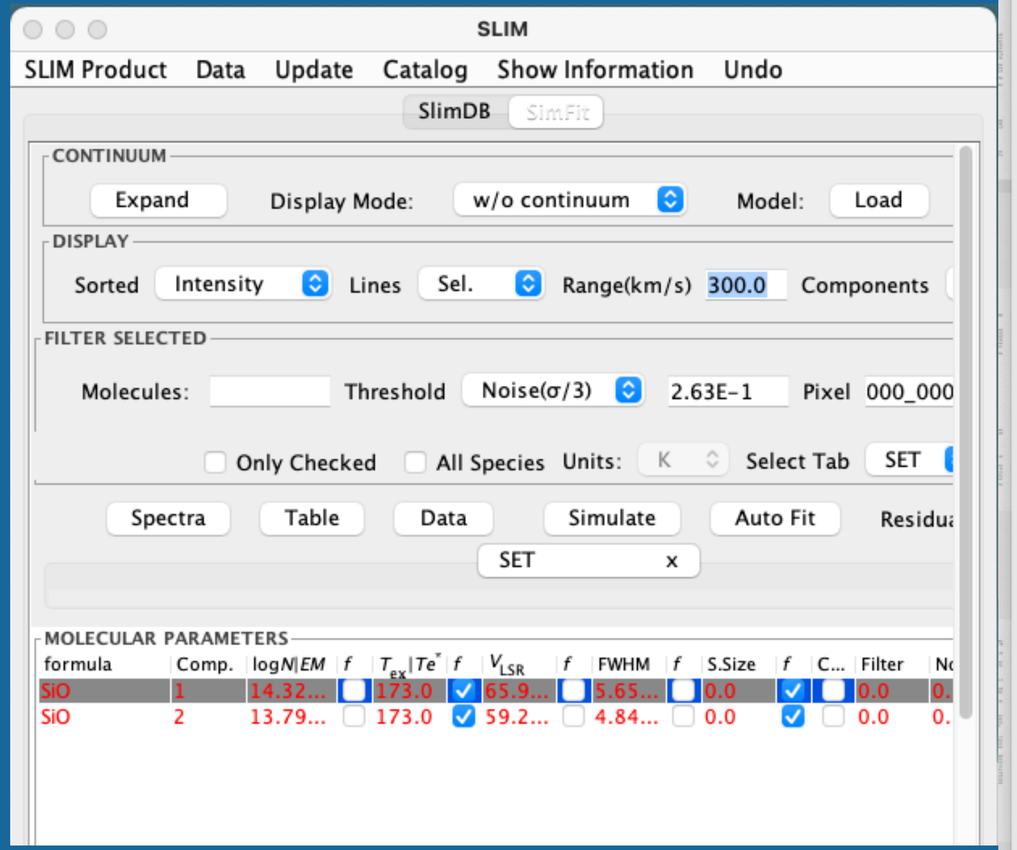
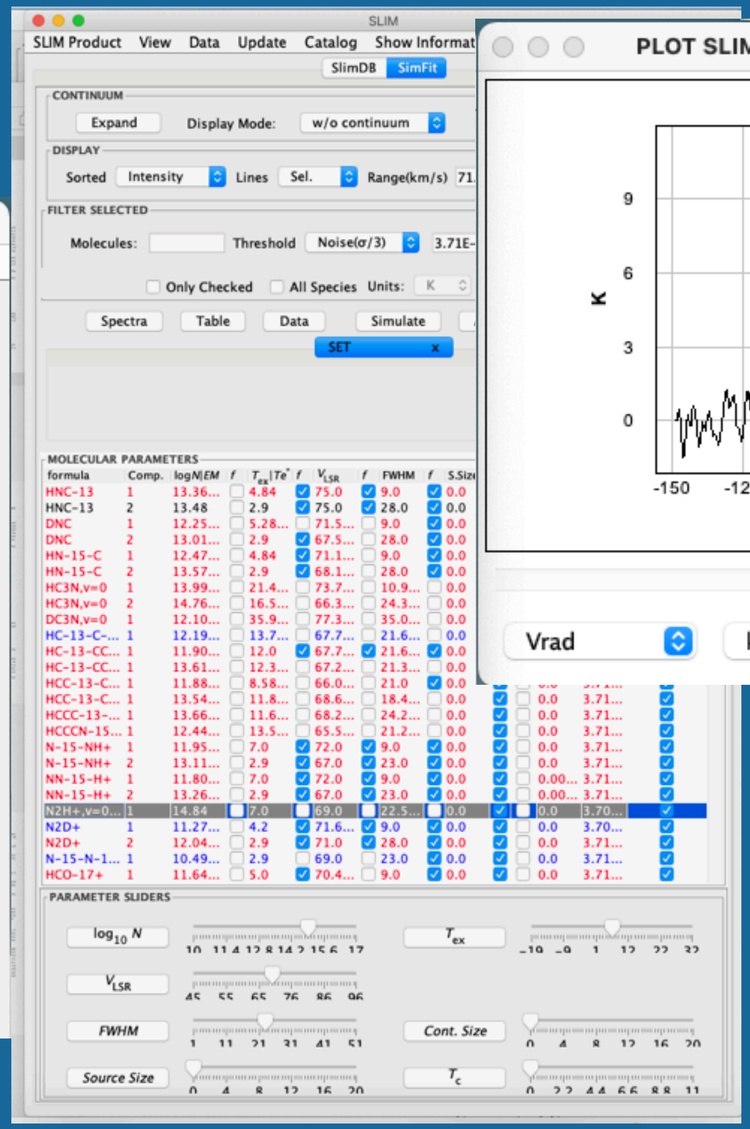
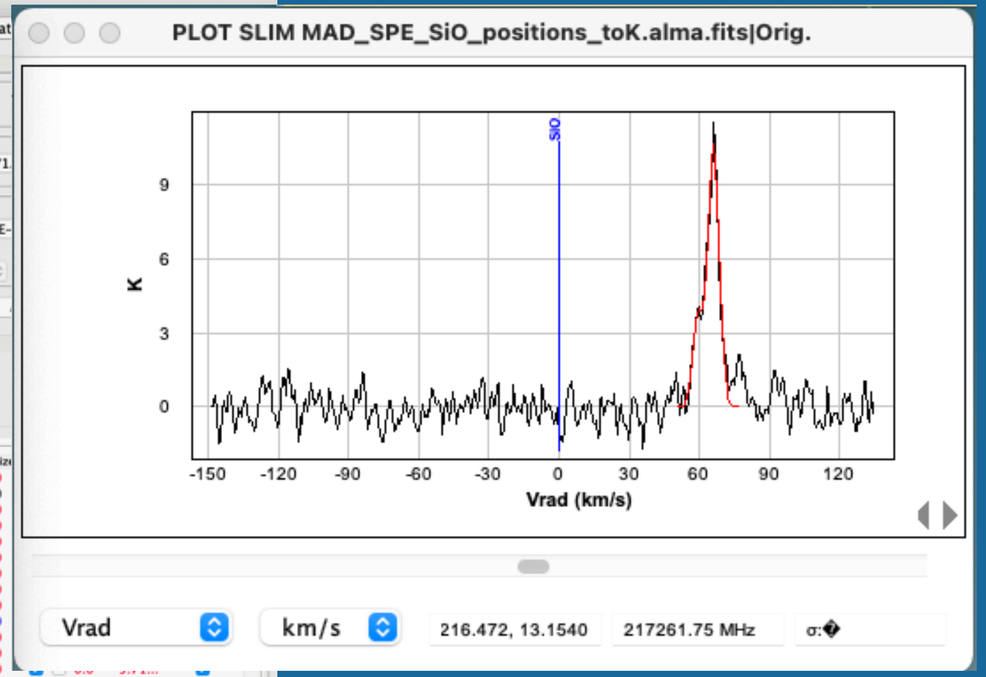
SLIM / AutoFit task

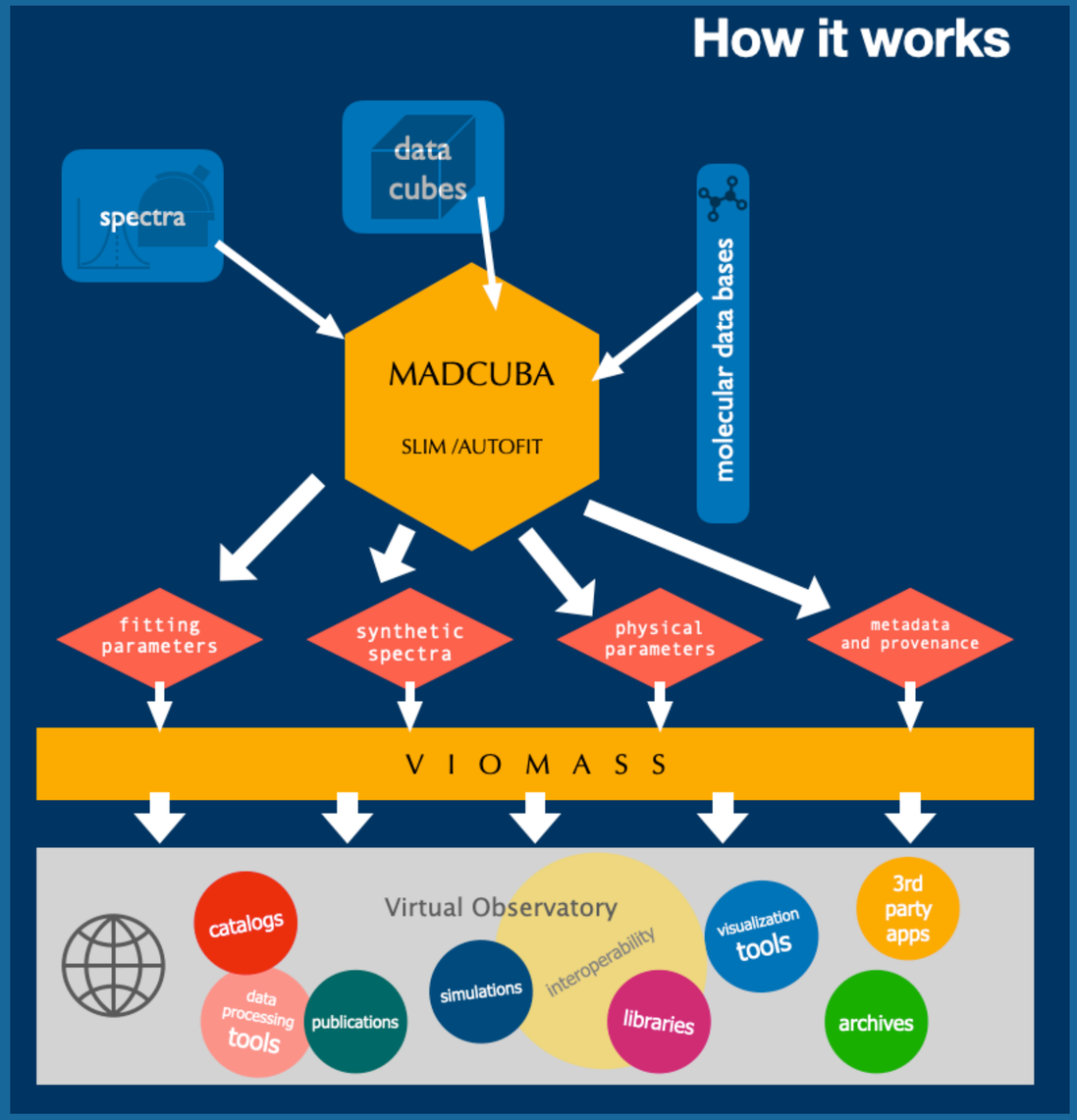






Virtual Observatory **I**ntegration **O**f **M**ADCUBA **A**nd **S**LIM **S**pectra

- Collaboration between MADCUBA and SVO groups
- Aims: to enhance the exploitation of MADCUBA and to build a new VO tool
- How: by transforming MADCUBA/SLIM outputs as VO-compliant
- Spectra as FITS files and tables as VOTables.



Spectra data model

- (Hybrid) FITS files containing both observed and modeled spectra.
- Formed by a generic primaryHDU followed by a set of imageHDUs
- ImageHDUs always considered as cubes, even for a 2D images (a one-channel cube) or a single spectrum (a one-pix cube).

```
No.    Name         Ver    Type      Cards   Dimensions   Format
  0  PRIMARY        1 PrimaryHDU      35   ()
  1  SPEC1          1 ImageHDU        60   (961, 1, 1, 1)   float64
  2  SPEC2          1 ImageHDU        60   (75, 1, 1, 1)   float64
  3  CUBE3          1 ImageHDU        58   (23, 23, 984)   float64

# HDU 0
SIMPLE  =                    T / Standard FITS format
BITPIX  =                    8 / Character data
NAXIS   =                    0 / No image, just extensions
EXTEND  =                    T / There are standard extensions

# HDU 1
XTENSION= 'IMAGE   '           / Image extension
BITPIX  =                  -64 / array data type
NAXIS   =                    4 / number of array dimensions
NAXIS1  =                  961
NAXIS2  =                    1
NAXIS3  =                    1
NAXIS4  =                    1
```

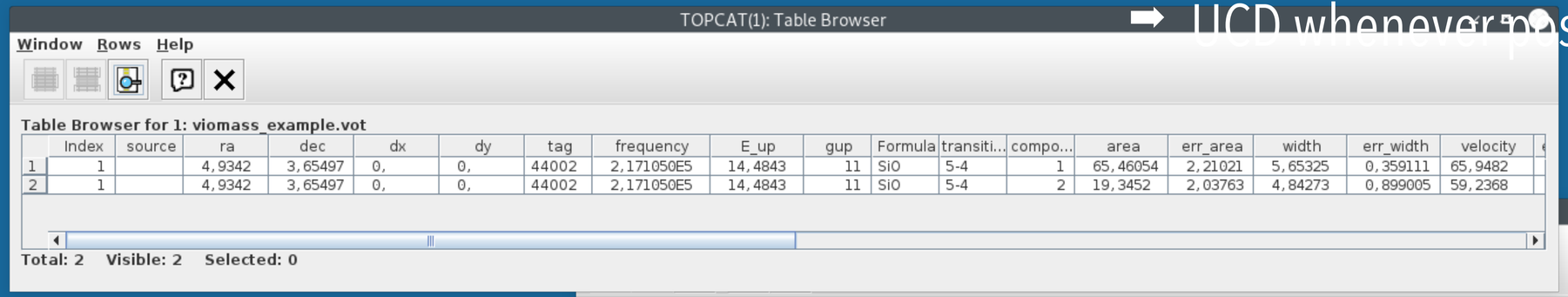
FITS headers

- Organized by categories:
  1. XTENSION and data type
  2. Physical units
  3. Array
  4. Times and dates
  5. Telescope
  6. Observed and/or synthetic spectra
  7. Comments, logs, and END
- Validity checked: FITS standard, VO-compliant
- Some mandatory keywords
- Units explicitly exposed in header

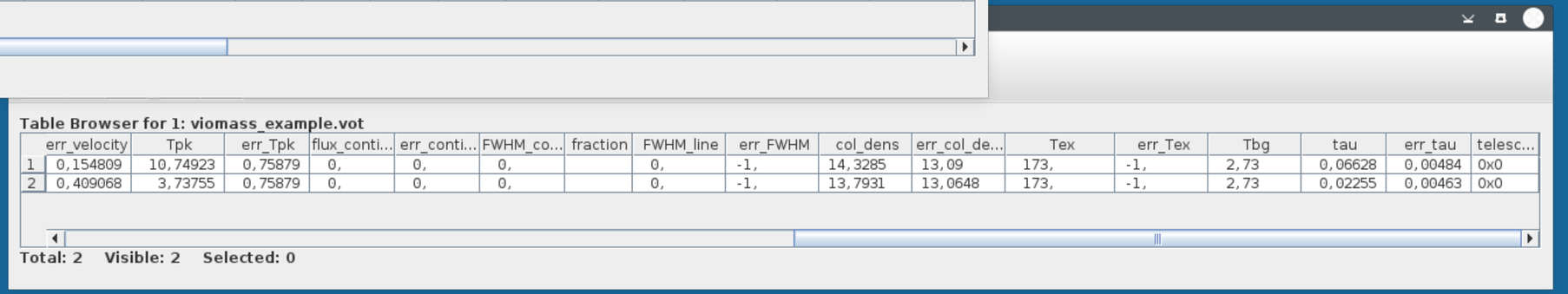
```
(1) Extension and data type ----------------------------------------------
XTENSION= 'IMAGE   '           / Type of extension
EXTNAME = 'DATA CUBE'          / Extension name
EXTVER  =                    1 / Version of extension
BITPIX  =                  -64 / Array data type

(2) Physical units -------------------------------------------------------
BSCALE  =                  1.0 / Scale
BZERO   =                  0.0 / Value corresponding to zero, in physical scale
BUNIT   = 'K       '           / Unit of physical values
BLANK   =                -1E8 /
DATAMIN = -0.196652002633E-001 /
DATAMAX =  0.267310943455E-001 /

(3) Array ----------------------------------------------------------------
NAXIS   =                    4 / Number of array dimensions
NAXIS1  =                  984 / Size of dimension 1
NAXIS2  =                   23 / Size of dimension 2
NAXIS3  =                   23 / Size of dimension 3
NAXIS4  =                    1 / Size of dimension 4
CTYPE1  = 'FREQ    '                   /

(4) Times and dates ------------------------------------------------------
DATE    = '2021-08-27T12:02:22.596'    / HDU creation date
ORIGIN  = 'MADCUBA v 1.1      '        / Created by SLIM-AUTOFIT
TIMESYS = 'UTC                '        /
DATE-OBS= '2017-07-25T02:59:33.655'    / Date observed
DATE-RED= '2021-06-24T00:00:00.000'    / Date reduced
OBSTIME =  6.0000000000000E+02         / [s] Integration time
UT      = '02:59:33.655'               / Universal time at start

(5) Telescope ------------------------------------------------------------
TELESCOP= 'IRAM-30M '                  / Radio telescope
INSTRUME= 'EMIR-0   '                  / Receiver
OBSMODE = 'PSW      '                  / Observing mode

(6) Observation and/or synthetic spectra ---------------------------------
OBJECT  = 'AFGL2298    '               /
RA      =  0.2850453750000E+03         / [deg] Right Ascension
DEC     =  0.3763083333333E+01         / [deg] Declination
RADESYS = 'FK5'                        / Equatorial coordinate system
SPECSYS = 'LSRK'                       / Reference frame of spectral coordinates
ELEVATIO=  0.264136238885E+002         / [rad] Telescope elevation

(7) Comments, logs, and END ----------------------------------------------
HISTORY Written by MADCUBA v0.5.0 on 2021/08/30-16:22:15
COMMENT Blah blah blah
END
```

Output tables

- Source information: name, coordinates, offset
- Line/s used for fitting: name/s, formulation, quantum numbers, frequency/ies, energy/ies
- Physical parameters: column density, n(H2), tau, Texc, velocity, line width, source size
- All in single or multiple (TBD) VOTables
- Careful definitions of column names
- Inclusion of units associated with all columns
- UCD whenever possible.



	Index	source	ra	dec	dx	dy	tag	frequency	E_up	gup	Formula	transiti...	compo...	area	err_area	width	err_width	velocity
1	1		4,9342	3,65497	0,	0,	44002	2,171050E5	14,4843	11	SiO	5-4	1	65,46054	2,21021	5,65325	0,359111	65,9482
2	1		4,9342	3,65497	0,	0,	44002	2,171050E5	14,4843	11	SiO	5-4	2	19,3452	2,03763	4,84273	0,899005	59,2368



	err_velocity	Tpk	err_Tpk	flux_conti...	err_conti...	FWHM_co...	fraction	FWHM_line	err_FWHM	col_dens	err_col_de...	Tex	err_Tex	Tbg	tau	err_tau	telesc...
1	0,154809	10,74923	0,75879	0,	0,	0,		0,	-1,	14,3285	13,09	173,	-1,	2,73	0,06628	0,00484	0x0
2	0,409068	3,73755	0,75879	0,	0,	0,		0,	-1,	13,7931	13,0648	173,	-1,	2,73	0,02255	0,00463	0x0

Output tables

TOPCAT(1): Table Columns

Window Columns Display Help

Table Columns for 1: viomass_example.vot

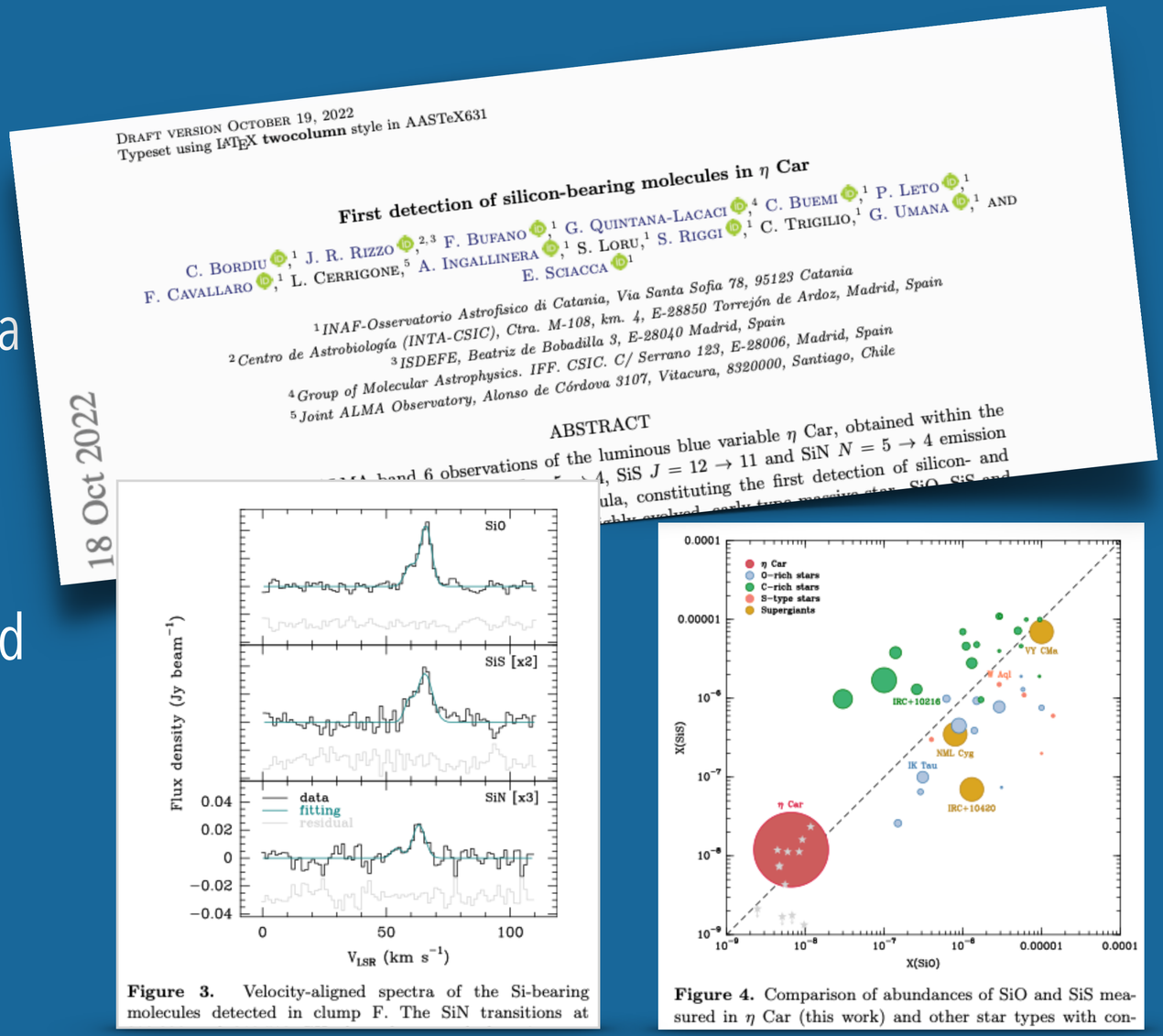
Δ	Index	Visible	Name	$ID	Class	Units	Description	UCD	Datatype
0		☐	Index	$0	Long		Table row index		
1	1	☑	Index	$1	Integer				int
2	2	☑	source	$2	String		Source name	src	char
3	3	☑	ra	$3	Double	deg	Right ascension (Expression: frequency/44000)	pos.eq.ra	double
4	4	☑	dec	$4	Double	deg	Declination (Expression: ra/1.35)	pos.eq.dec.	double
5	5	☑	dx	$5	Double	arcsec	RA offset from source position	pos.eq.offset	double
6	6	☑	dy	$6	Double	arcsec	Dec offset from source position	pos.eq.offset	double
7	7	☑	tag	$7	String		Molecule tag		char
8	8	☑	frequency	$8	Double	MHz	Frequency	em.freq	double
9	9	☑	E_up	$9	Double	cm-1	upper level energy		double
10	10	☑	gup	$10	Integer		Upper level degeneracy		int
11	11	☑	Formula	$11	String		Chemical formulation		char
12	12	☑	transition	$12	String		Spectral line transition	spect.line	char
13	13	☑	component	$13	Integer		Velocity component		int
14	14	☑	area	$14	Double	K km/s	Integrated line intensity	spect.line.strength	double
15	15	☑	err_area	$15	Double	K km/s	Uncertainty		double
16	16	☑	width	$16	Float	km/s	Line width	spect.line.width	float
17	17	☑	err_width	$17	Float	km/s	Uncertainty		float
18	18	☑	velocity	$18	Float	km/s	Central velocity of the component	spect.dopplerVeloc... ...radio	float
19	19	☑	err_velocity	$19	Float	km/s	Uncertainty		float
20	20	☑	Tpk	$20	Double	K	Peak intensity	spect.line.intensity	double
21	21	☑	err_Tpk	$21	Double	K	Uncertainty		double
22	22	☑	flux_continuum	$22	Double	Jy	Continuum flux density		double
23	23	☑	err_continuum	$23	Double	Jy	Uncertainty		double
24	24	☑	FWHM_continuum	$24	Double	arcsec	Diameter of the continuum source	src.fwhm	double
25	25	☑	fraction	$25	Double		Fraction covered by the beam		double
26	26	☑	FWHM_line	$26	Float	arcsec	FWHM of the source size		float
27	27	☑	err_FWHM	$27	Float	arcsec	Uncertainty		float
28	28	☑	col_dens	$28	Float	cm-2	Column density	phys.columnDensity	float
29	29	☑	err_col_dens	$29	Float	cm-2	Uncertainty		float
30	30	☑	Tex	$30	Float	K	Excitation temperature	phys.temperature	float
31	31	☑	err_Tex	$31	Float	K	Uncertainty		float
32	32	☑	Tbg	$32	Float	K	Background temperature		float
33	33	☑	tau	$33	Double		Optical depth / Line opacity	phys.absorption... ...opticalDepth	double
34	34	☑	err_tau	$34	Double		Uncertainty		double
35	35	☑	telescope	$35	String		Telescope	instr.tel	char

Interoperability

- Spectra successfully opened by CASSIS
- Cubes visible within Aladin, with channels in the ‘movie’ mode
- Tables recognized by Topcat
- Not all features tested yet

First science case

- astro-ph 2210.09774 (Oct 18 2022)
- Discovery of Si-bearing molecules in eta Carina
- Si, SiS and SiN found in twelve clumps
- Other molecules: 13CO, 13CN
- Column densities and abundances determined by the VO-compliant MADCUBA output
- SiO formed by shocks. Complex chemistry, grain destruction and formation.



Draft version October 19, 2022
Typeset using LaTeX twocolumn style in AASTeX631

18 Oct 2022

First detection of silicon-bearing molecules in η Car

C. Bordiu [1], J. R. Rizzo [2,3], F. Bufano [1], G. Quintana-Lacaci [4], C. Buemi [1], P. Leto [1], F. Cavallaro [1], L. Cerrigone [5], A. Ingallinera [1], S. Loru [1], S. Riggi [1], C. Trigilio [1], G. Umana [1], and E. Sciacca [1]

[1] INAF-Osservatorio Astrofisico di Catania, Via Santa Sofia 78, 95123 Catania
[2] Centro de Astrobiología (INTA-CSIC), Ctra. M-108, km. 4, E-28850 Torrejón de Ardoz, Madrid, Spain
[3] ISDEFE, Beatriz de Bobadilla 3, E-28040 Madrid, Spain
[4] Group of Molecular Astrophysics. IFF. CSIC. C/ Serrano 123, E-28006, Madrid, Spain
[5] Joint ALMA Observatory, Alonso de Córdova 3107, Vitacura, 8320000, Santiago, Chile

ABSTRACT

...band 6 observations of the luminous blue variable η Car, obtained within the ...4, SiS $J = 12 \rightarrow 11$ and SiN $N = 5 \rightarrow 4$ emission ...ula, constituting the first detection of silicon- and ...

Figure 3. Velocity-aligned spectra of the Si-bearing molecules detected in clump F. The SiN transitions at

Figure 4. Comparison of abundances of SiO and SiS measured in η Car (this work) and other star types with con-

To do list

- History logs and provenance
- Testing on interoperability
- UCDs (semantics)
- Fine tuning definitions for the output tables
- Documentation and tutorials.

Concluding remarks

- MADCUBA and SLIM are powerful radio astronomy tools
- Efforts are being made to convert their output in VO-compliant
- Spectra as hybrid FITS and tables as VOTables
- Interoperability being tested with good results
- First succesful science use
- To do: provenance, interoperability, UCD, fine tuning, documentation.