



# The analysis of high spectral resolution observations in the far-infrared

With a focus on the interstellar medium (ISM)

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SOFIA Infrared School

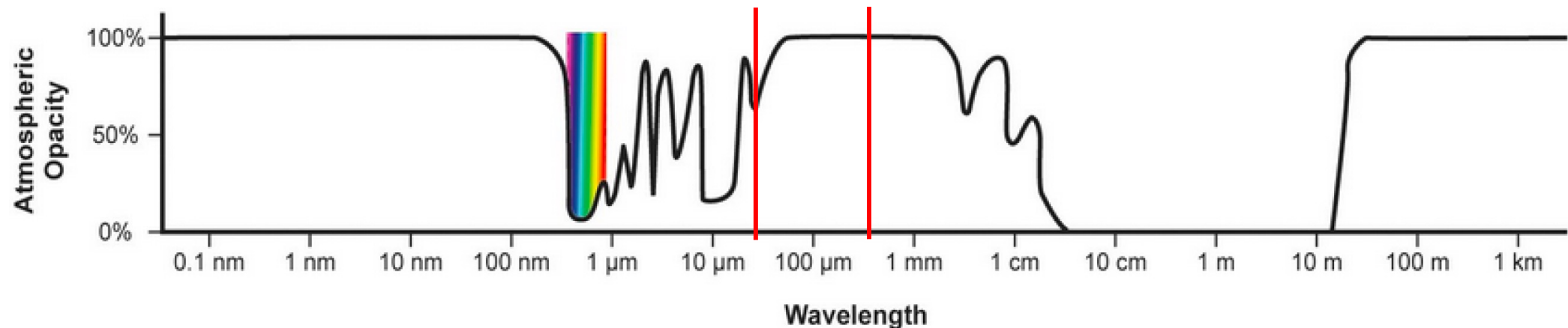
April 21<sup>st</sup> 2023

# Outline

- Short overview: high-resolution spectroscopy in the far-infrared
- ISM studies: far-infrared spectra
  - Dynamics, chemical abundances and excitation conditions
- ISM studies: far-infrared spectral data cubes
  - Visualizing and quantifying the data
  - Segmenting the data for analysis

# Far-infrared astronomy

- Far-infrared astronomy: 30 – 300 (or 450)  $\mu\text{m}$
- Observe from space or at least in the stratosphere
  - Mostly water absorption in the atmosphere (also  $\text{CO}_2$  contribution)

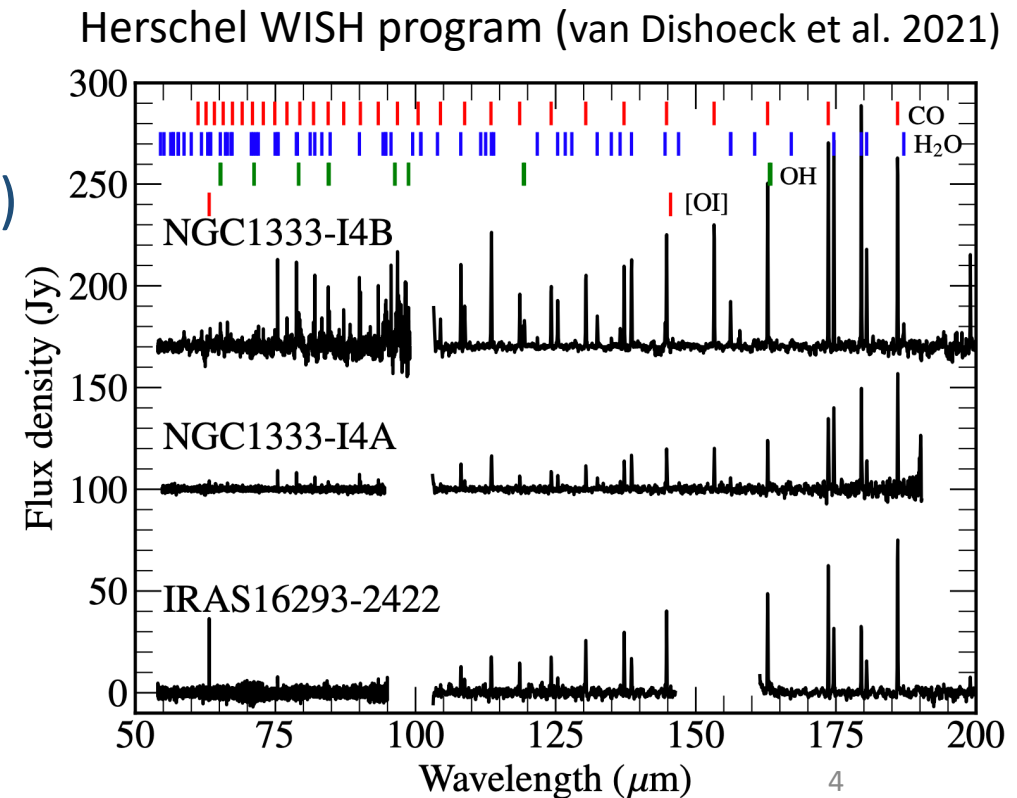


# Spectral lines in the far-infrared

- Far-infrared spectral lines contain a lot of information
  - Dynamics, excitation conditions, chemical abundances,...

## ➤ Spectral lines:

- H<sub>2</sub>O (proto-planetary disks, atmospheres)
- [CII] (galaxies, ISM)
- HD (proto-planetary disks)
- CO (shocks, galaxies, ISM)
- [NII], [OI], [OIII], HeH<sup>+</sup>, H<sub>2</sub>D<sup>+</sup>, OH, CH,...



# Far-infrared spectroscopy (history)

## ➤ ISO - LWS (1995-1998)

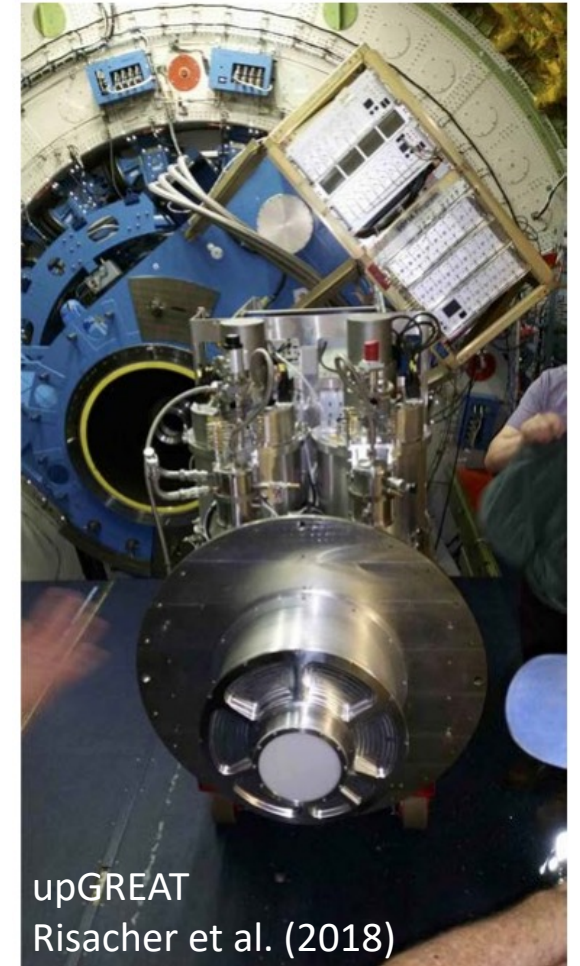
- Spectral resolution:  $\sim 10 \text{ km s}^{-1}$  (Swinyard et al. 1998)

## ➤ Herschel - HIFI (2009-2013)

- Spectral resolution:  $\sim 0.1 \text{ km s}^{-1}$  (de Graauw et al. 2010)

## ➤ SOFIA - (up)GREAT/4GREAT (2010-2022)

- Spectral resolution:  $\sim 0.1 \text{ km s}^{-1}$  (Heyminck et al. 2012; Risacher et al. 2016; Duran et al. 2021)



# The up/4GREAT receiver

## ➤ Heterodyne far-infrared receivers

- upGREAT: 2-band receiver, 7 pixels
- 4GREAT: 4-band receiver, 1 pixel

## ➤ Data reduction

- see talk R. Higgins (up next)

GREAT Configurations

Front-End	Frequencies (GHz)	Lines of Interest	DSB <sup>6</sup> Receiver Temperatures (K)	Main beam efficiencies
HFA <sup>1</sup>	4744.77749	[OI] 63 $\mu\text{m}$	1250	0.63
LFAH <sup>2</sup>	1835–2007	[CII] 158 $\mu\text{m}$ , CO, OH, $^2\Pi_{1/2}$ , $^{12}\text{CH}$ , $^{13}\text{CH}$	1000	0.69
LFAV <sup>2</sup>	1835–2007 2060–2065	Same as LFAH, plus [OI] 145 $\mu\text{m}$		
4G4	2490–2590	OH $^2\Pi_{3/2}$ , $^{18}\text{OH}^2$ $\Pi_{3/2}$	3300	0.57
4G3	1240–1395 1427–1525	[NII] 205 $\mu\text{m}$ , CO, OD, HCN, SH, $\text{H}_2\text{D}^+$	1100	0.70
4G2 <sup>3,4</sup>	890–984 990–1092	CO, CS	> 600 300	0.59
4G1 <sup>4</sup>	491–555 560–635	$\text{NH}_3$ , [CI] 609 $\mu\text{m}$ , CO, CH	< 150	0.51

# Far-infrared spectroscopy (the future)

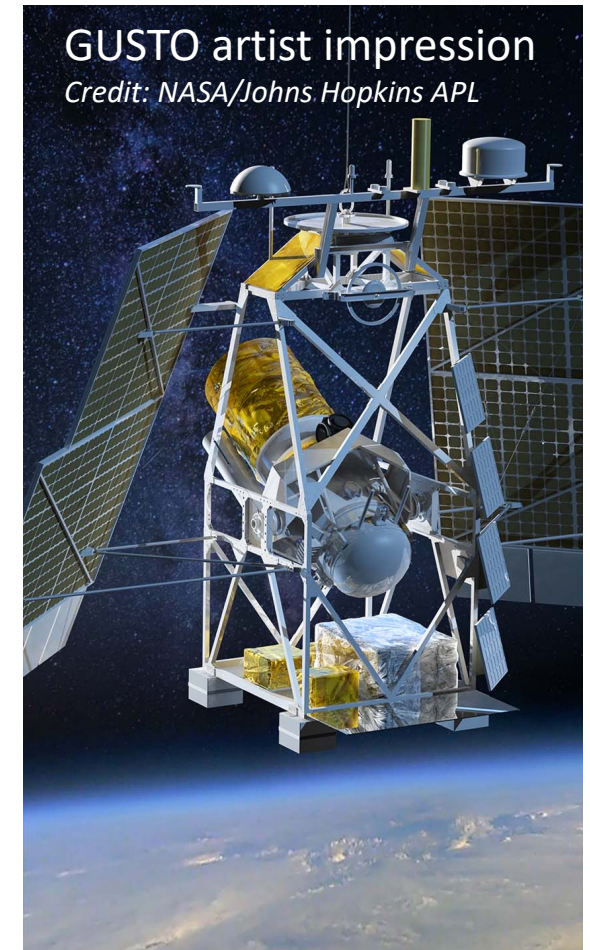
## ➤ Stratospheric balloon missions

- GUSTO (2023-2024: see e.g. Goldsmith et al. 2022)
  - [NII] @ 205  $\mu\text{m}$ , [CII] @ 158  $\mu\text{m}$  and [OI] @ 63  $\mu\text{m}$
- ASTHROS (2024-2025: see e.g. Pineda et al. 2022)
  - Includes [NII] @ 205  $\mu\text{m}$  and 122  $\mu\text{m}$ , and HD @ 112  $\mu\text{m}$
- Probe mission in 2030-2040?

## ➤ Herschel & SOFIA archive

<http://archives.esac.esa.int/hsa/whsa/>

[https://irsa.ipac.caltech.edu/applications/sofia/?\\_action=layout.showDropDown&](https://irsa.ipac.caltech.edu/applications/sofia/?_action=layout.showDropDown&)



# Units

➤ ‘Brightness temperature – T (K)’ or ‘(milli/mega-)Jansky – (m/M)Jy’

- As in submillimeter and radio astronomy

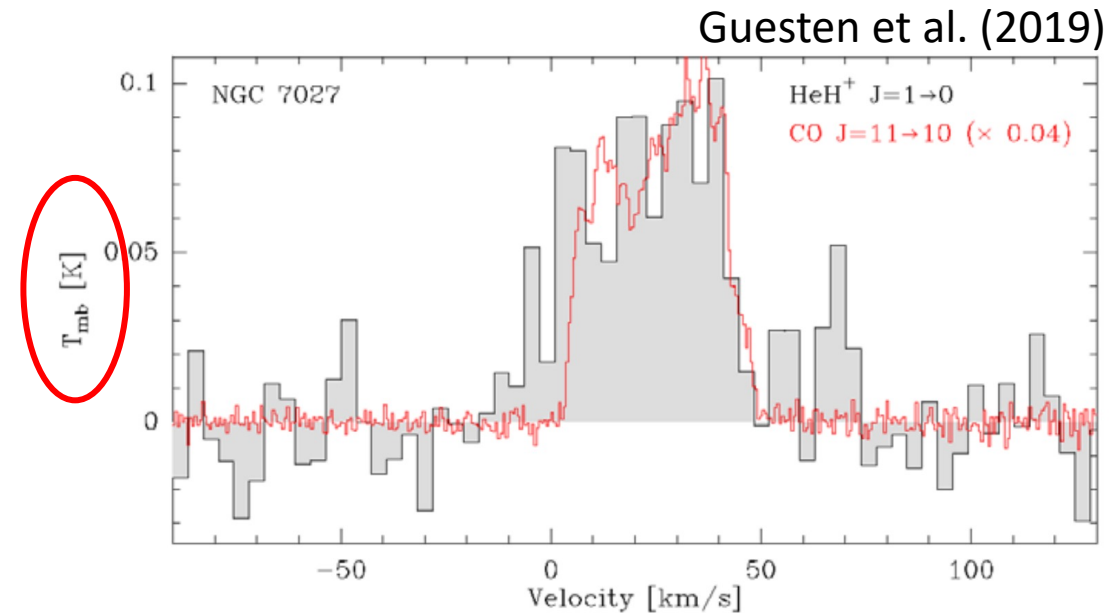
➤ Flux density (S):  $1 \text{ Jy} = 10^{-26} \text{ W m}^{-2} \text{ Hz}^{-1}$

➤ Brightness temperature:  $T = \frac{\lambda^2}{2 k \Omega} S$

- Rayleigh-Jeans law

<https://science.nrao.edu/facilities/vla/proposing/TBconv>

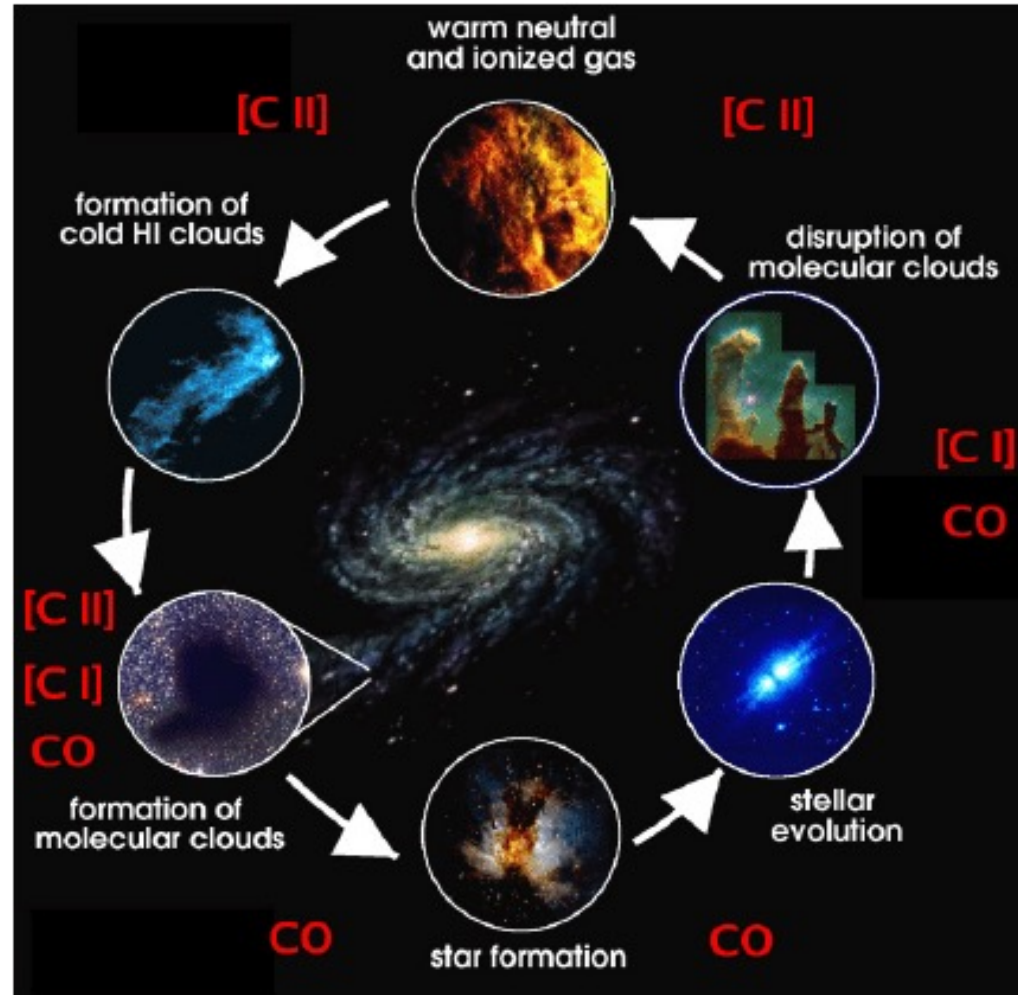
<https://www.atnf.csiro.au/research/radio-school/2011/talks/Parkes-school-Fundamental-II.pdf>





# The cycle of matter in galaxies

Kulesa et al. (2013)

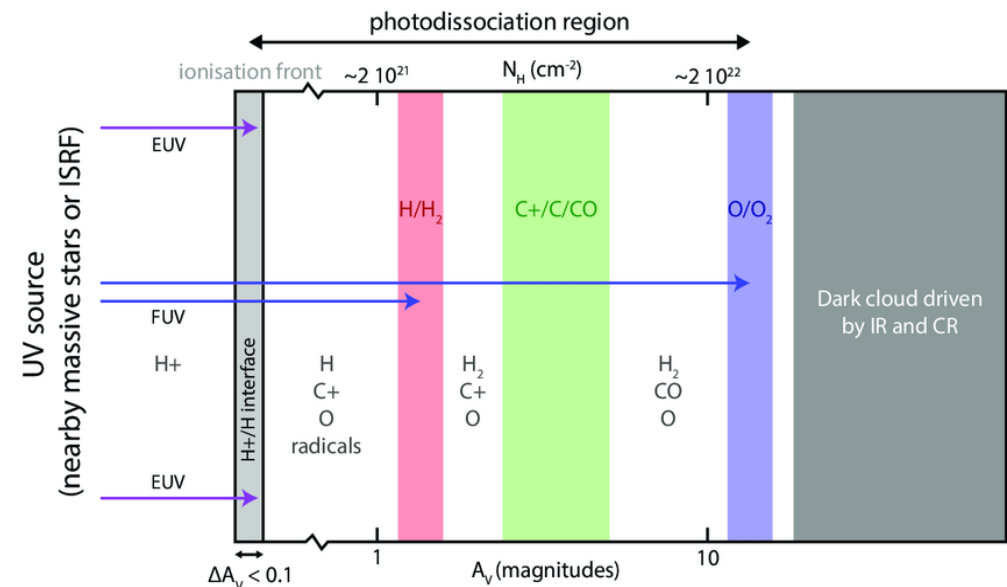


# The [CII] fine structure line

- The ionization potential of carbon is 11.3 eV
  - Can trace neutral regions in the ISM ( $< 13.6$  eV)
  - Fine-structure line emits at  $158 \mu\text{m}$  ([CII])

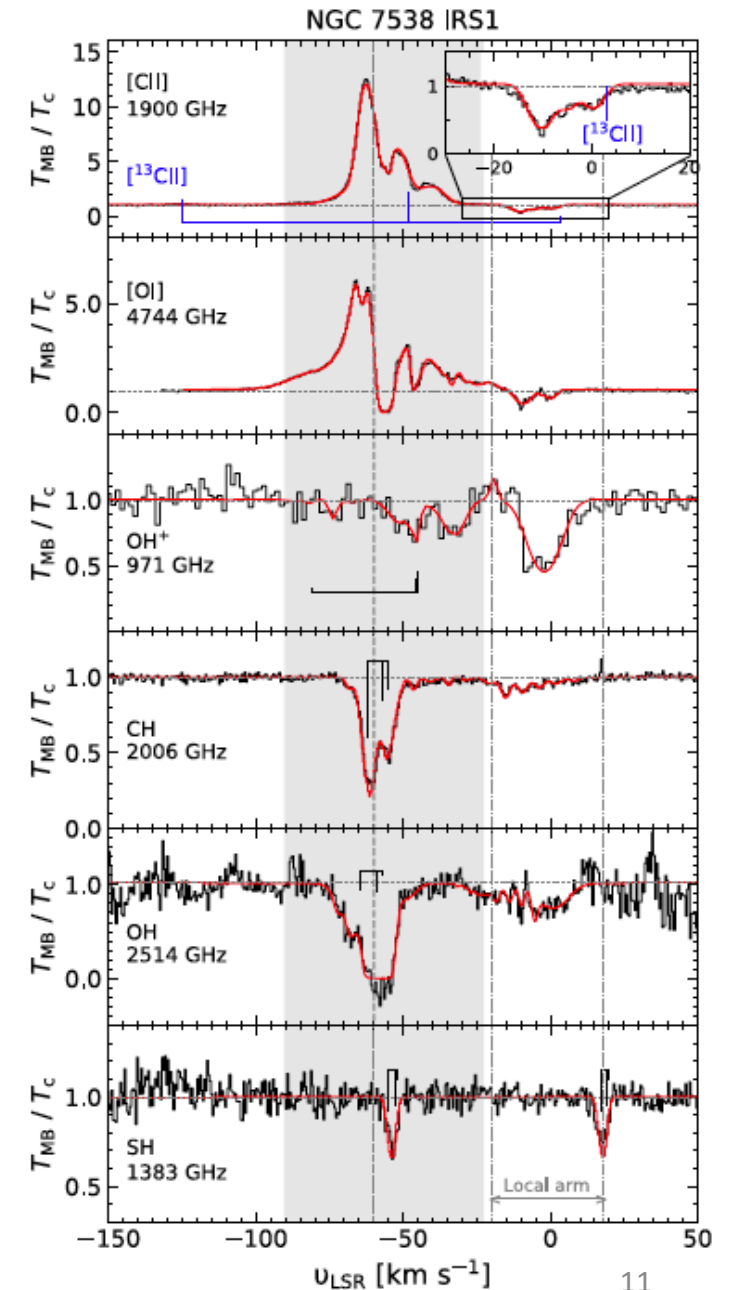
- Dominant cooling line in the neutral ISM
  - [CII] mostly originates from photodissociation regions (PDRs) (e.g. Pineda et al. 2013; Tarantino et al. 2021)
  - PDRs: see talks M. Wolfire, J. Sutter

- FEEDBACK Legacy survey: large [CII] maps (Schneider et al. 2020)



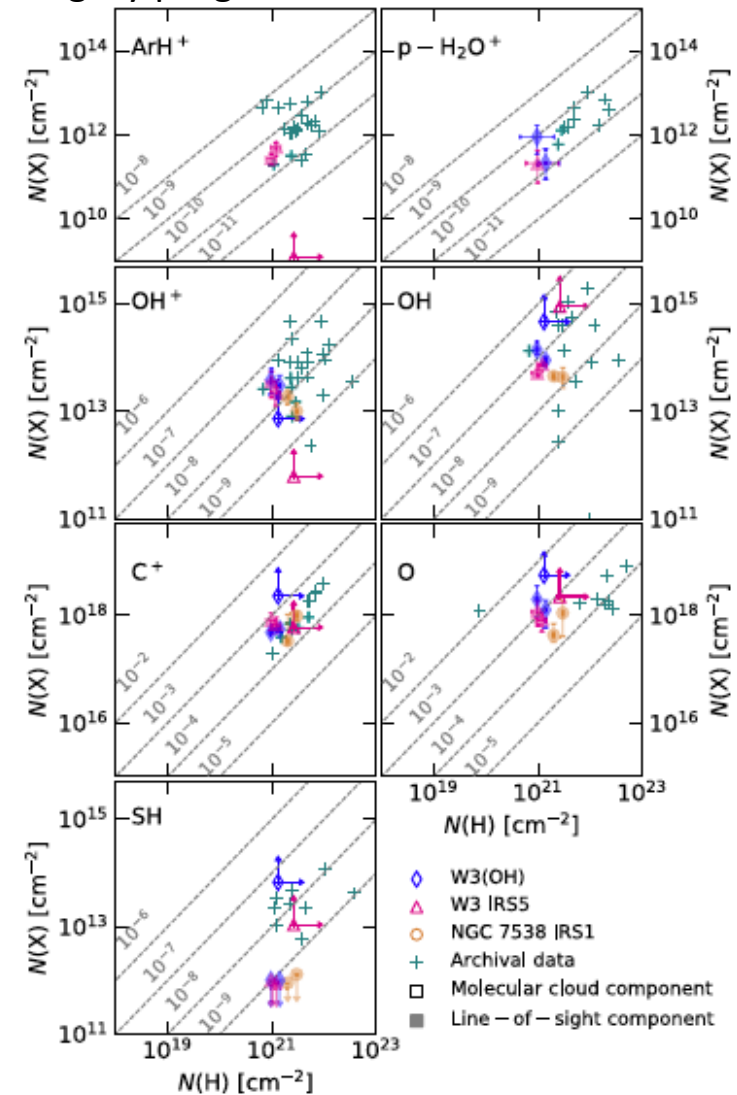
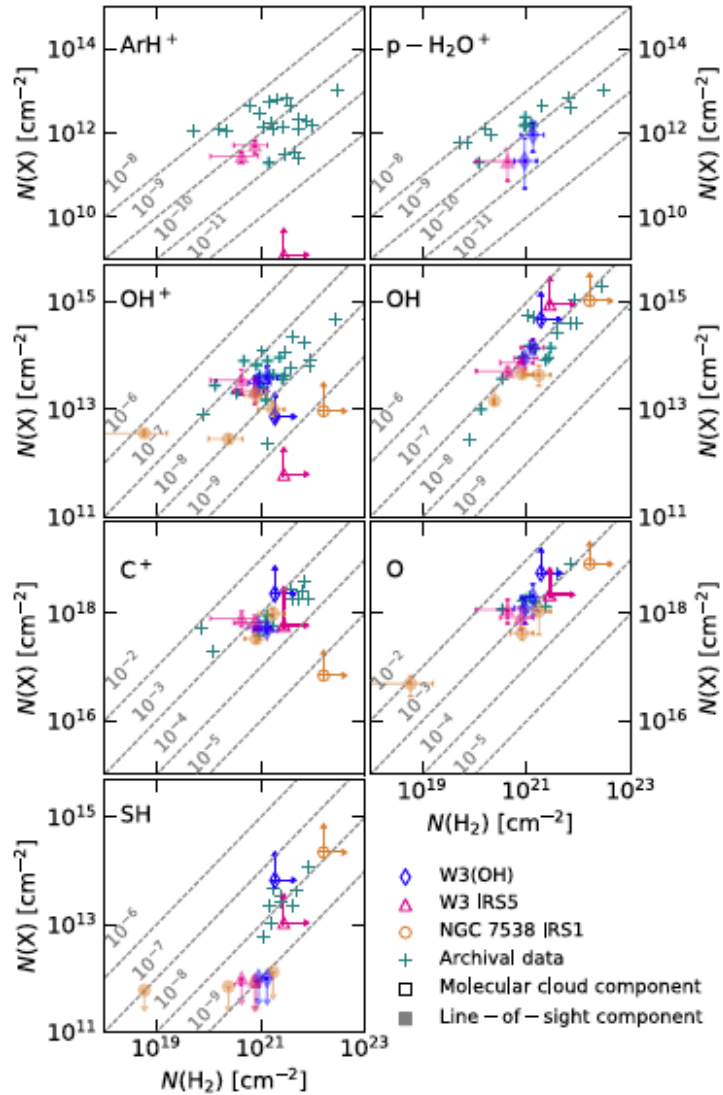
# Spectral features

- (Self/foreground-)absorption + emission
  - Spectra modelled with XCLASS (Möller et al. 2017)
  - Automated fitting routine: MAGIX (Möller et al. 2013)
  
- XCLASS: A tool for CASA <https://casa.nrao.edu/>
  - Models spectral lines by solving the radiative transfer equation assuming LTE
  - Spectroscopic data from CDMS & JPL



# Abundances in the ISM

Jacob et al. (2022): Hygal Legacy program



# Dynamics in the ISM

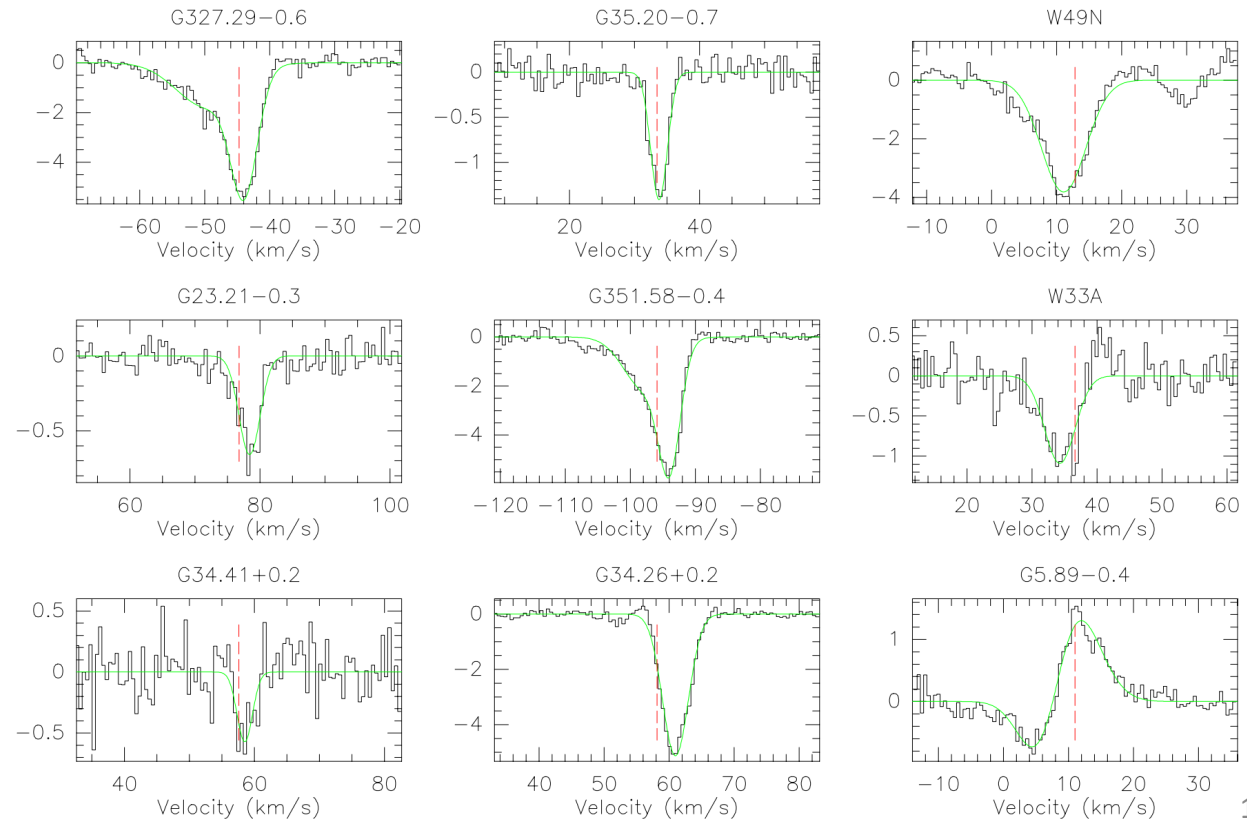
- Expansion and infall in massive star forming clumps (Wyrowski et al. 2012; 2016)
  - $\text{NH}_3$  absorption shift relative to the centroid velocity of  $\text{C}^{17}\text{O}(3-2)$

- Fitting with CLASS

- A GILDAS package
- Can be coupled to Python

- GILDAS: see talk R. Higgins

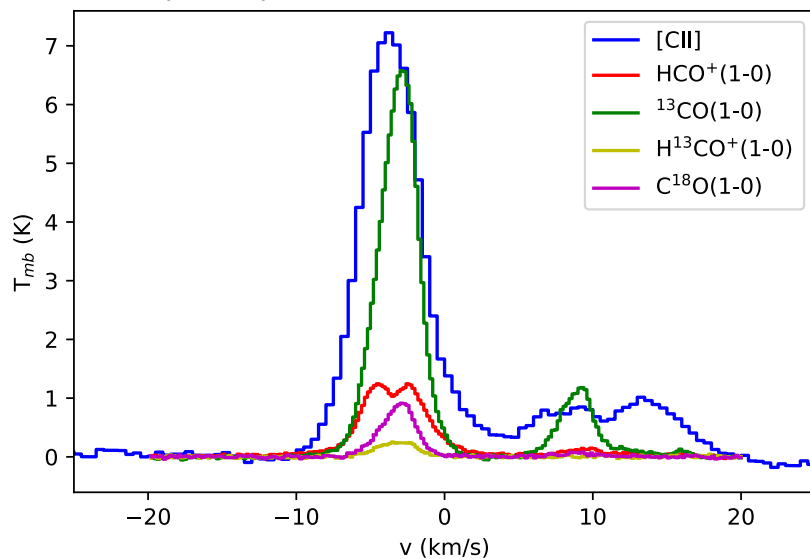
<https://www.iram.fr/IRAMFR/GILDAS/doc/html/class-html/class.html>



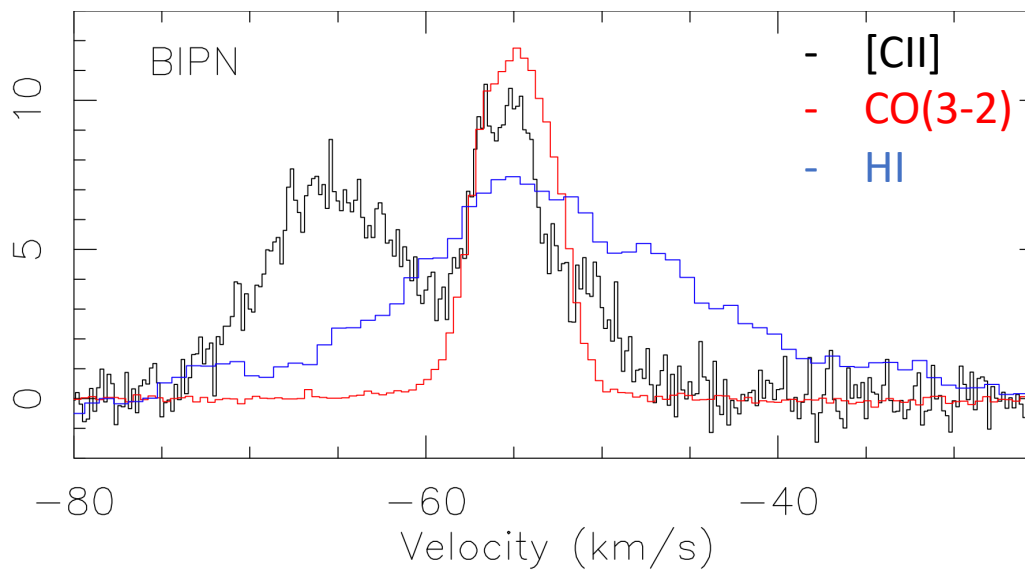
# Dynamics in the ISM

- Emission: unveils previously unseen dynamics
  - Which gas phase does it trace?
  - Implications for ISM evolution?

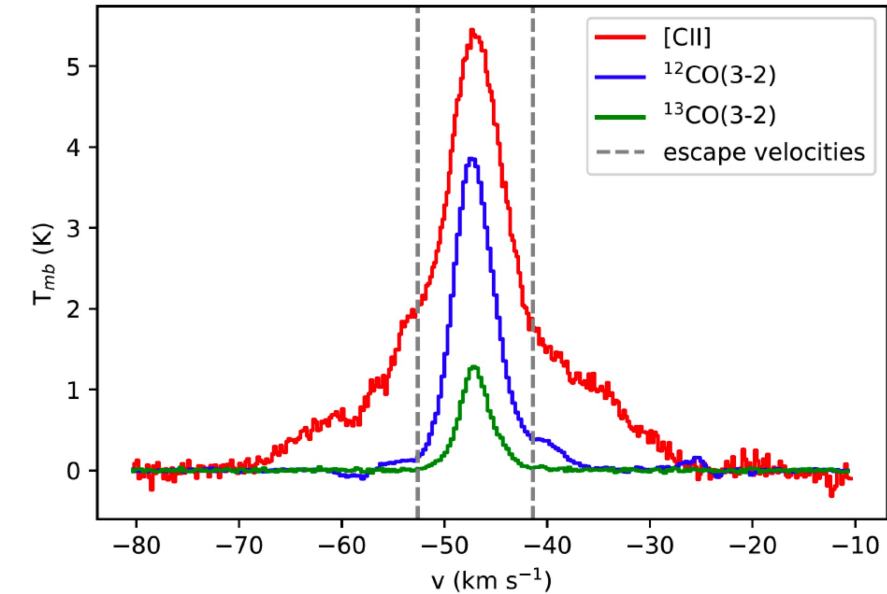
DR21: Bonne et al. in review; Schneider et al. (2023)



NGC 7538: Beuther et al. (2022)



RCW 79: Bonne et al. in prep.



# Self-absorption

## ➤ Self-absorption in [CII]

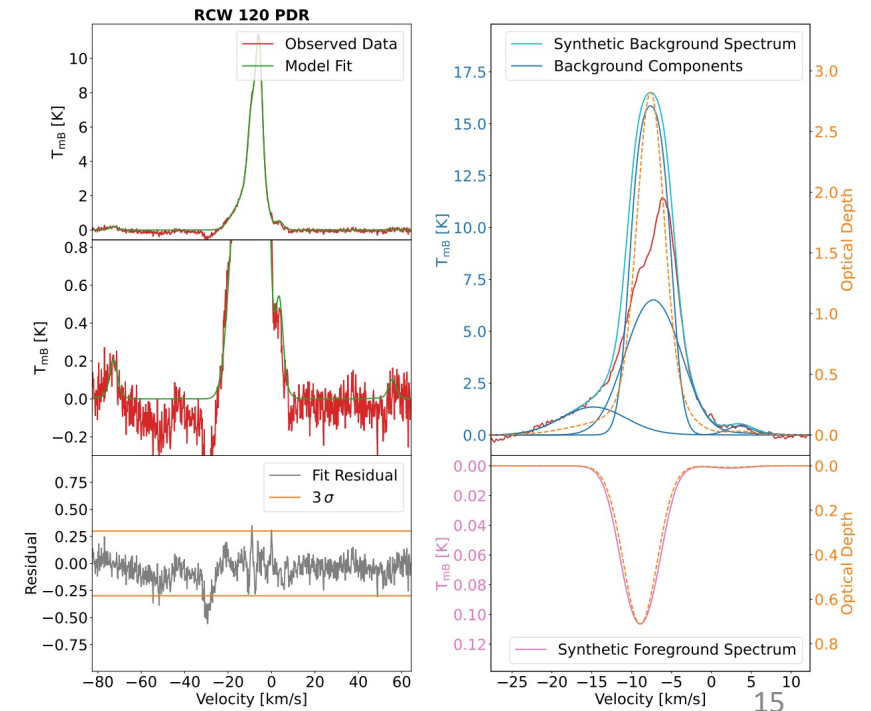
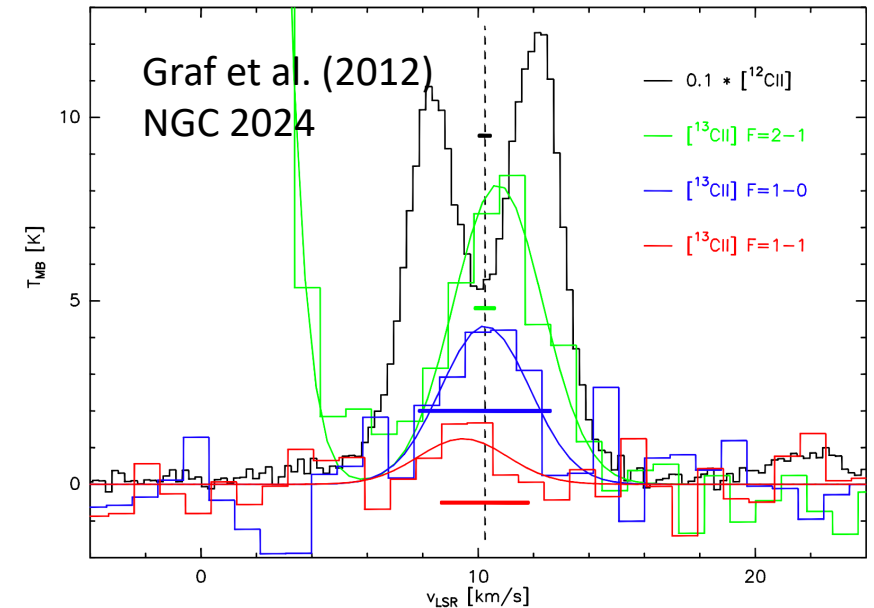
- Identified with  $[^{13}\text{CII}]$
- Origin of this self-absorption?

## ➤ Fit with a multi-layer model (see Guevara et al. 2020; Kabanovic et al. 2022)

- Warm & cold layers of gas at different velocities
- Also applicable to CO observations (Bonne et al. 2020)

## ➤ Also seen in [OI] @ 63 $\mu\text{m}$ (e.g. Goldsmith et al. 2021)

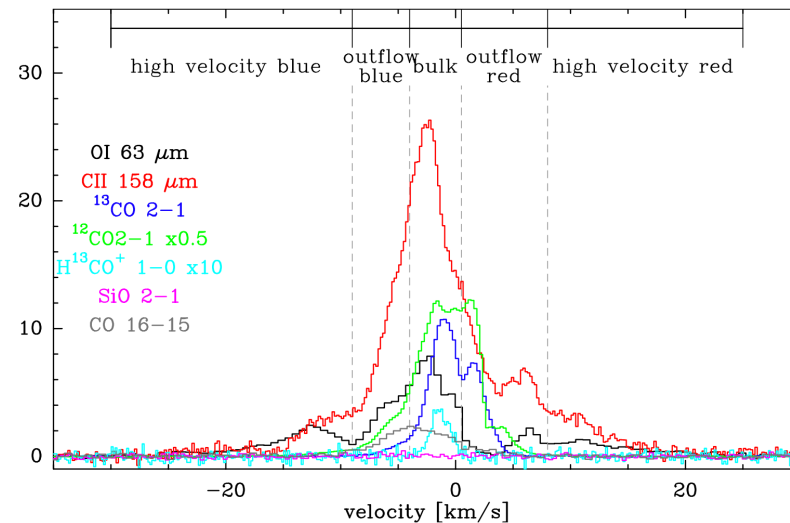
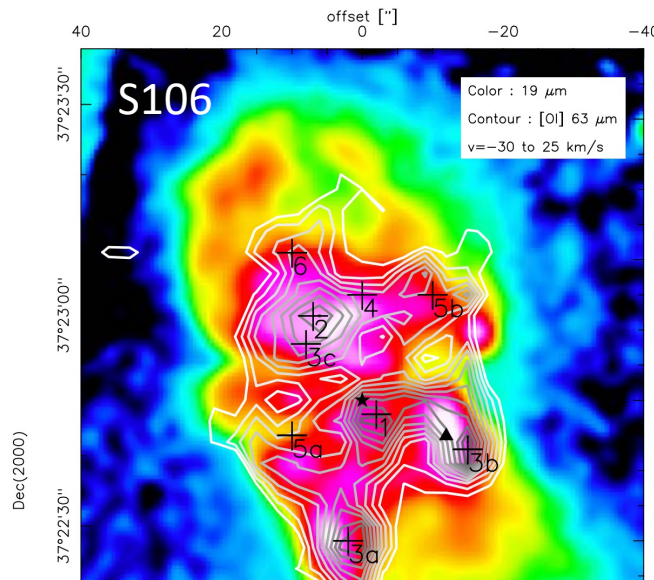
- Best identified with [OI] @ 145  $\mu\text{m}$



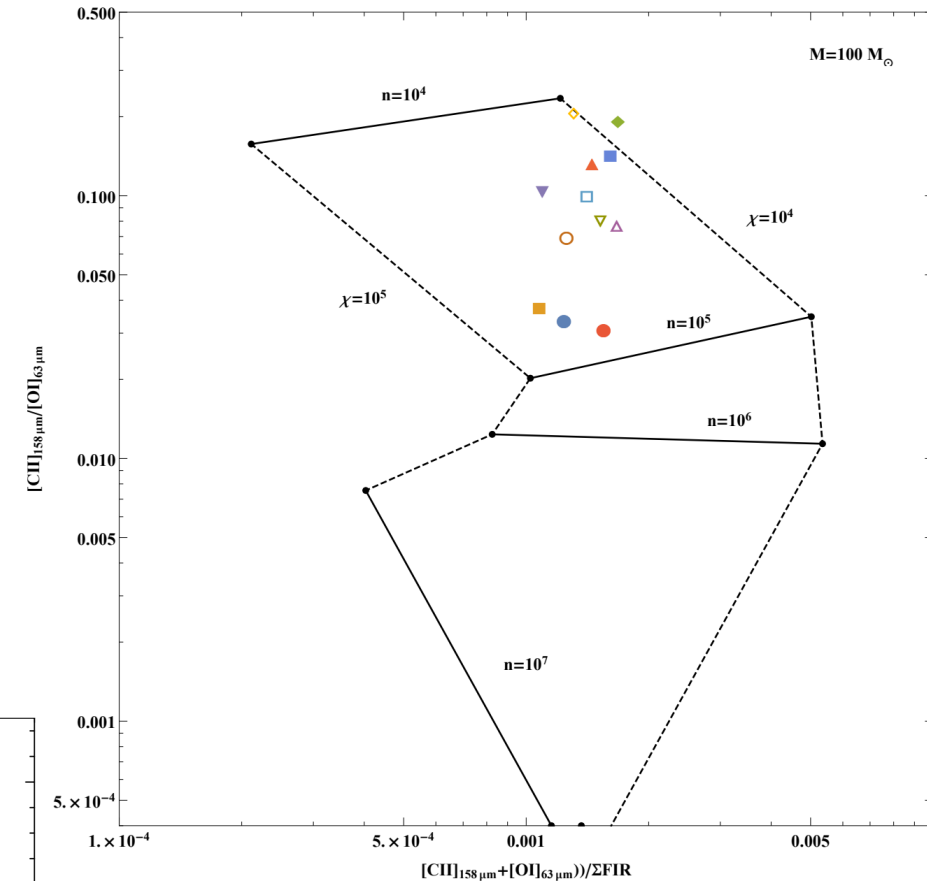


# PDR modeling

- PDR analysis at high spectral resolution
  - Can provide 3D information
- KOSMA-tau models (Stoerzer et al. 1996; Roellig et al. 2006)
  - Available in the PDR Toolbox (see talk M. Pound)



S106: Schneider et al. (2018)





# PDR modeling

➤ There are a wide variety of PDR codes (Roellig et al. 2007)

- PDR Toolbox (Pound & Wolfire 2008; 2023)
- Meudon PDR (Le Petit et al. 2006; Le Bourlot et al 2012)
- CLOUDY (Ferland et al. 1998; 2017)
- ...

➤ Meudon code

- Online model fitting (on the ISMDB)
- ISMDB: also hosts shock code

<https://pdr.obspm.fr/>

1 – Search among two parameters

x	<input type="text" value="nH"/>	cm <sup>-3</sup>	<input checked="" type="checkbox"/> log scale
y	<input type="text" value="chi front"/>	ISRF	<input checked="" type="checkbox"/> log scale

2 – Fix all the other parameters (reset all)

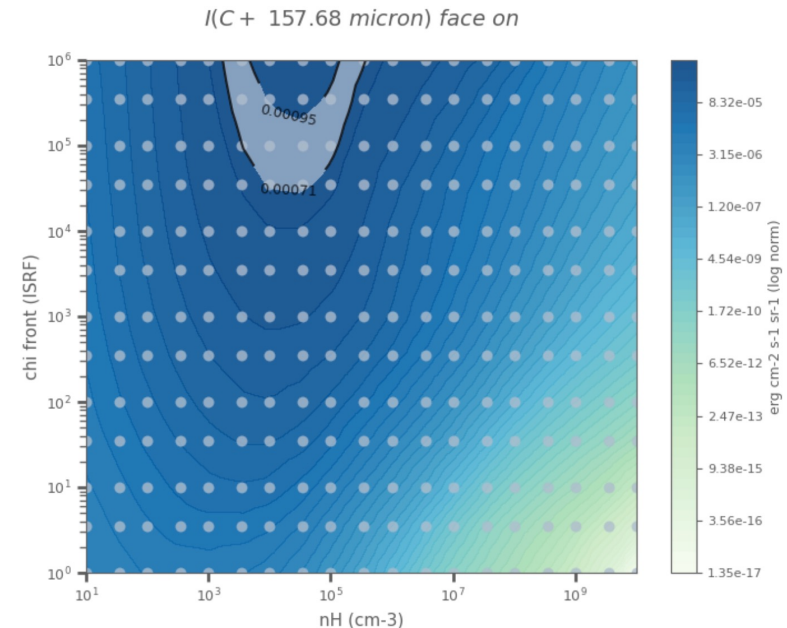
<input type="text" value="AVmax"/>	mag	<input type="text" value="5"/>
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Selected observational constraints

"I(C+ 157.68 micron) face on" > 70.8e-5  
"I(C+ 157.68 micron) face on" < 94.8e-5

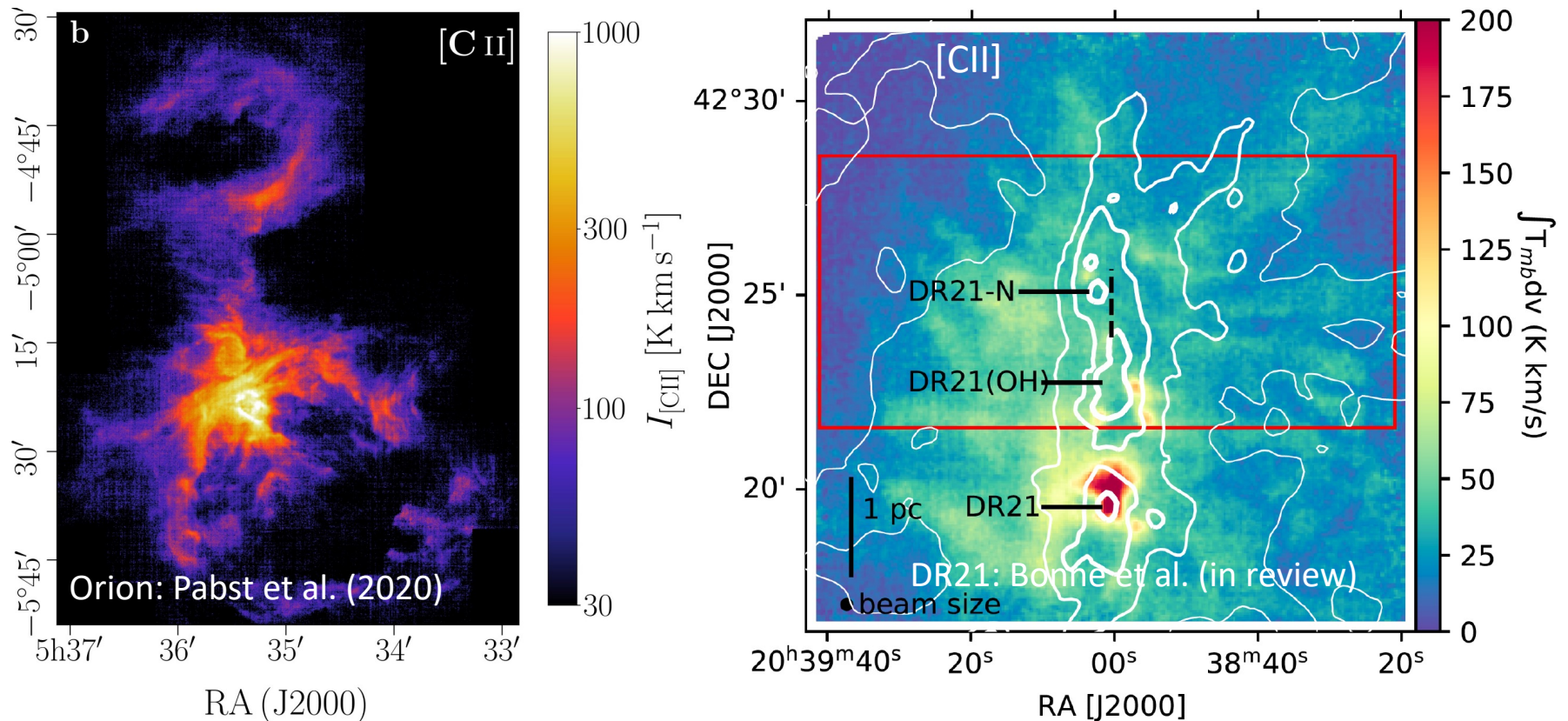
Values from S106 (Schneider et al. 2018)

Search



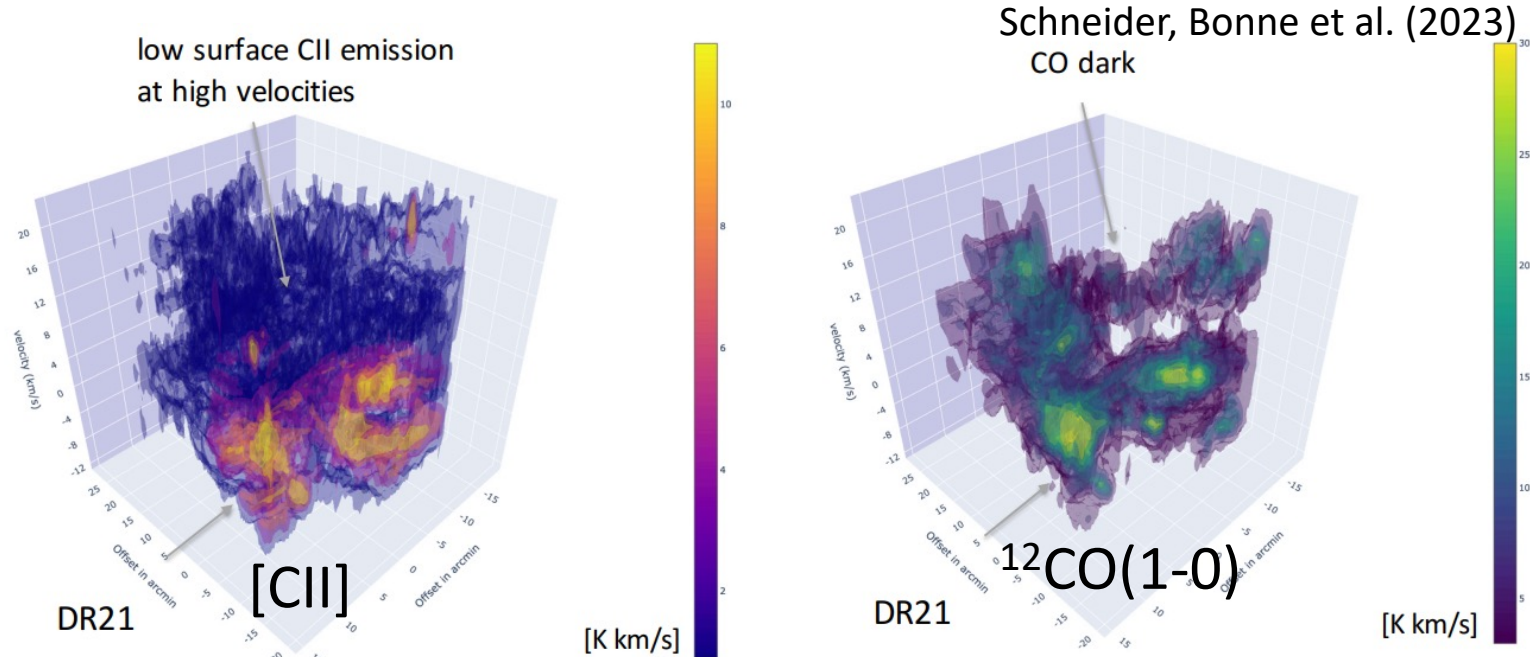
# Spectral data cubes

- A lot of information in a single spectrum
  - Spectral cubes: up to millions of ([CII]) spectra



# A 3D view of the spectral cube

- Isosurface plots with plotly in Python <https://plotly.com/python/3d-isosurface-plots/>
  - A relatively simple way to visualize the 3D cube
  - In Cygnus-X/DR21: unveils colliding flows forming molecular clouds





# Position-velocity (PV) diagrams

- Extract velocity information along one axis
  - Function in astropy: pvextractor
  - X-ray & radio/optical data: stellar wind driven?

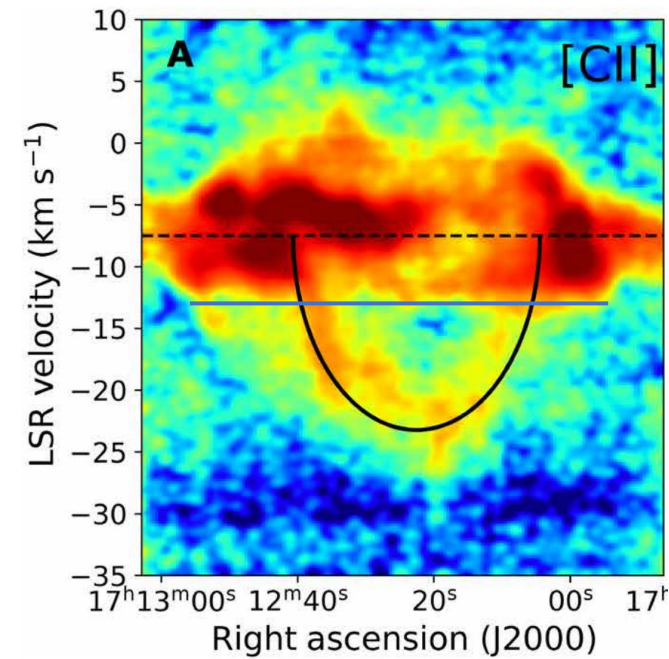
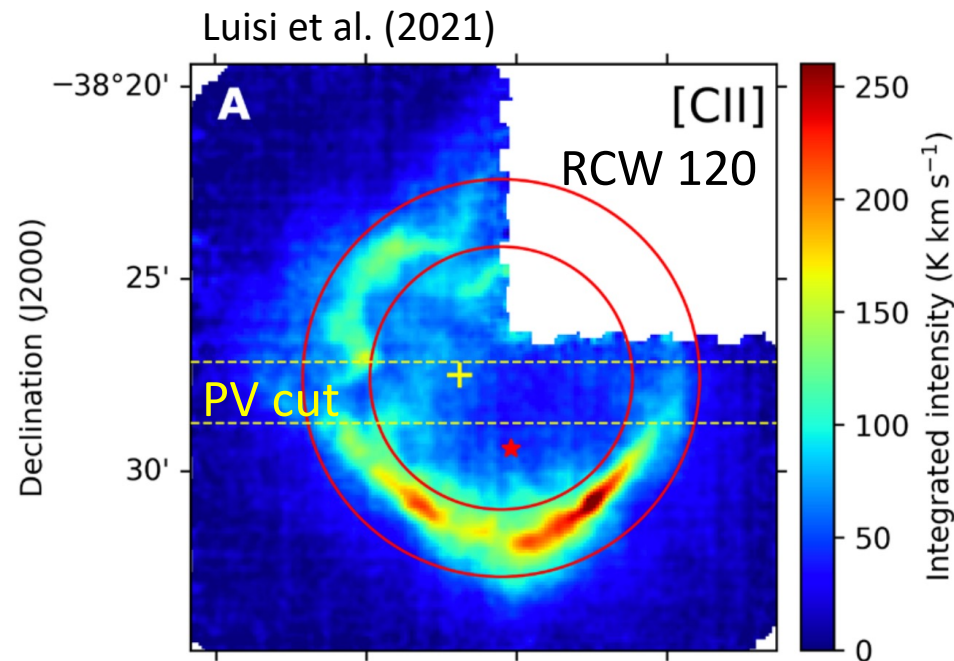
<https://pvextractor.readthedocs.io/en/latest/>  
<https://github.com/radio-astro-tools/pvextractor>

$$v_{\text{LSR}} = v_{\text{cloud}} + v_{\text{exp}} * \cos(bx)$$

Mass: Goldsmith et al. (2012) + Sofia et al. (2004)

$N(\text{C}^+)$

$[\text{C}^+]/[\text{H}]$

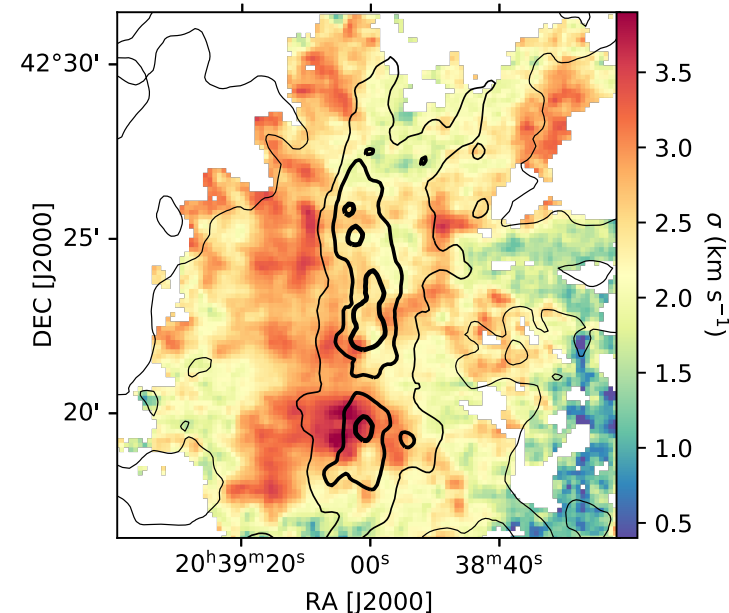
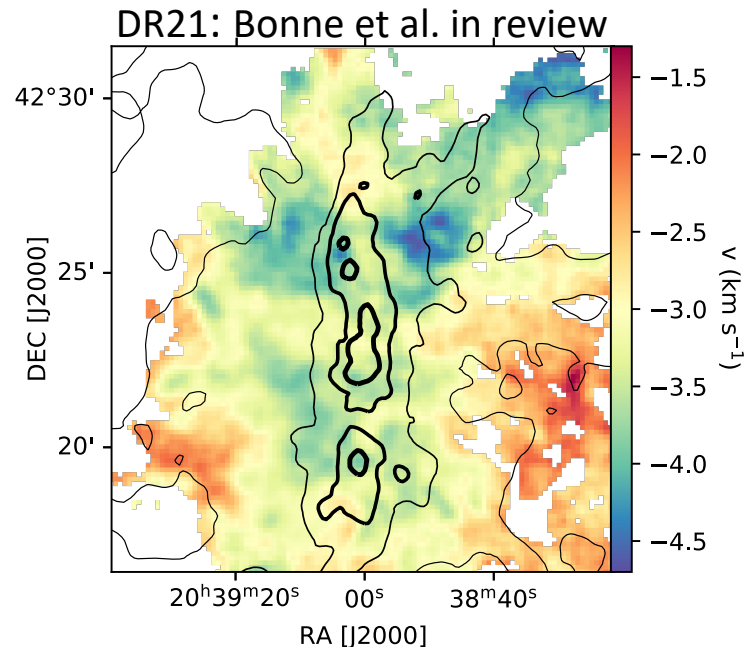


# Moment maps

- Gives a perspective on the global velocity field and linewidth
  - Remarkable change in linewidth across the DR21 ridge
  - Use ‘SpectralCube’ package in Astropy
  - Be aware of S/N (see e.g. Teague et al. 2019)

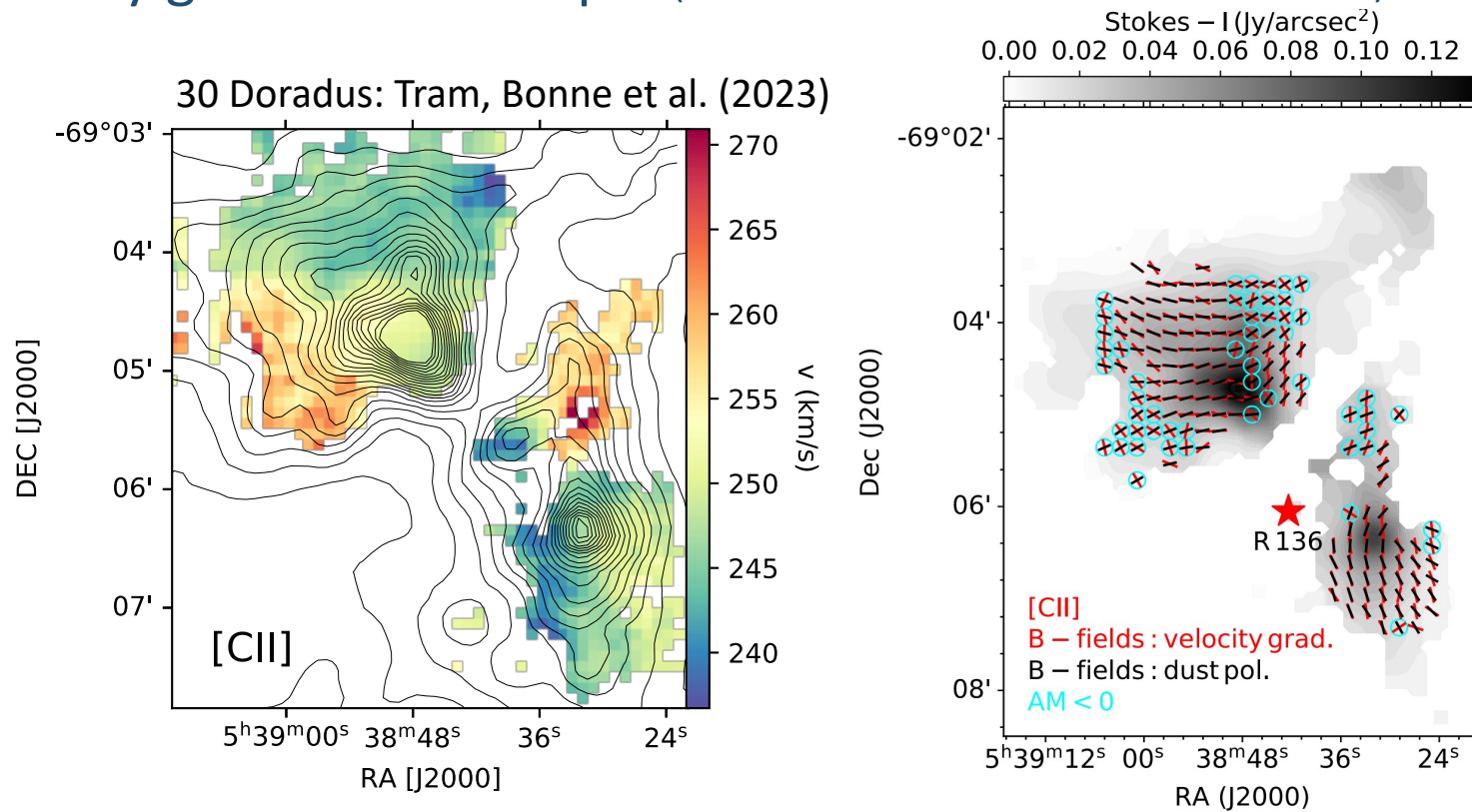
```
>>> moment_0 = cube.moment(order=0)
>>> moment_1 = cube.moment(order=1)
>>> moment_2 = cube.moment(order=2)
```

<https://spectral-cube.readthedocs.io/en/latest/moments.html>



# Synergy with the magnetic field observations

- Provides more comprehensive view of the ISM evolution
  - Determine the magnetic field strength (see talk V. Le Gouellec)
  - Velocity gradient technique (see Gonzalez-Casanova & Lazarian 2017)



# Multi-Gaussian fitting

➤ Extract more information from the spectra

➤ Don't reinvent the wheel

- Beyond The Spectrum (BTS) (Clarke et al. 2018)

- Fully automated

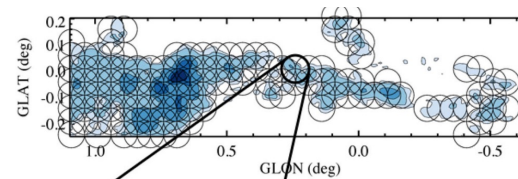
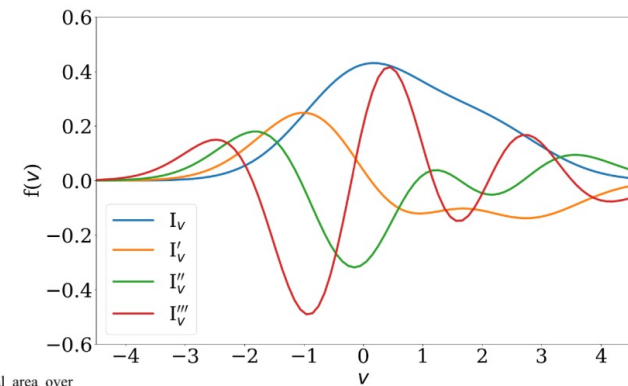
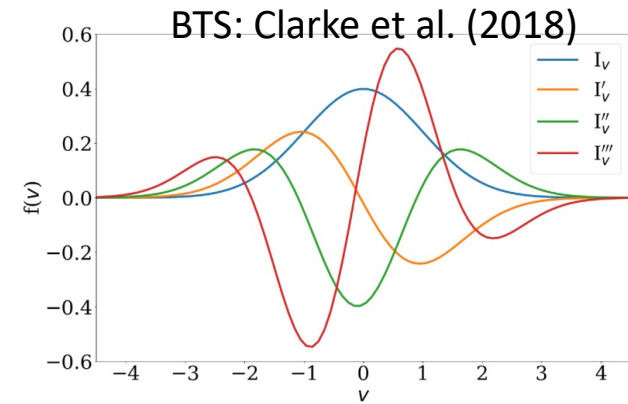
- Scouse(Py) (Henshaw et al. 2016; 2019)

- Semi-automated

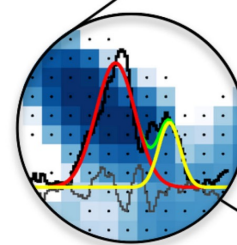
- Hierarchical approach

- Also exists in IDL

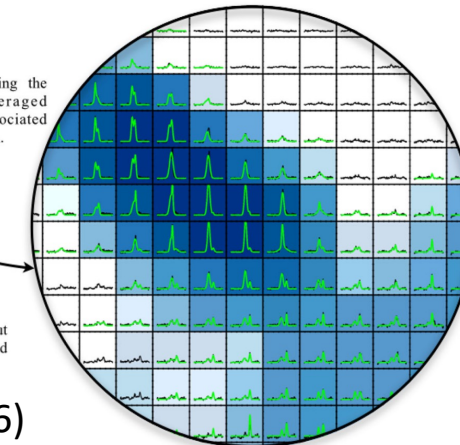
- ...



Stage 1: Identify the spatial area over which to implement SCOUSE - A grid of Spectral Averaging Areas (SAAs; black circles where 50% of the enclosed positions have a non-zero integrated intensity).



Stage 2: Fitting the spatially-averaged spectrum associated with each SAA.



Stages 3 & 4: Fitting the individual spectra using output parameters from stage 2 as free-parameter inputs, and selecting the "best-fits" to each spectrum.

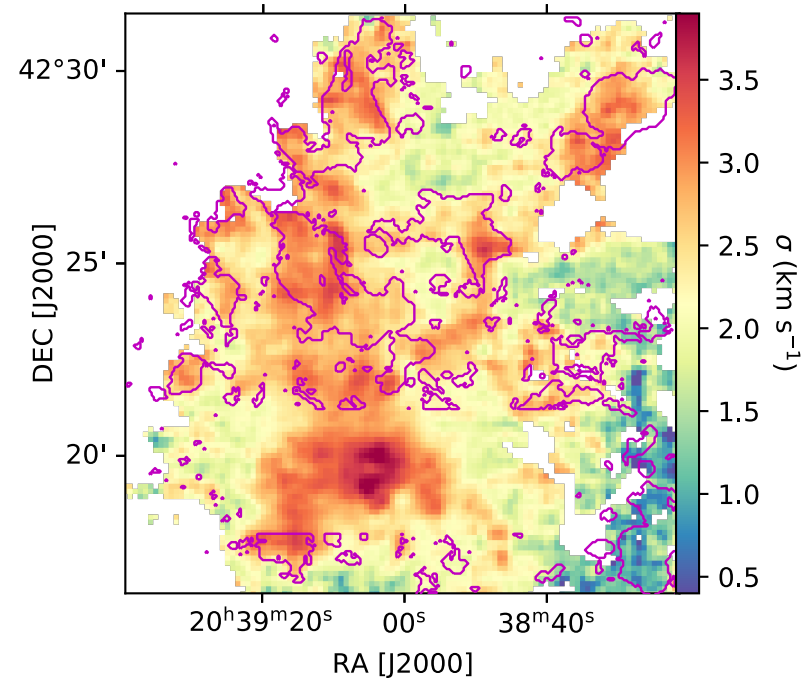
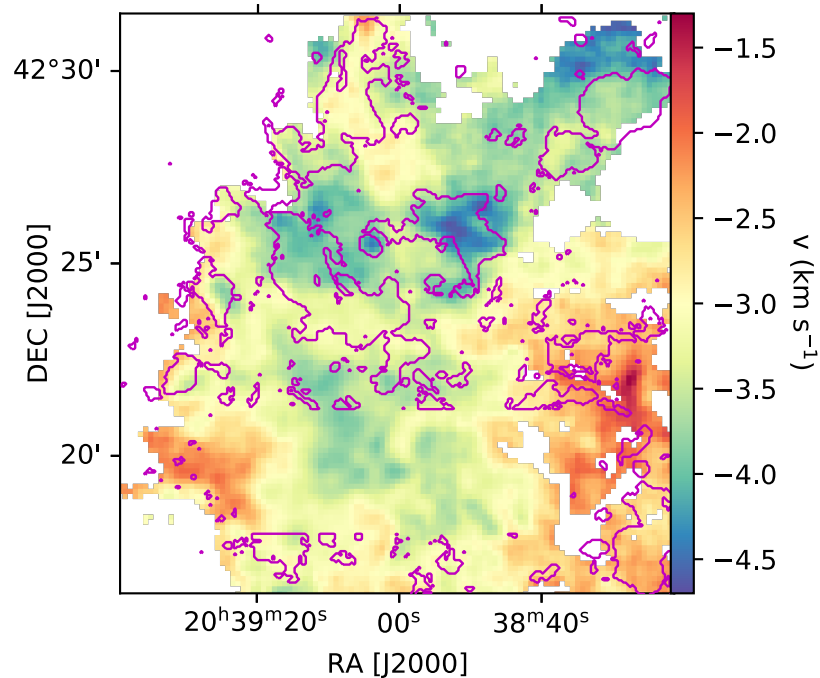
Scouse: Henshaw et al. (2016)

# Multi-Gaussian fitting

- Dynamic features associated with multiple components
  - Need to be careful: self-absorption

Results from BTS (Bonne et al. in review)

Magenta: regions with two velocity components





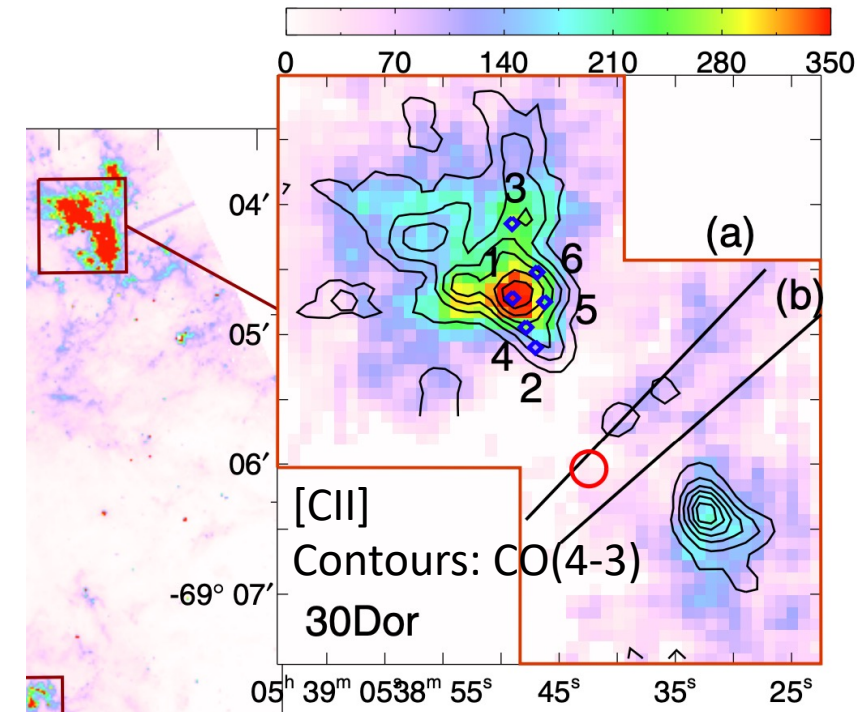
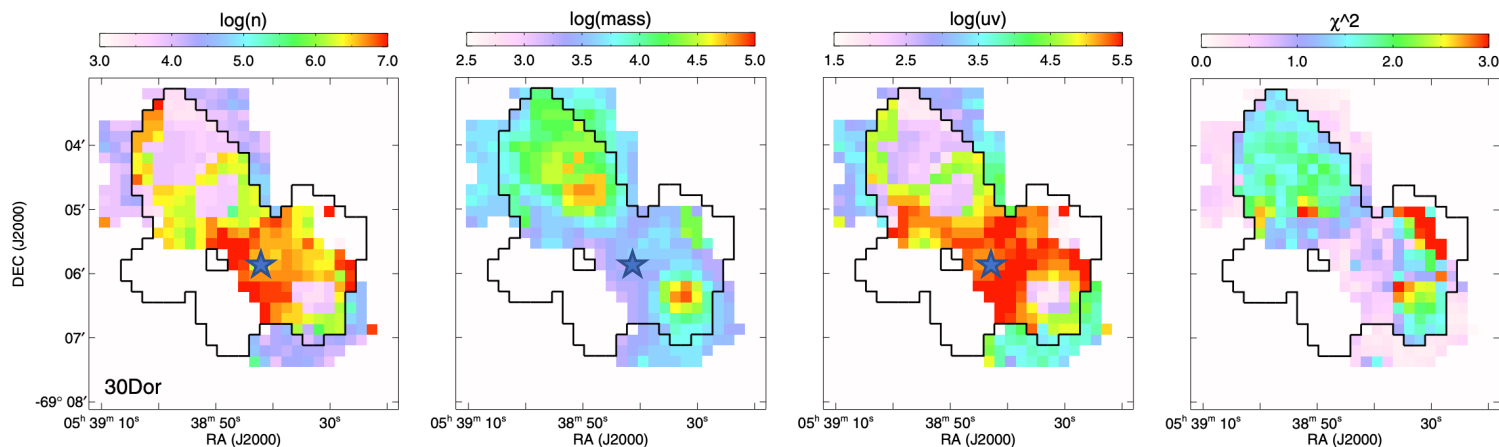
# PDR analysis of far-infrared maps

## ➤ Fit pixel-by-pixel fitting

- Kosma-tau (e.g. Okada et al. 2019)
- PDR Toolbox (see talk M. Pound)

## ➤ Maps the (best fitting) excitation conditions

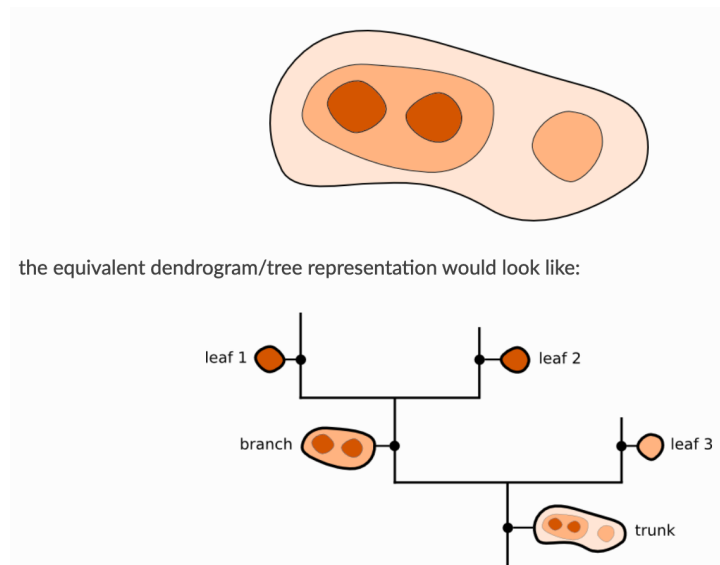
- Using: [CII], [OI], [CI] & CO lines



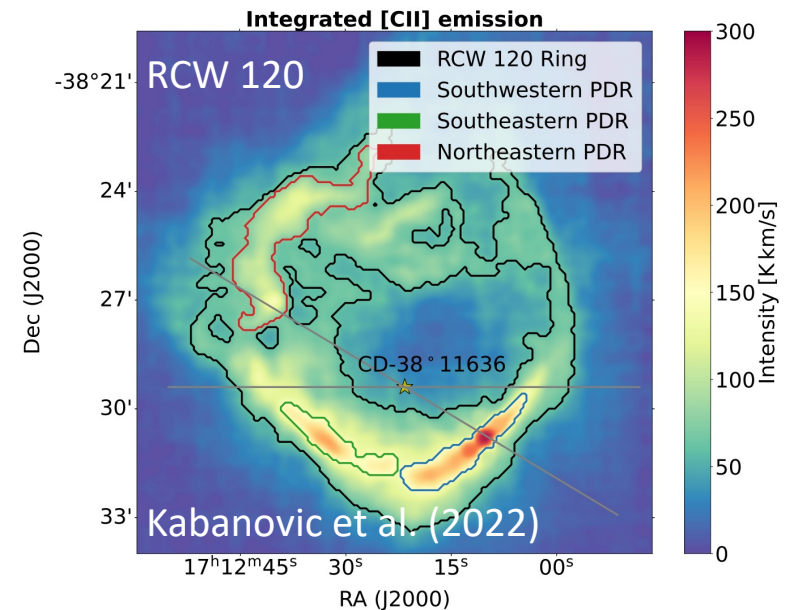
# Segmenting data cubes: spatially

## ➤ Dendrograms: hierarchical structure (Rosolowsky et al. 2008)

- Astrodendro package in Python <https://dendrograms.readthedocs.io/en/stable/>
- Also applicable to PPV
- Basis for: e.g. SCIMES (Colombo et al. 2015), Acorns (Henshaw et al. 2019)



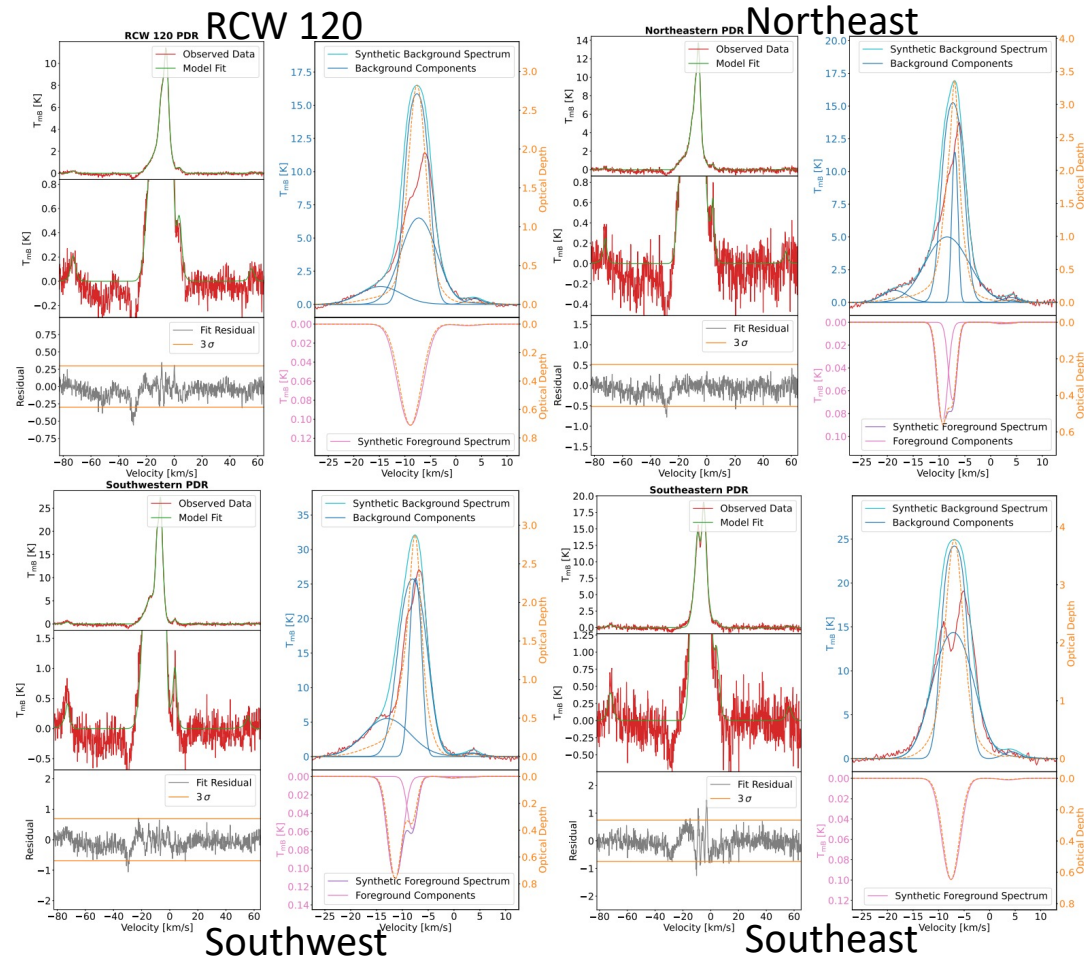
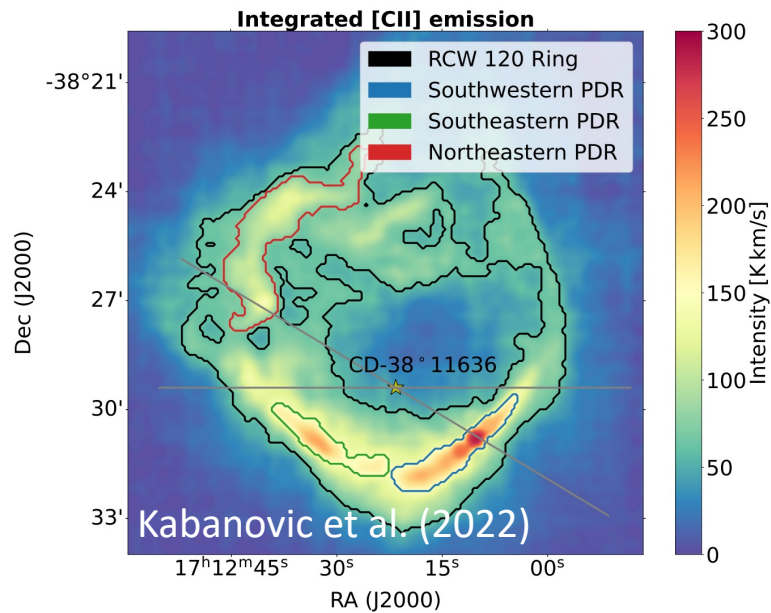
Adapted from: <https://dendrograms.readthedocs.io/en/stable/>



# Segmenting data cubes: spatially

➤ Can analyze the different structures

- [CII] self-absorption
- Due to the cold atomic halo?

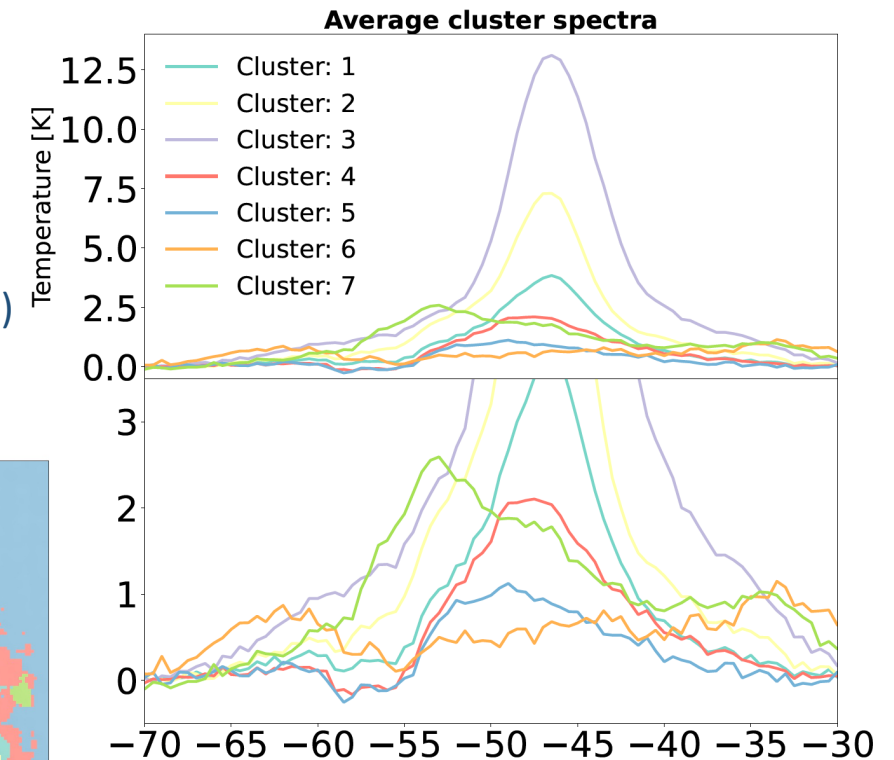
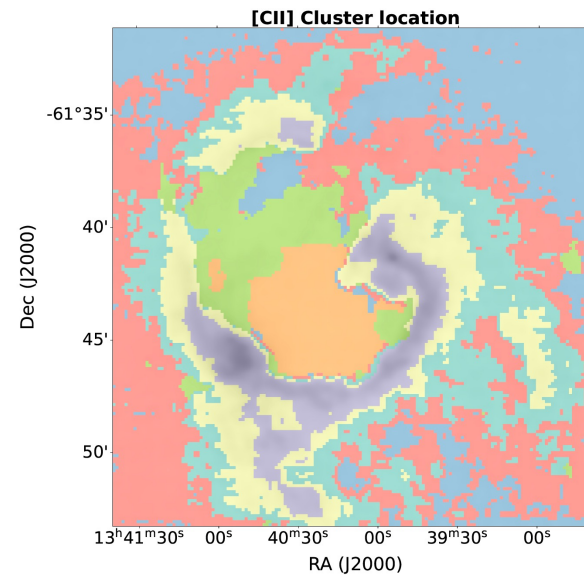
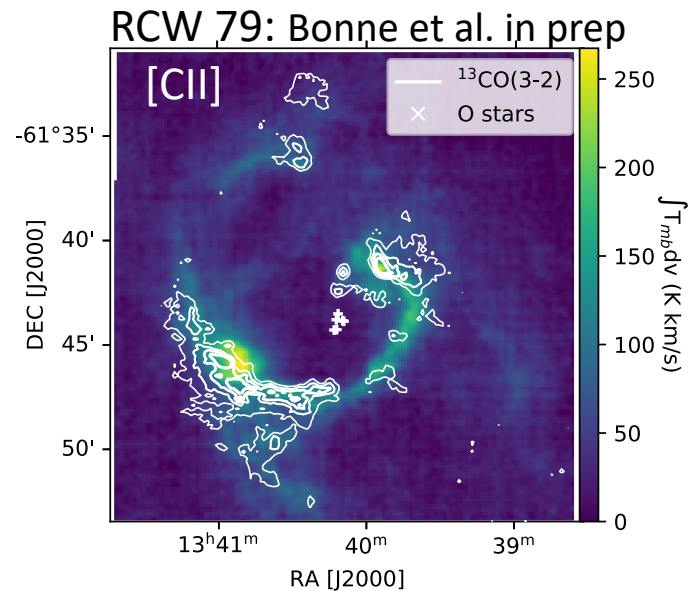


# Segmenting data cubes: spectrally

➤ Segment map based on the spectra

➤ Gaussian Mixture Model (GMM)

- Unsupervised machine learning (see Kabanovic et al. 2022)



# Conclusion

- Provides a unique view (on the ISM)
  - Work is only starting
- High spectral resolution provides detailed information
  - Dynamics
  - Chemical abundances
  - Excitation conditions
- Several analysis tools are already available