PDR Modelling

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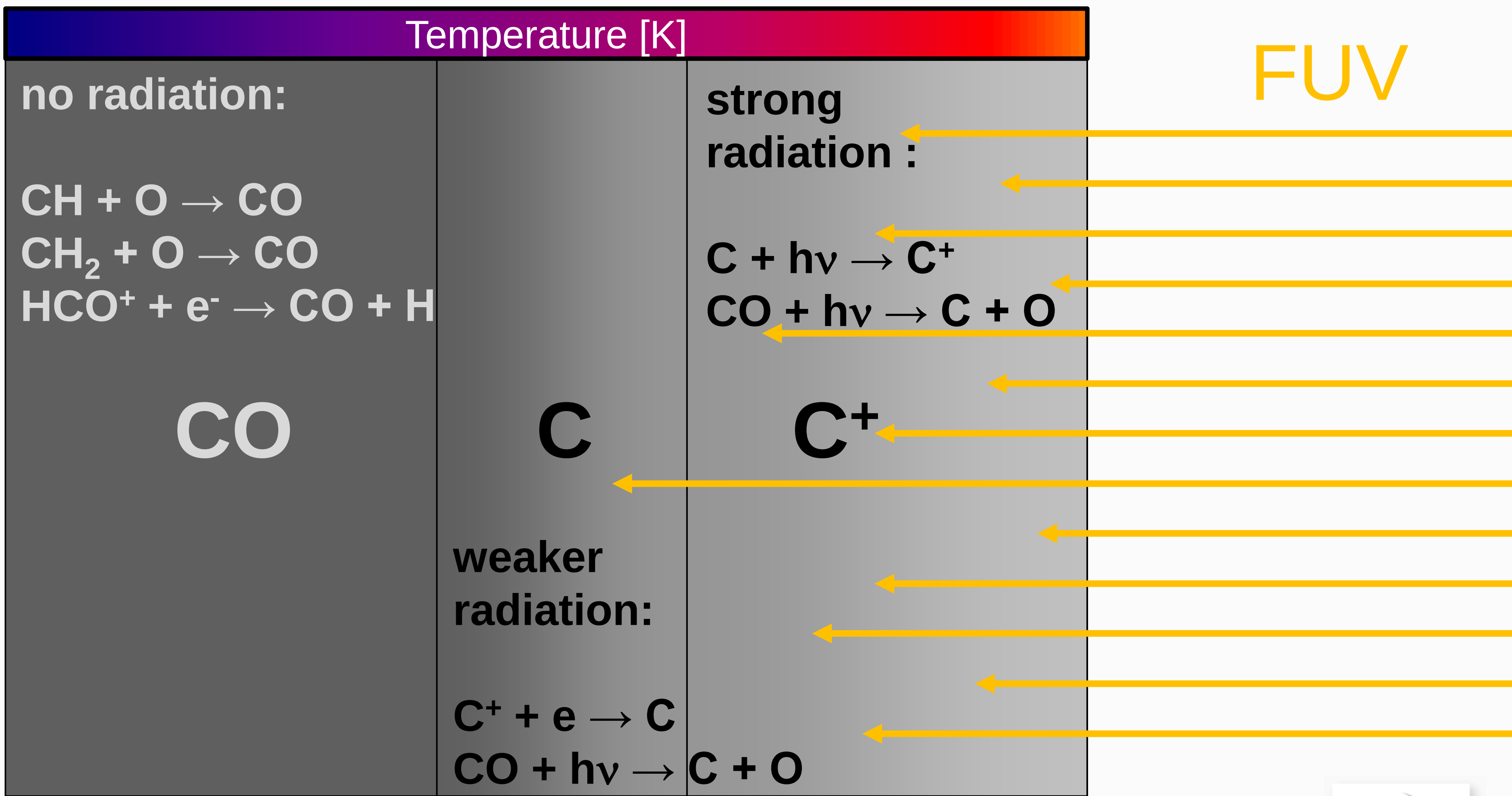
PDR - Photodissociation Region

- A region where far-ultraviolett (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.

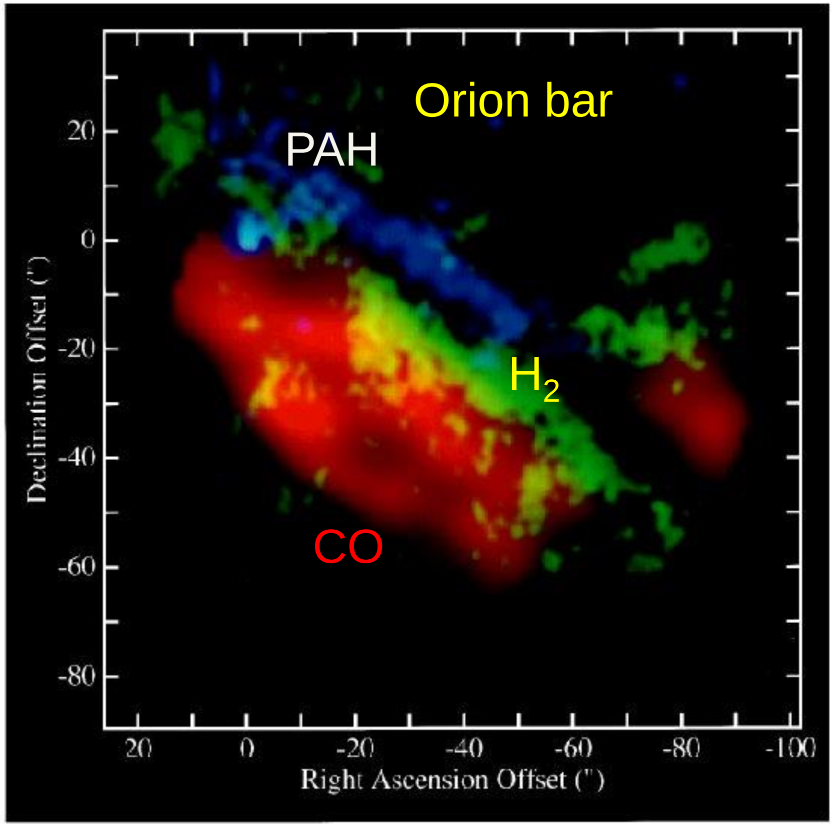
– **6 eV (2066 Å)**	~ionization potential of dust/PAHs
11.1 eV (1117 Å)	dissociation energy of CO
11.3 eV (1097 Å)	ionization potential of C
– **13.6 eV (912 Å)**	ionization potential of H
	ionization potential of O
14.5 eV (855 Å)	ionization potential of N

Photodissociation Region



Interstellar cloud surface (cross section)

Photodissociation Region



Tielens & Hollenbach 1998

Motte et al. 2010

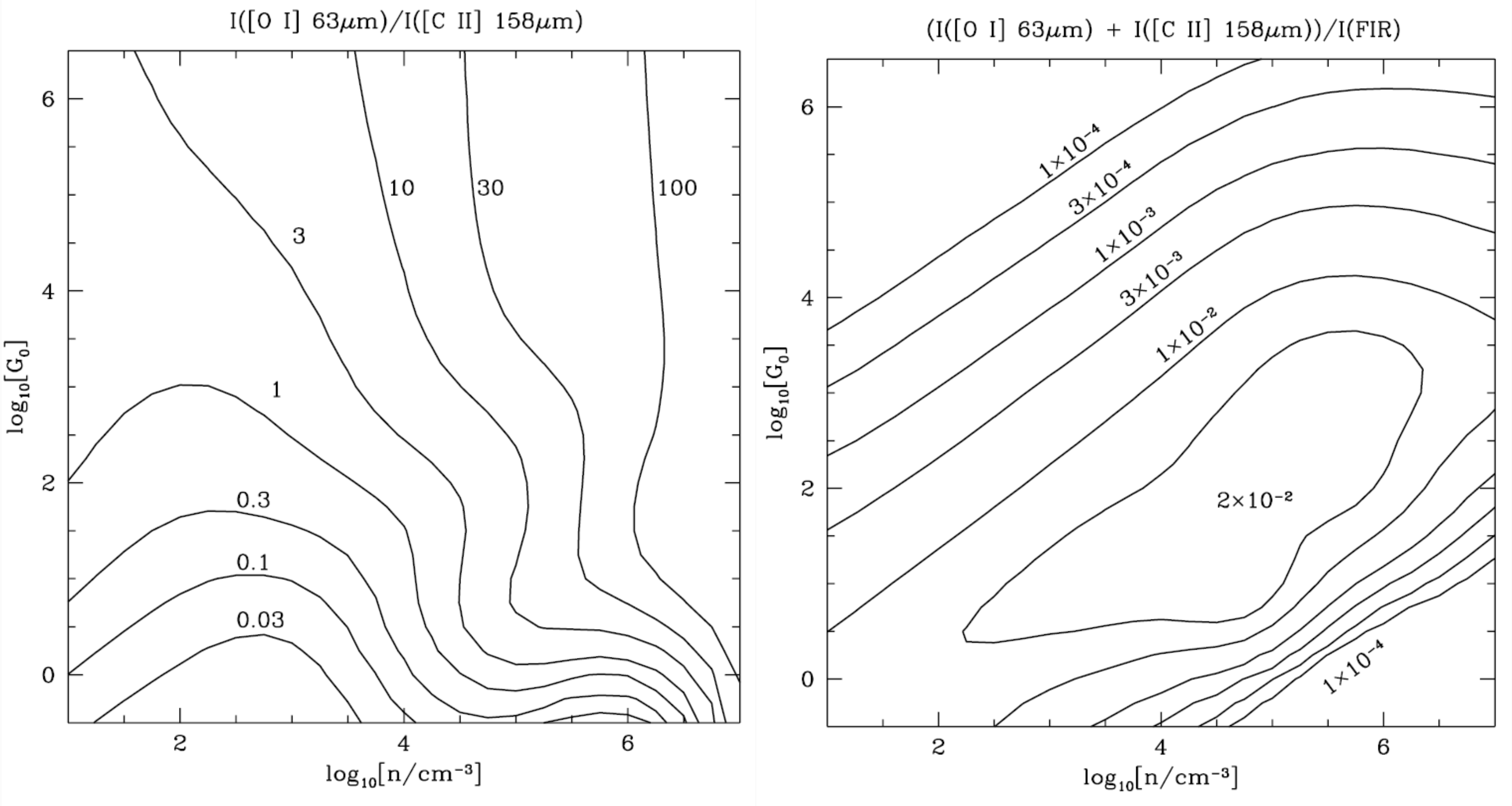
PDR Model Complexity

- Geometry
  - plane parallel slab
    - 1-sided / 2-sided
  - sphere (new parameter: mass)
  - circular paraboloid (outflow)
  - 3-D
  - clumpy, fractal
- Radiation field (int & ext)
  - isotropic and/or directed/inclined
  - spectral shape of FUV field
    - physics and chemistry λ-dependent
  - detailed photon cross-section
  - full λ-resolving radiative transfer
- Dust content
  - dust composition, size distribution (practically unknown)
  - very small grains, PAHs
PE efficiency, charge exchange
  - grain surface characterization
E_{bind} ??
- Chemistry
  - nonlinear chemical networks
~10-20% reaction rates known
  - coupling to heating & cooling & RT
  - ice & surface & gas chemistry
  - coupling to FUV & CR & XR
  - state-to-state reaction rates

PDR Model Complexity

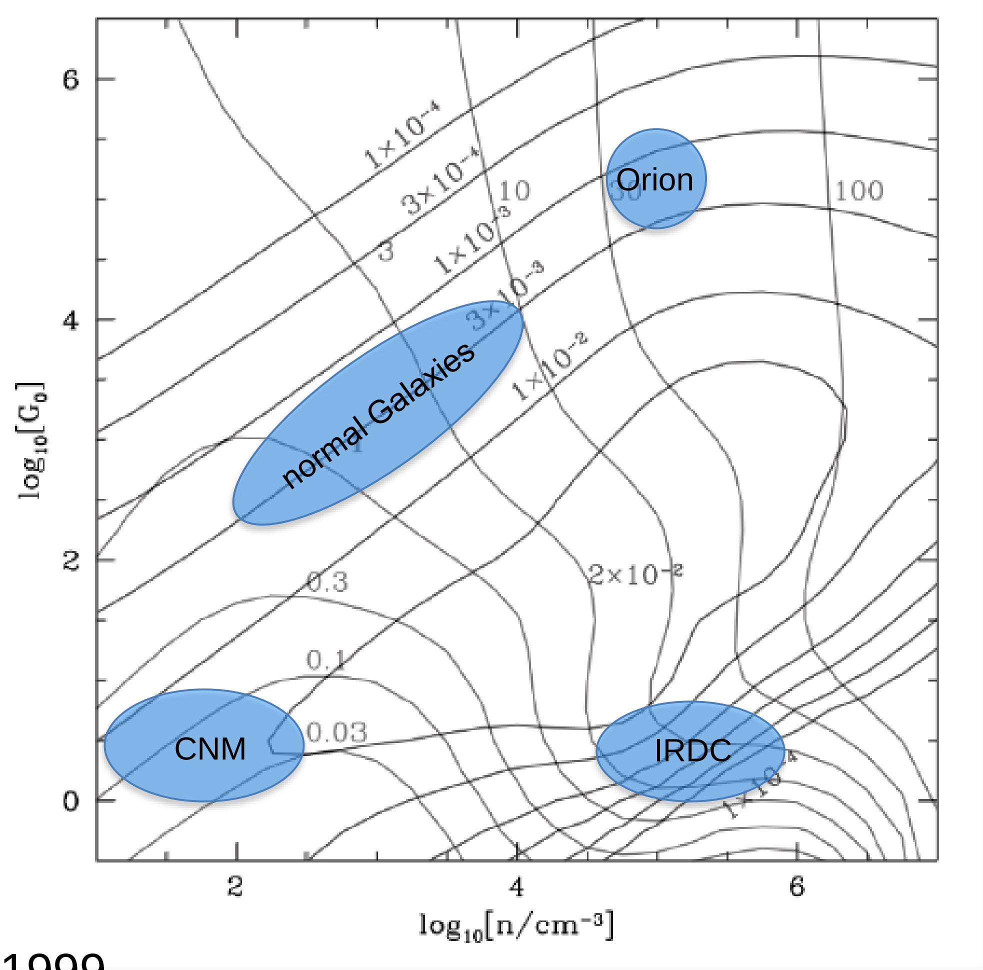
- Energetics / Thermodynamics
  - heating couples to FUV RT & dust
  - cooling couples to chemistry & RT
  - full treatment of H2, HD, CO, H2O,….
  - detailed internal RT vs. approx.
  - isobaric (p constant) vs. isochoric (n constant)
  - chemical heating & cooling
  - multi-stability solutions?
- Stationarity
  - stationary vs. time-dep solution
    - initial conditions?
    - rate uncertainties more important
  - non-stationary model parameters!
    - UV field, geometry, pressure/density
- Numerics
  - non-linear coupling of geometry RT & energetics & chemistry
  - horrible scaling with problem size chemistry: $N^{3.5}$
  - interpolation introduces large uncertainties
  - n-dim global root finding/minimization
  - existance of (multiple) solutions?

Line ratio analysis



Kaufman et al. 1999

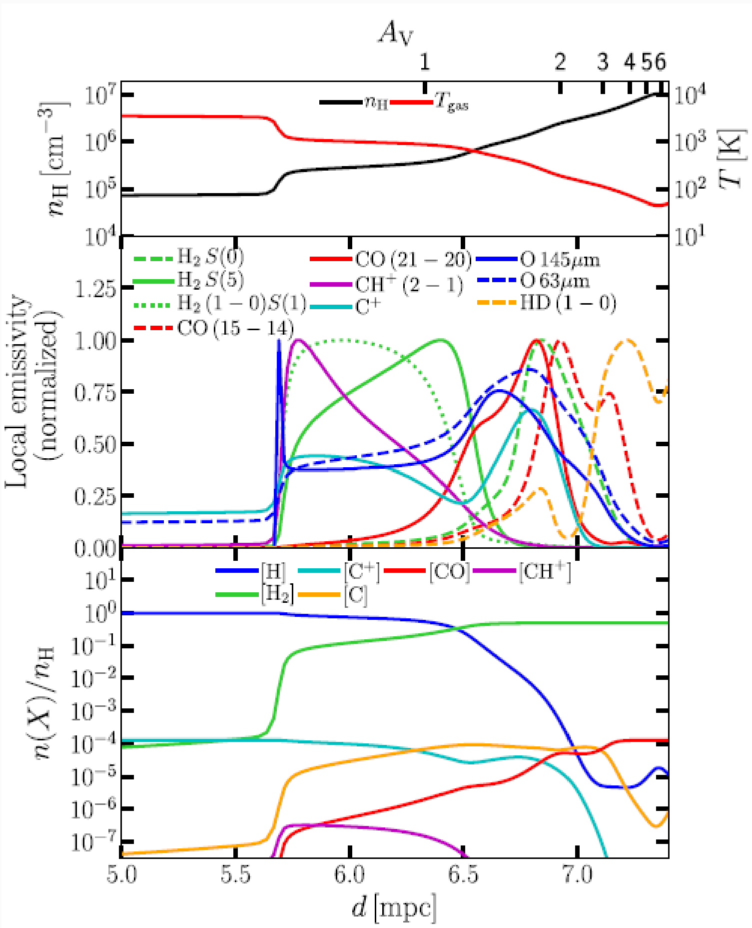
Line ratio analysis

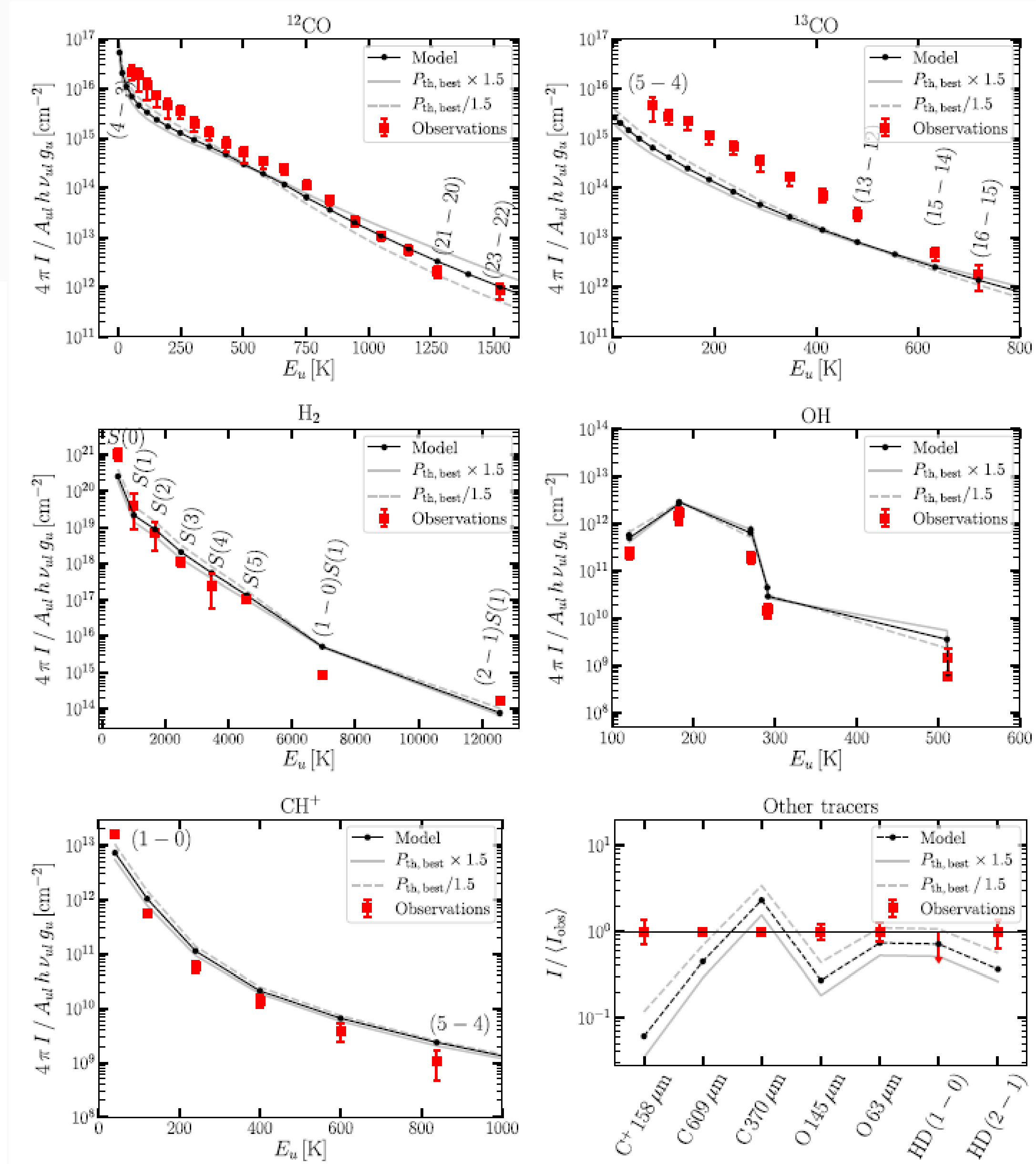


Kaufman et al. 1999

Orion Bar Modelling

Meudon PDR Code, isobaric

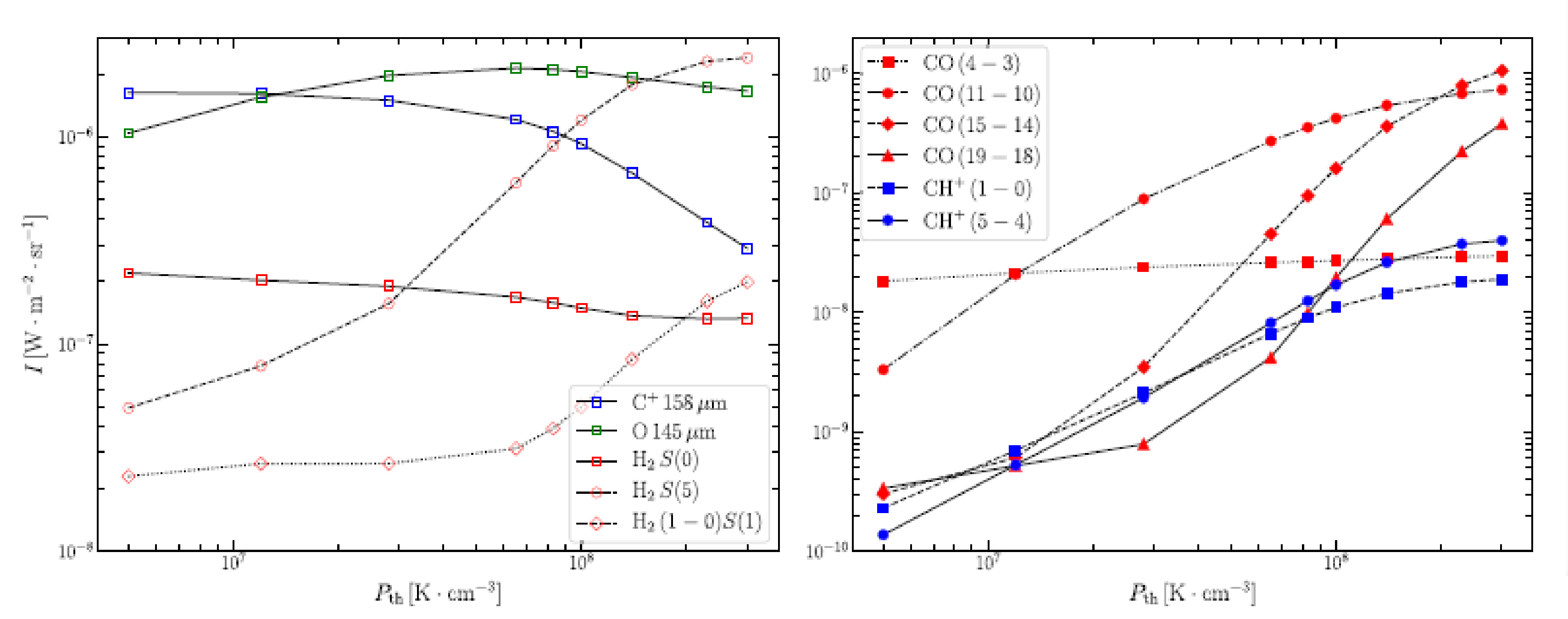




Joblin et al. 2018

Isobaric PDR Models

- Orion Bar model
- PDR energetics in terms of pressure
- Model emission strong function of thermal pressure

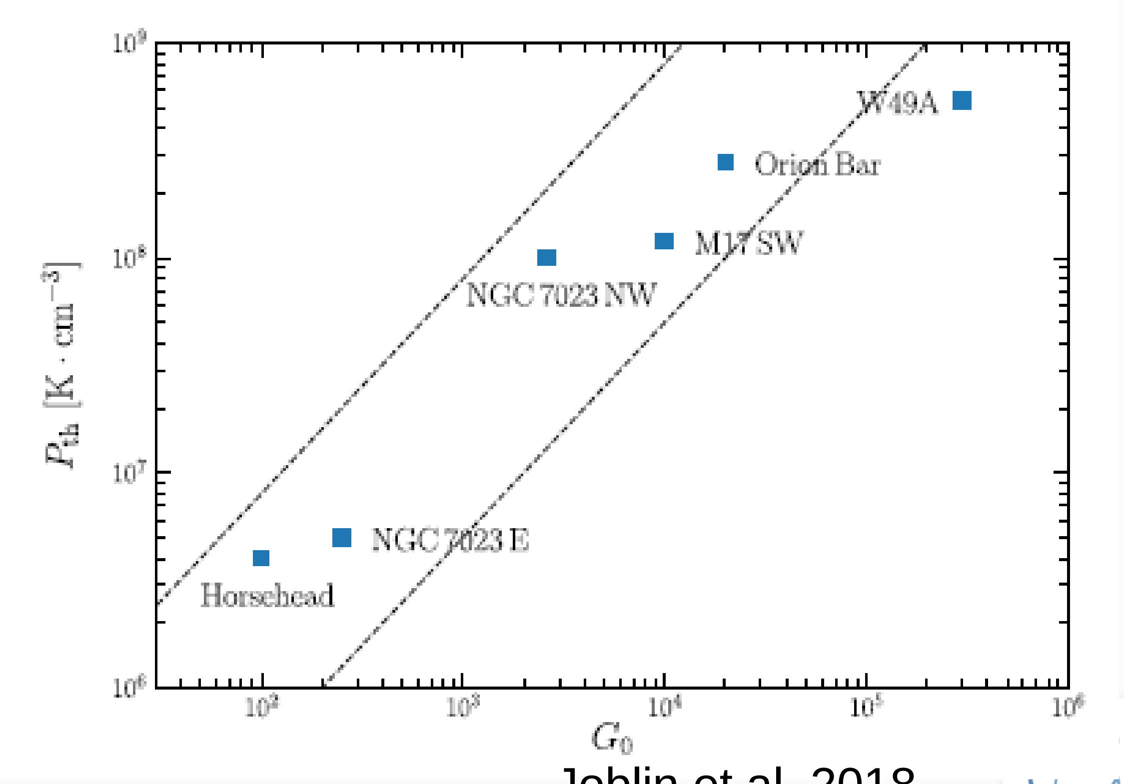


Joblin et al. 2018

Isobaric PDR Models

- Thermal PDR pressure derrived from observations correlates with FUV illumination strength.

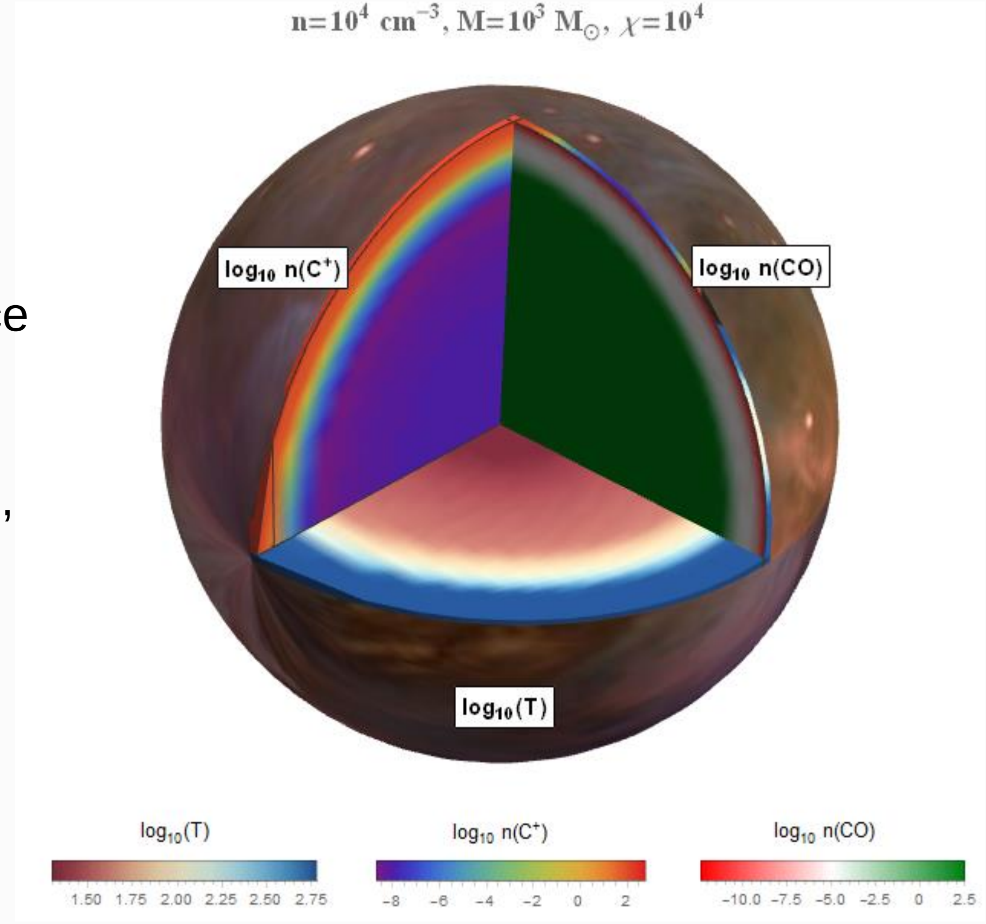
- Can be emulated by density profile, e.g. B.E.-Sphere, Plummer-profile



Joblin et al. 2018

The KOSMA-τ PDR Code

- 1-D, spherical geometry
  - power-law density profile
  - isotropic illumination
- self-consistent solution of energy- and chemical balance and radiative transfer
- self-shielding of H_2, CO (FGK, Draine & Bertoldi 1997, Visser et al. 2009)
- full dust RT and temp. computation for varying dust distribution



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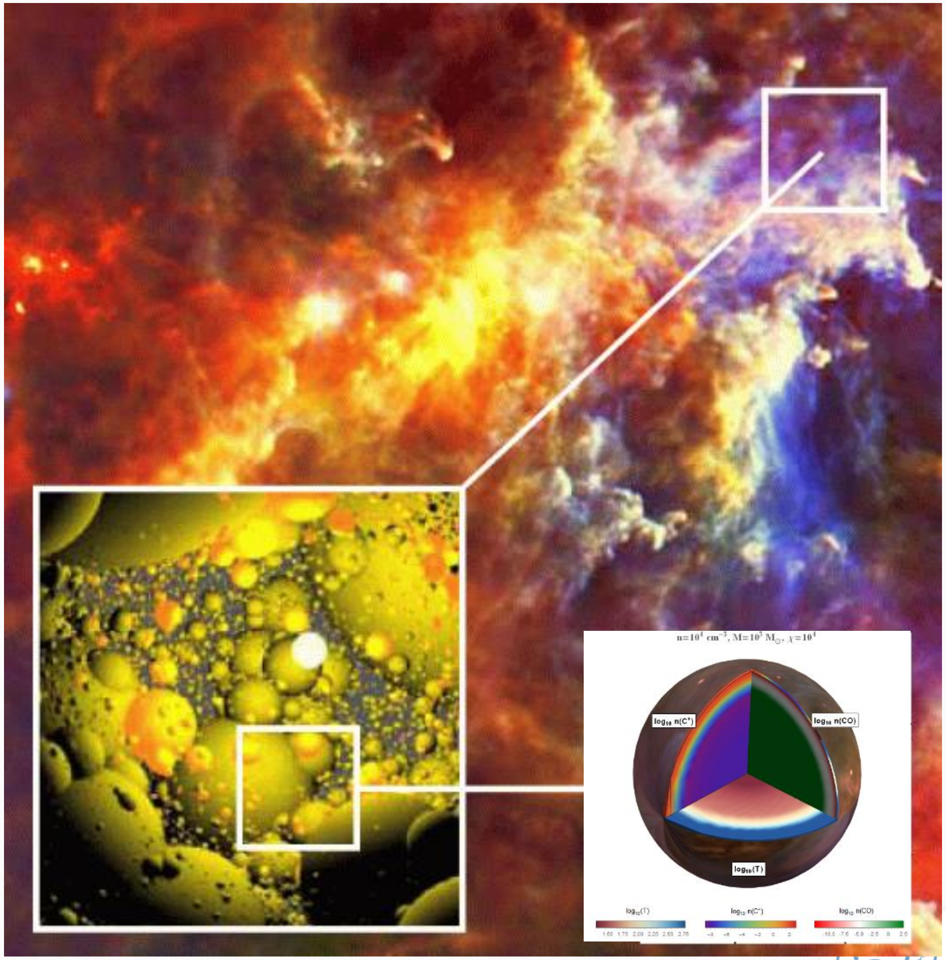
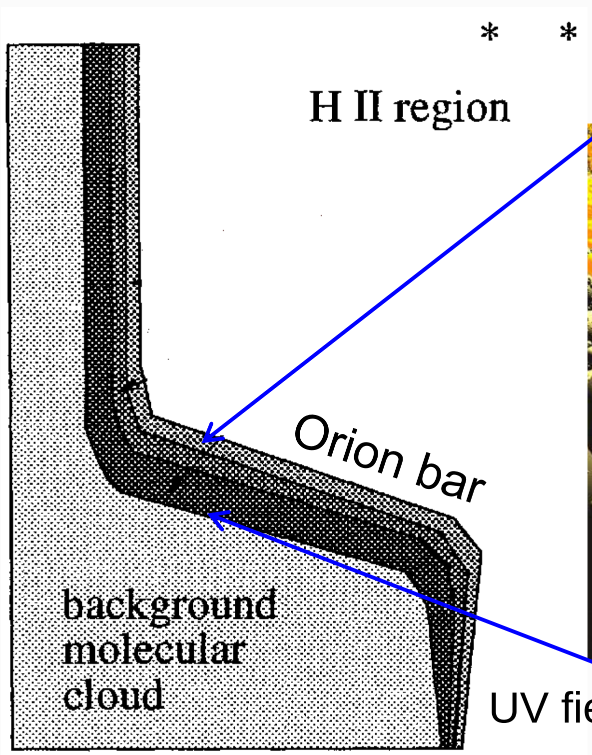
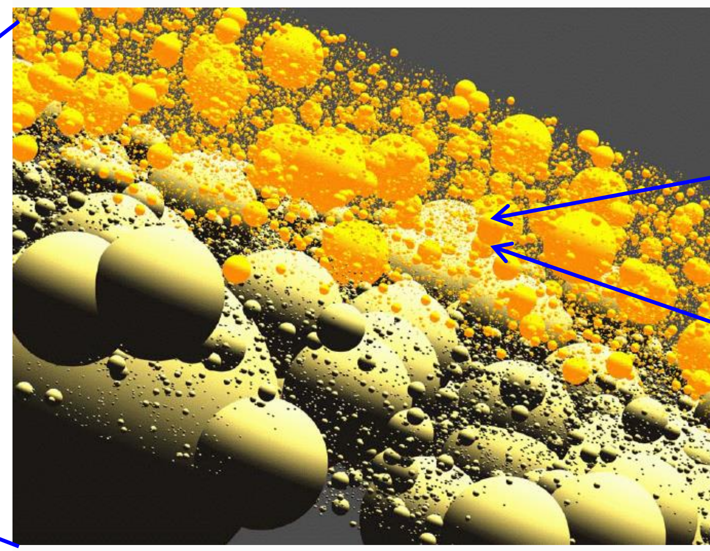
- self-consistent solution of energy- and chemical balance and radiative transfer
- self-shielding of H_2, CO (FGK, Draine & Bertoldi 1997, Visser et al. 2009)
- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
  - stochastic clump ensemble
  - **KOSMA-τ 3D** (Andree-Labsch et al. 2017)

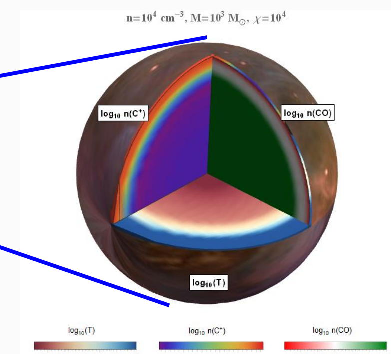


Applications: KOSMA-τ 3D

- Arbitrary 3-dim structure, each voxel populated by PDR clump ensembles with full size distribution (embedded in interclump medium)



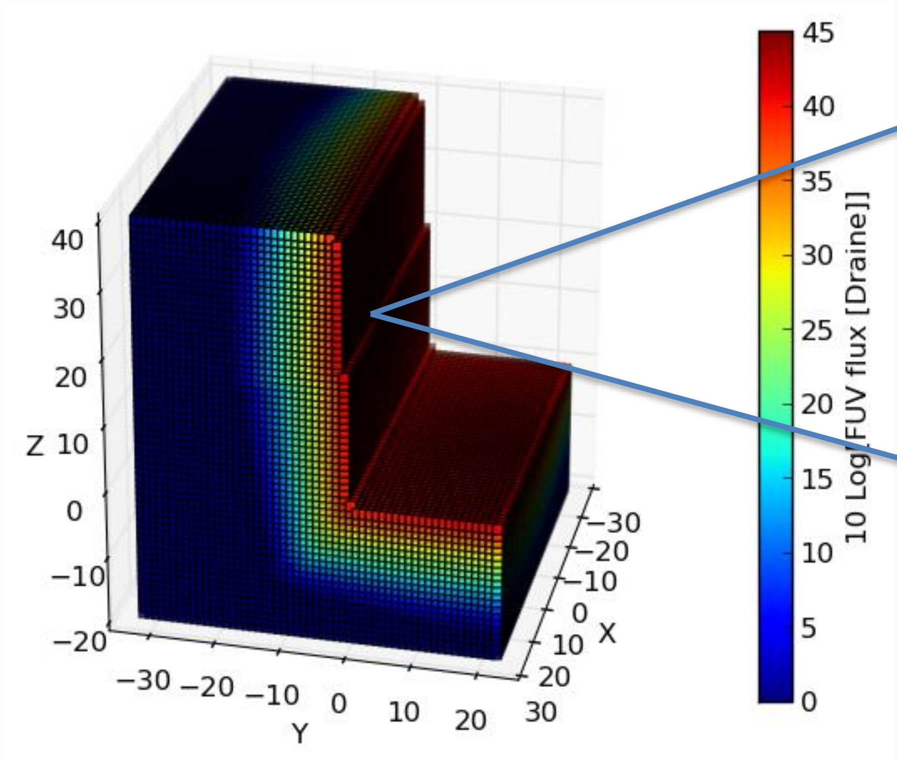


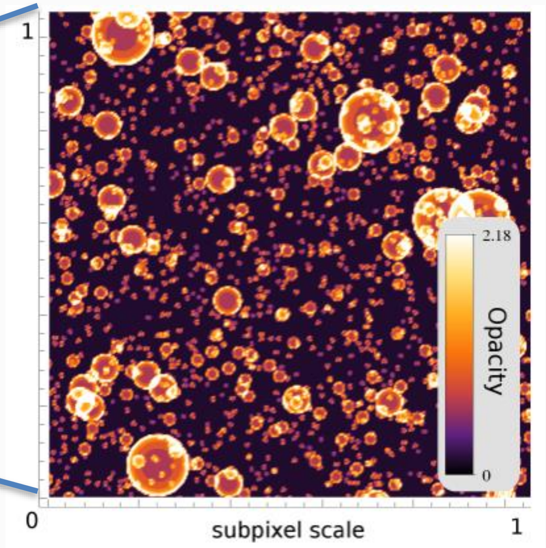


UV field attenuated in the cloud by foreground clumps

Applications: KOSMA-τ 3D

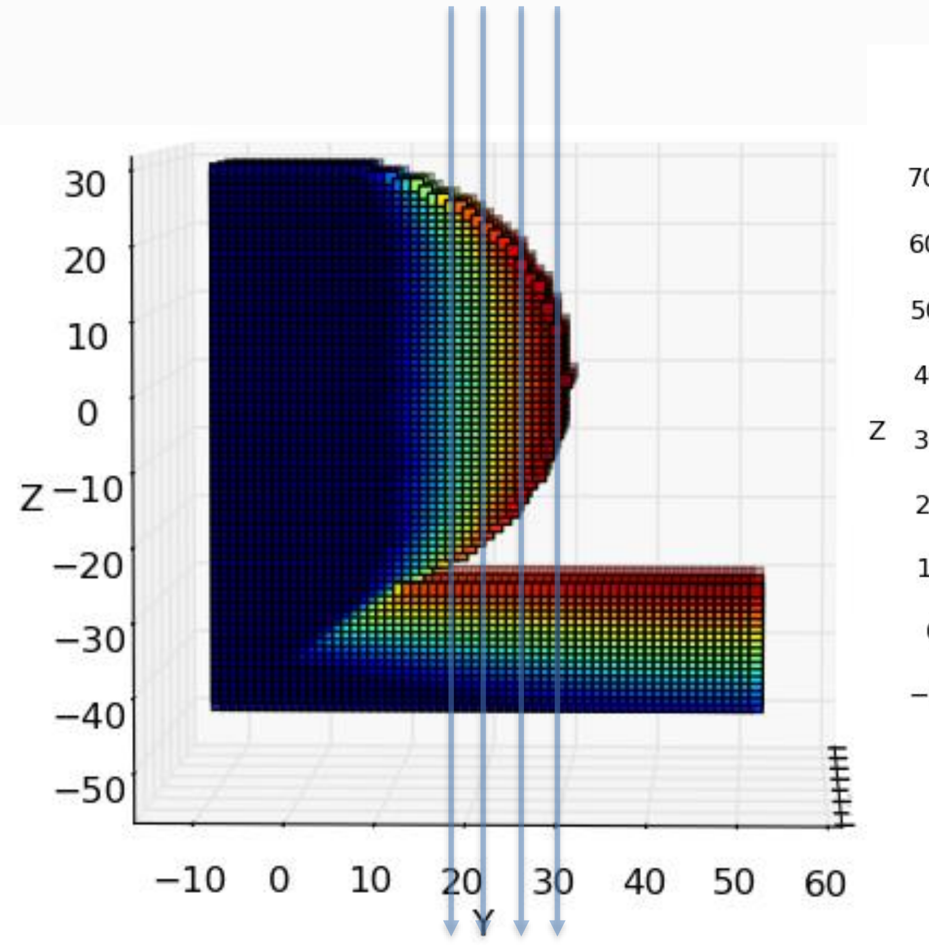
- Radiative transfer through all voxel (including shielding) allows to simulate observations from any direction, distance, …

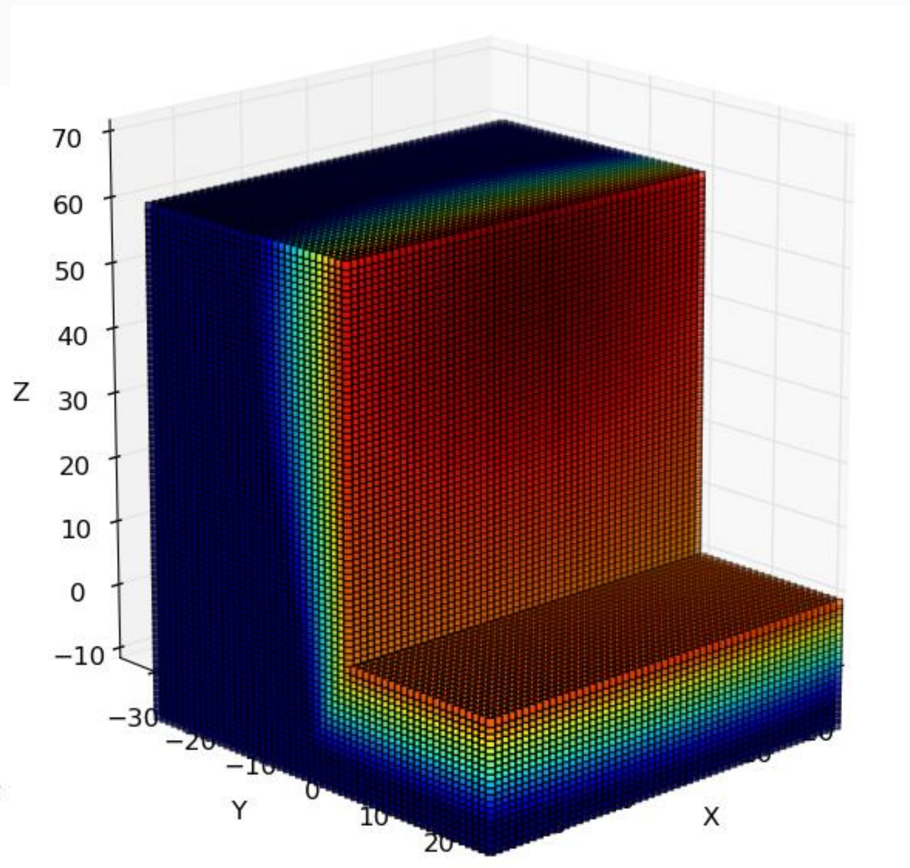




Andree-Labsch et al. 2017

Applications: KOSMA-τ 3D



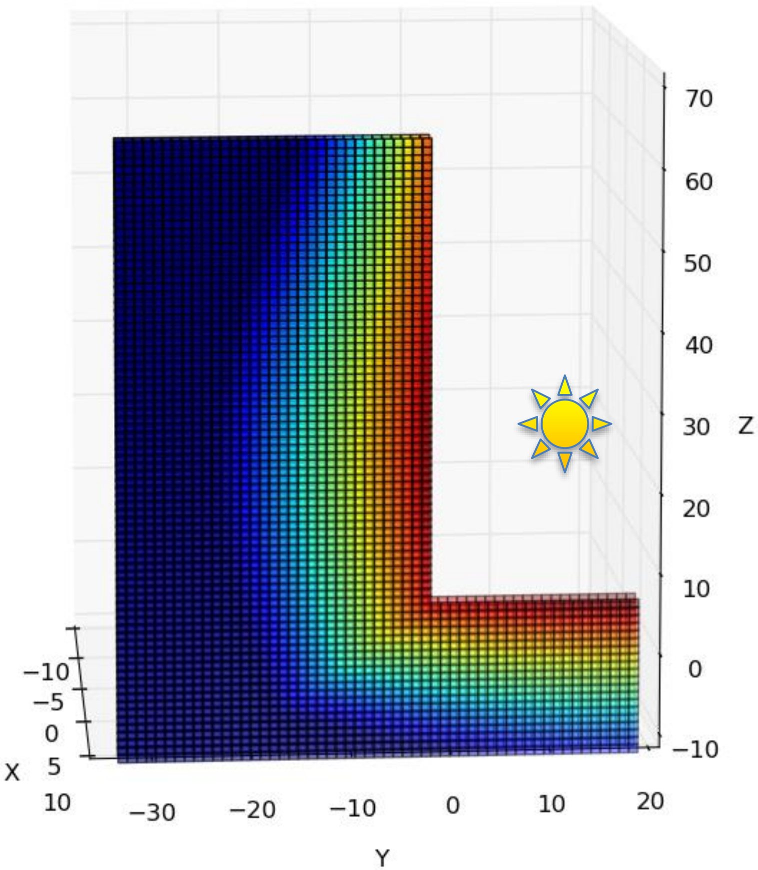


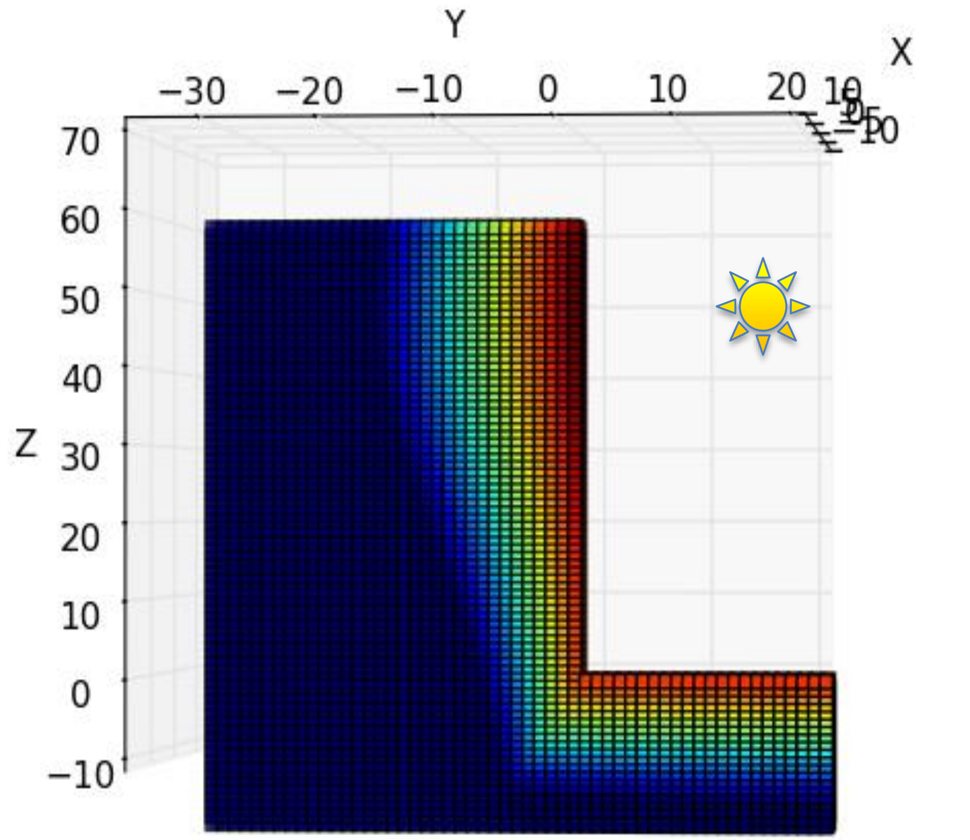
no chemical stratification

Andree-Labsch et al. 2017

Applications: KOSMA-τ 3D

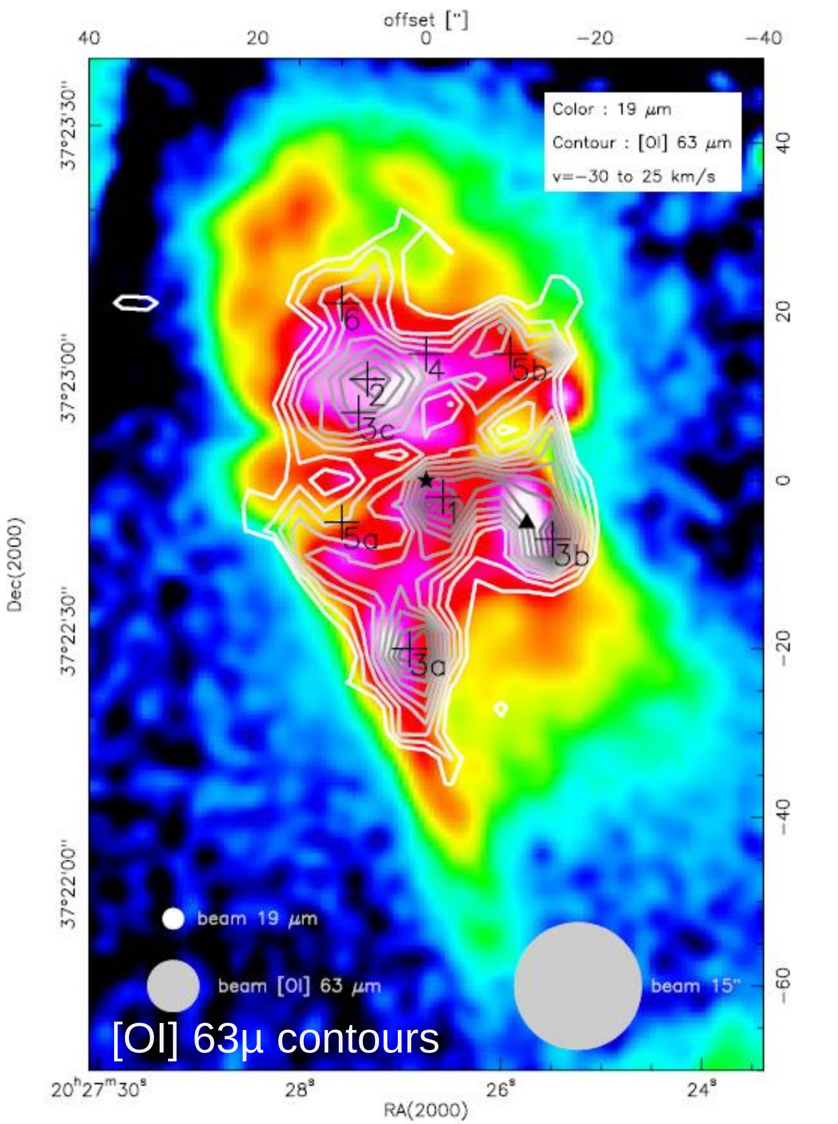
foreground absorption
by cool material in front of hot gas



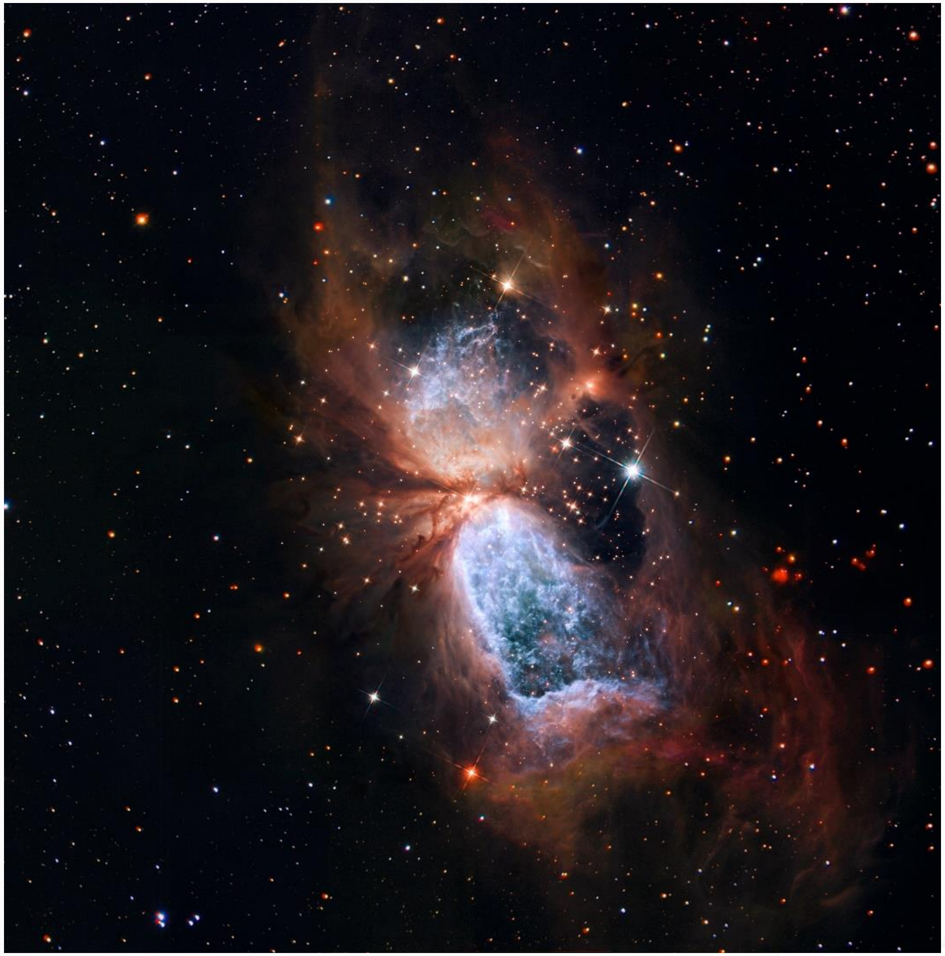


Andree-Labsch et al. 2017

S106



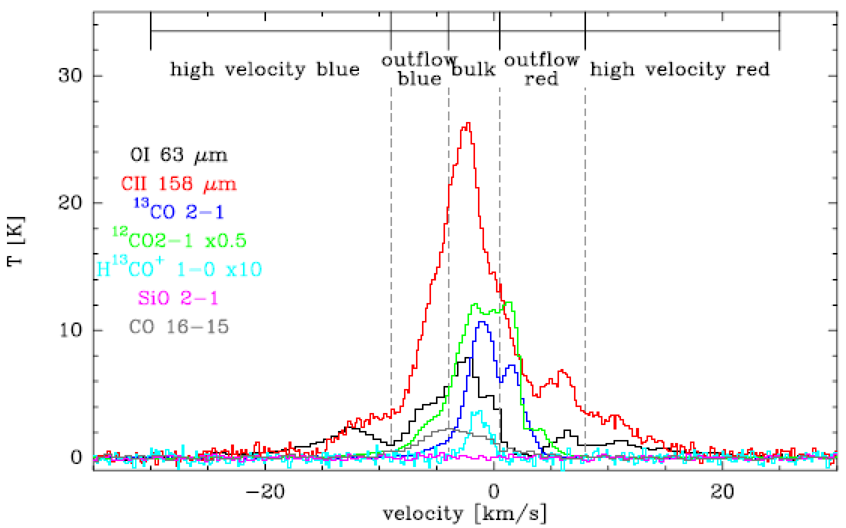
Schneider et al. 2018

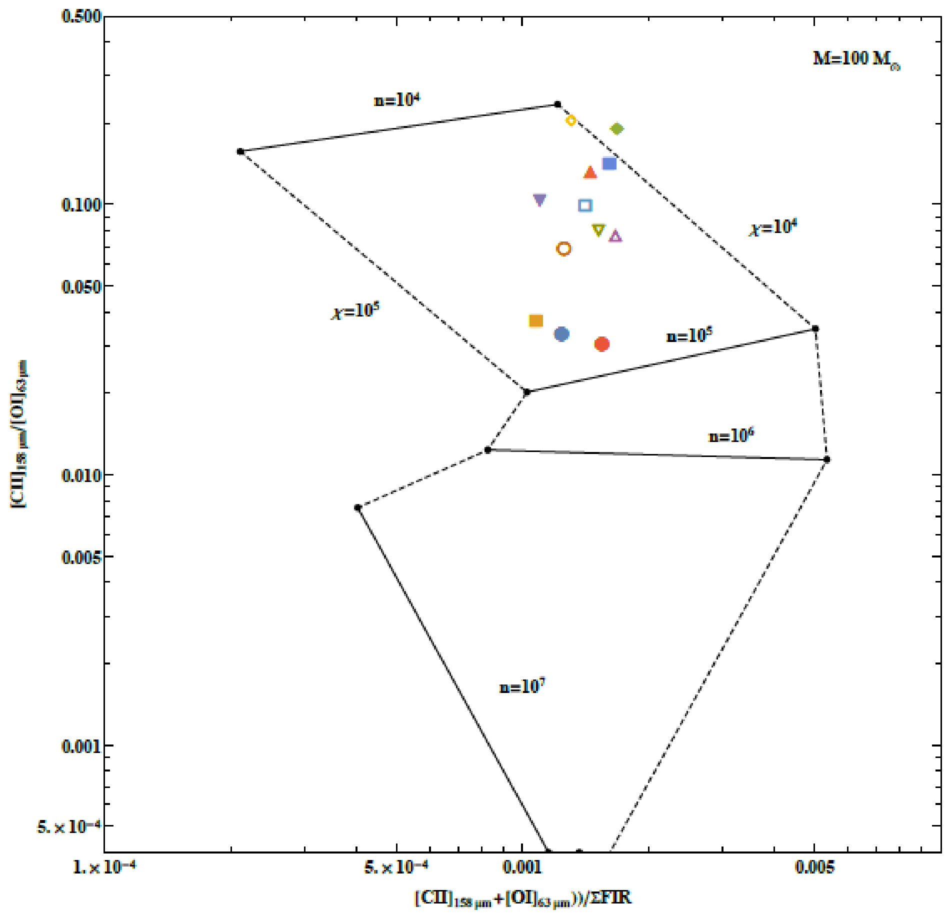


S106

High spectral resolution of (up)**GREAT on SOFIA** allows the spectral identification of various kinematic components

Tomography of 3-D structure





Schneider et al. 2018

S106

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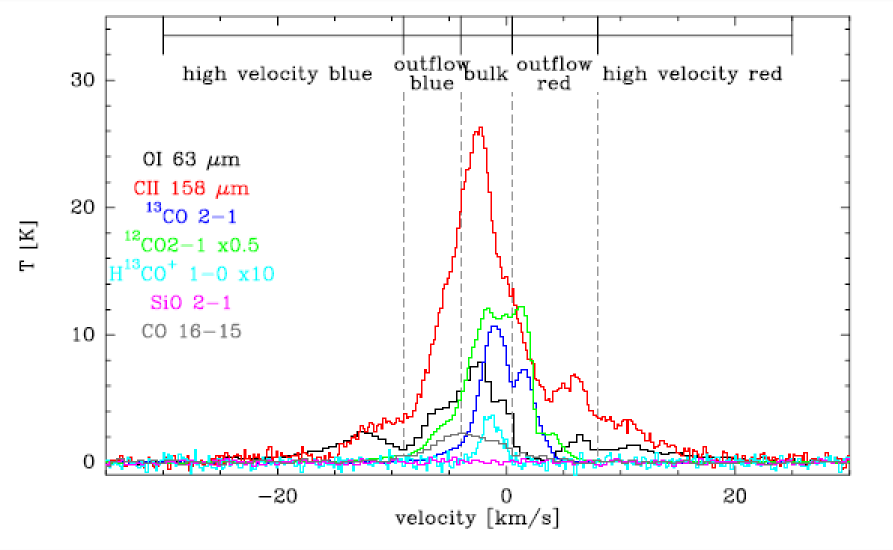
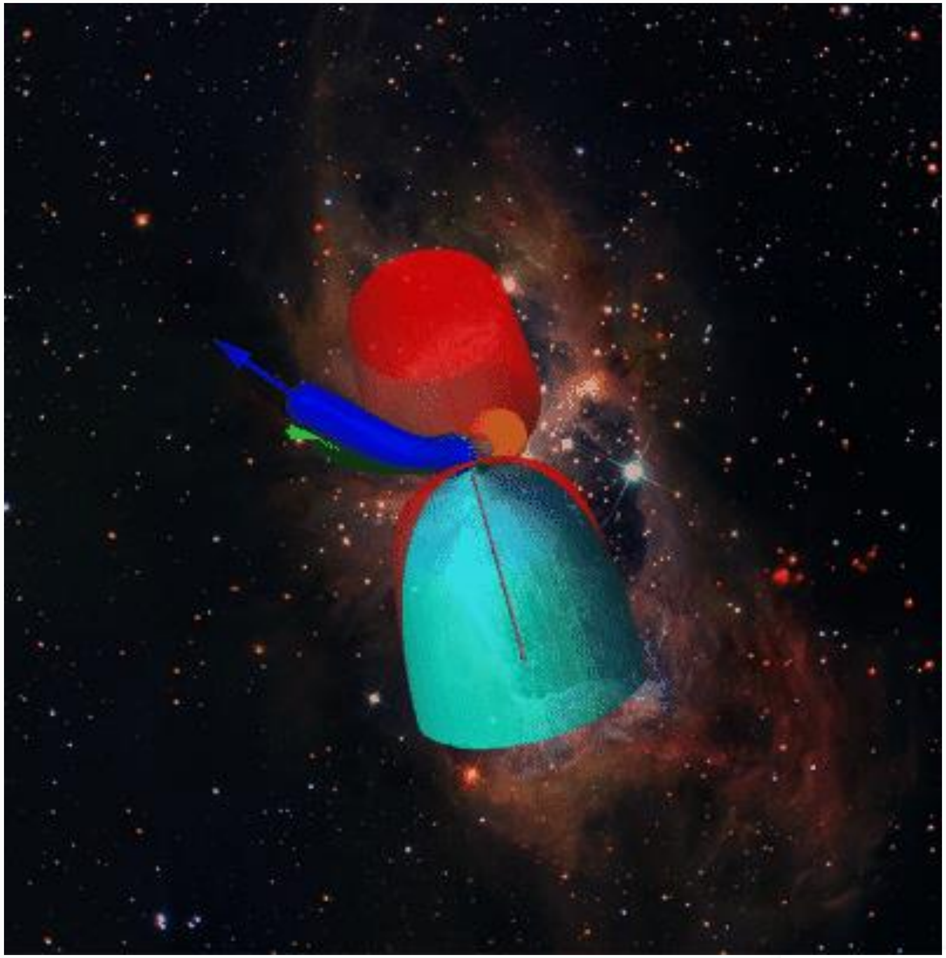
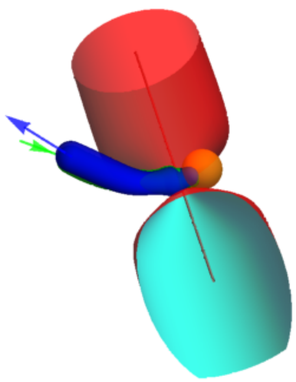
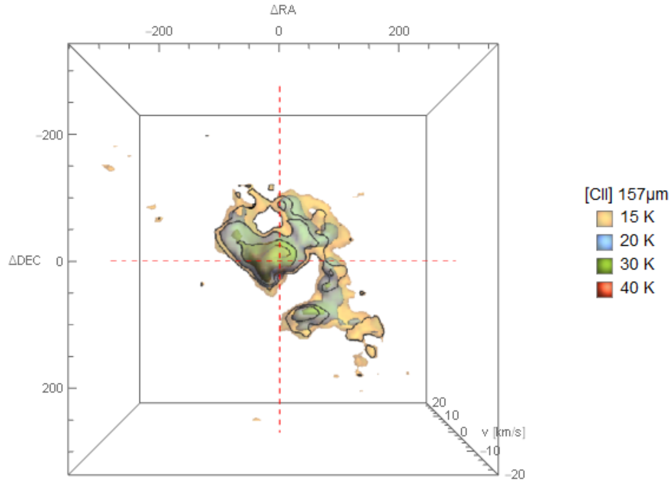


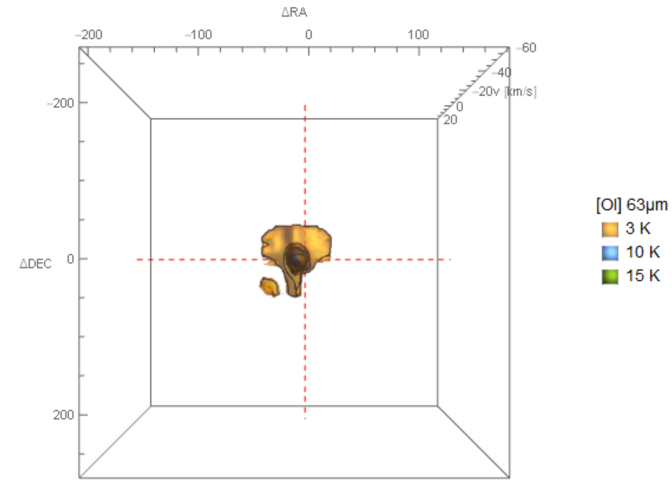


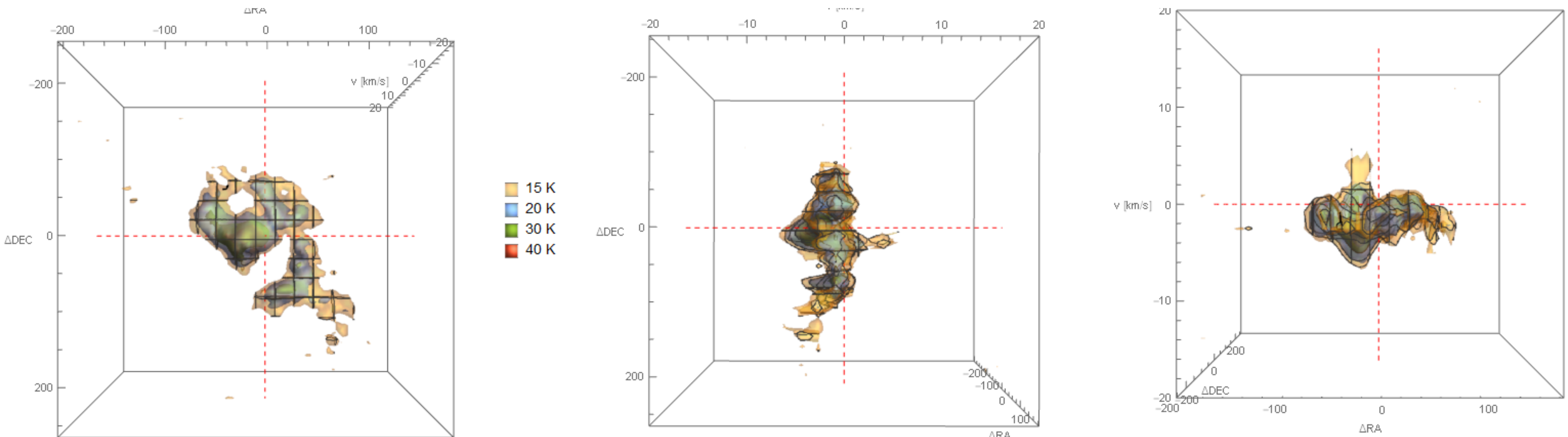
Schneider et al. 2018

[CII] and [OI] contours in (RA,Dec,v) space





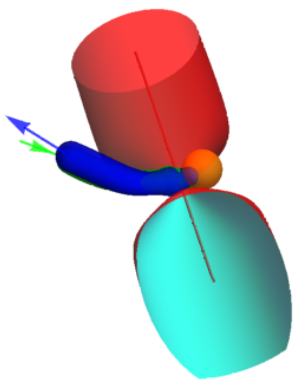


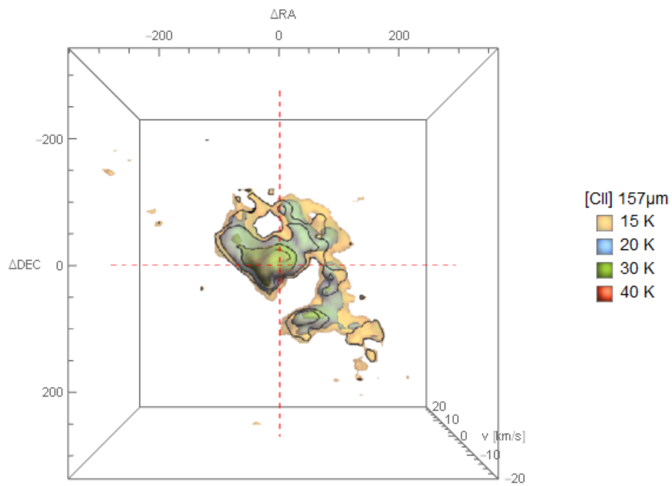


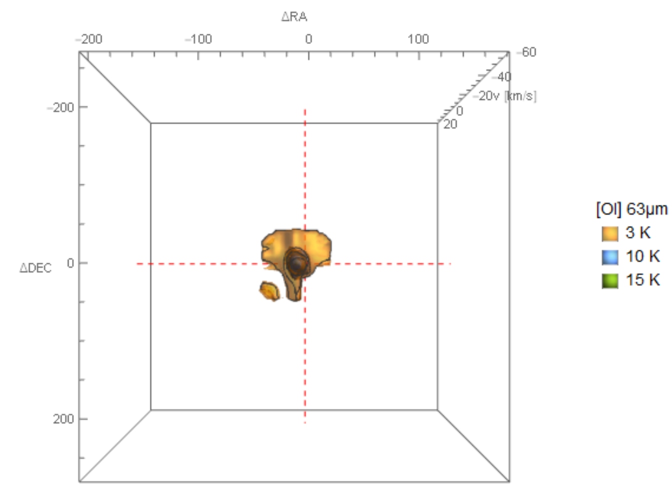
[CII] contours

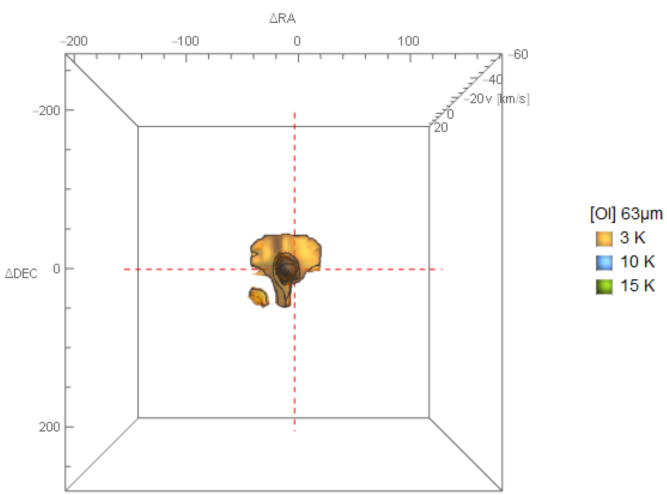
SFB 956 Cologne | Bonn

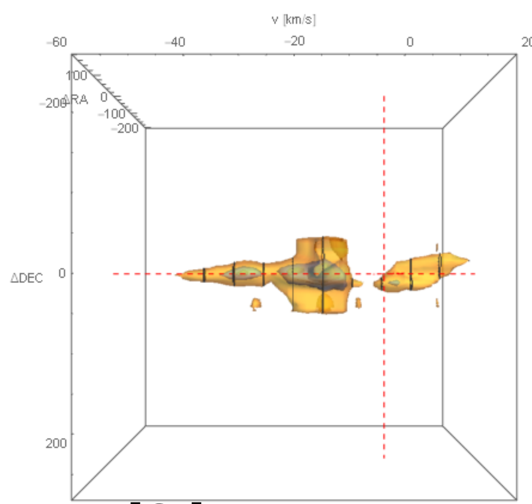
[CII] and [OI] contours in (RA,Dec,v) space

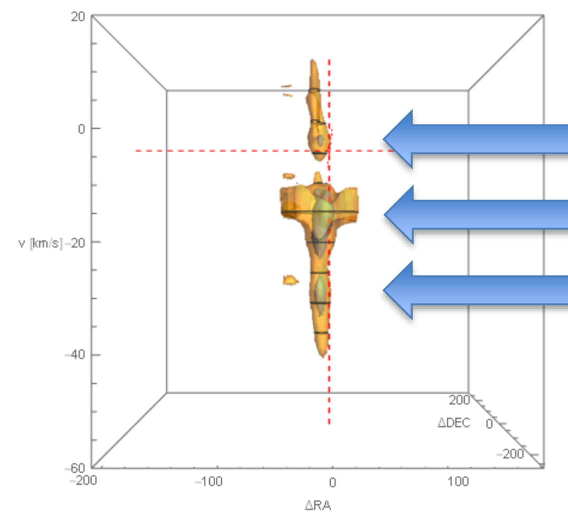




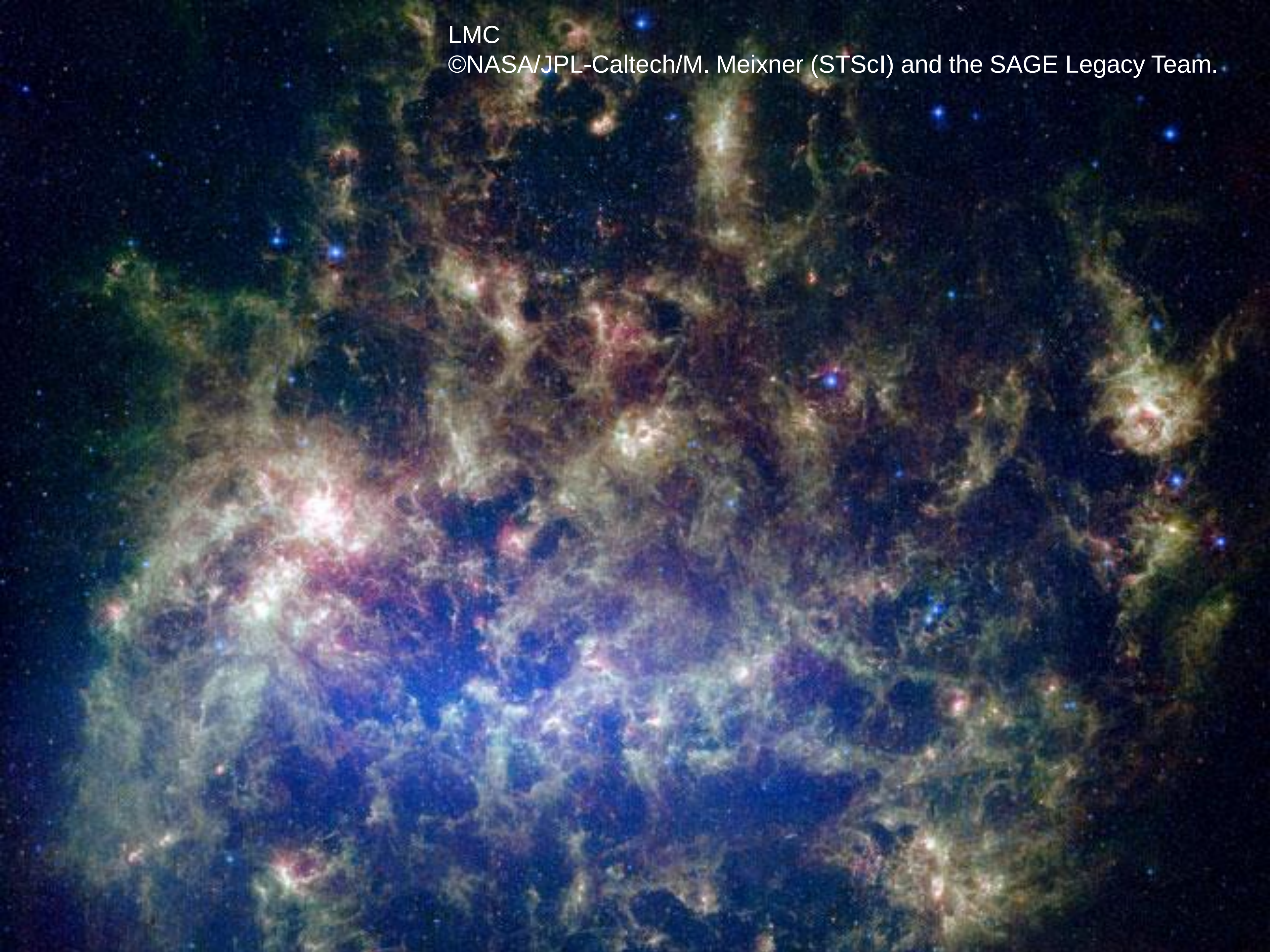








[OI] contours


LMC
©NASA/JPL-Caltech/M. Meixner (STScI) and the SAGE Legacy Team.


LMC
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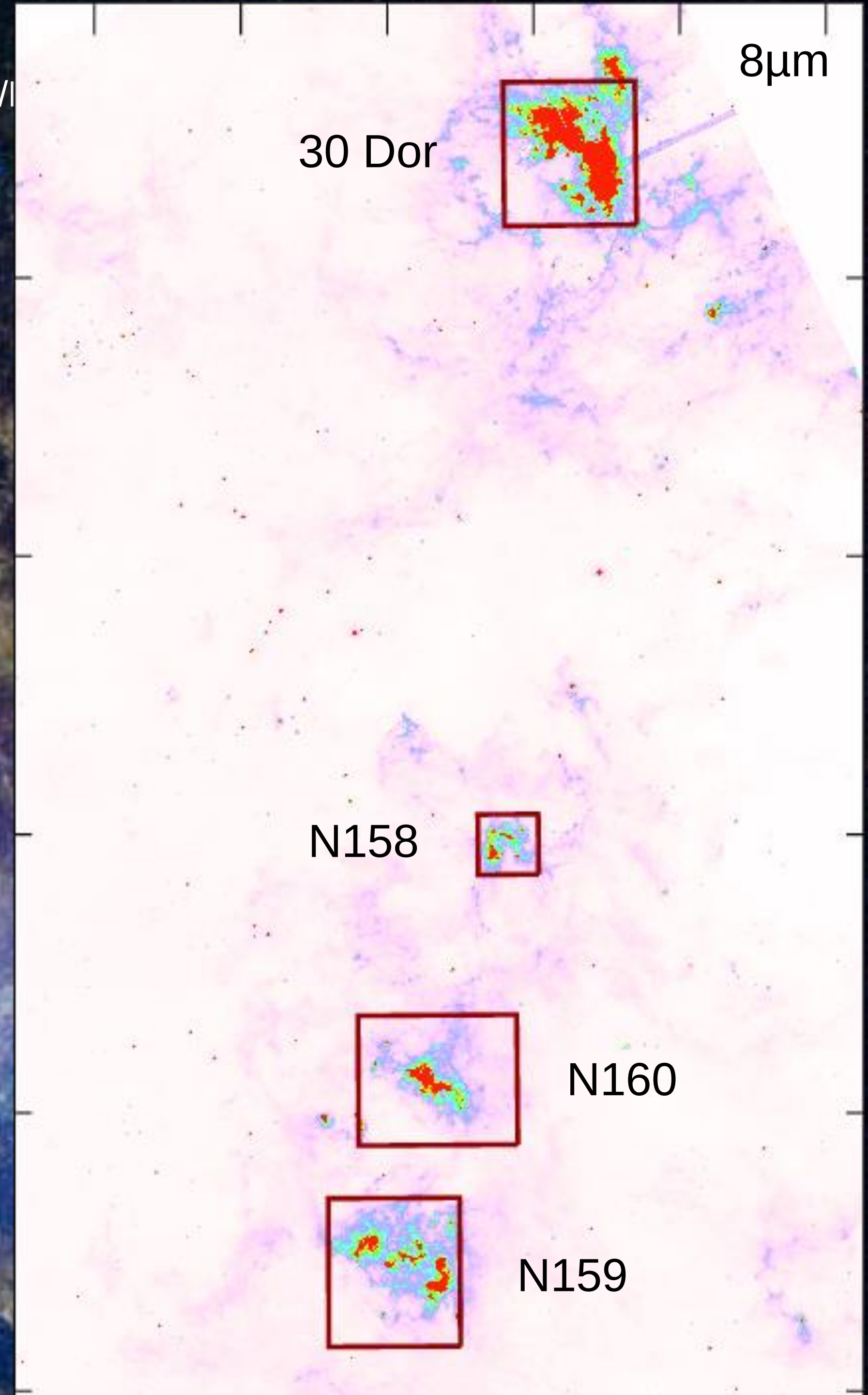
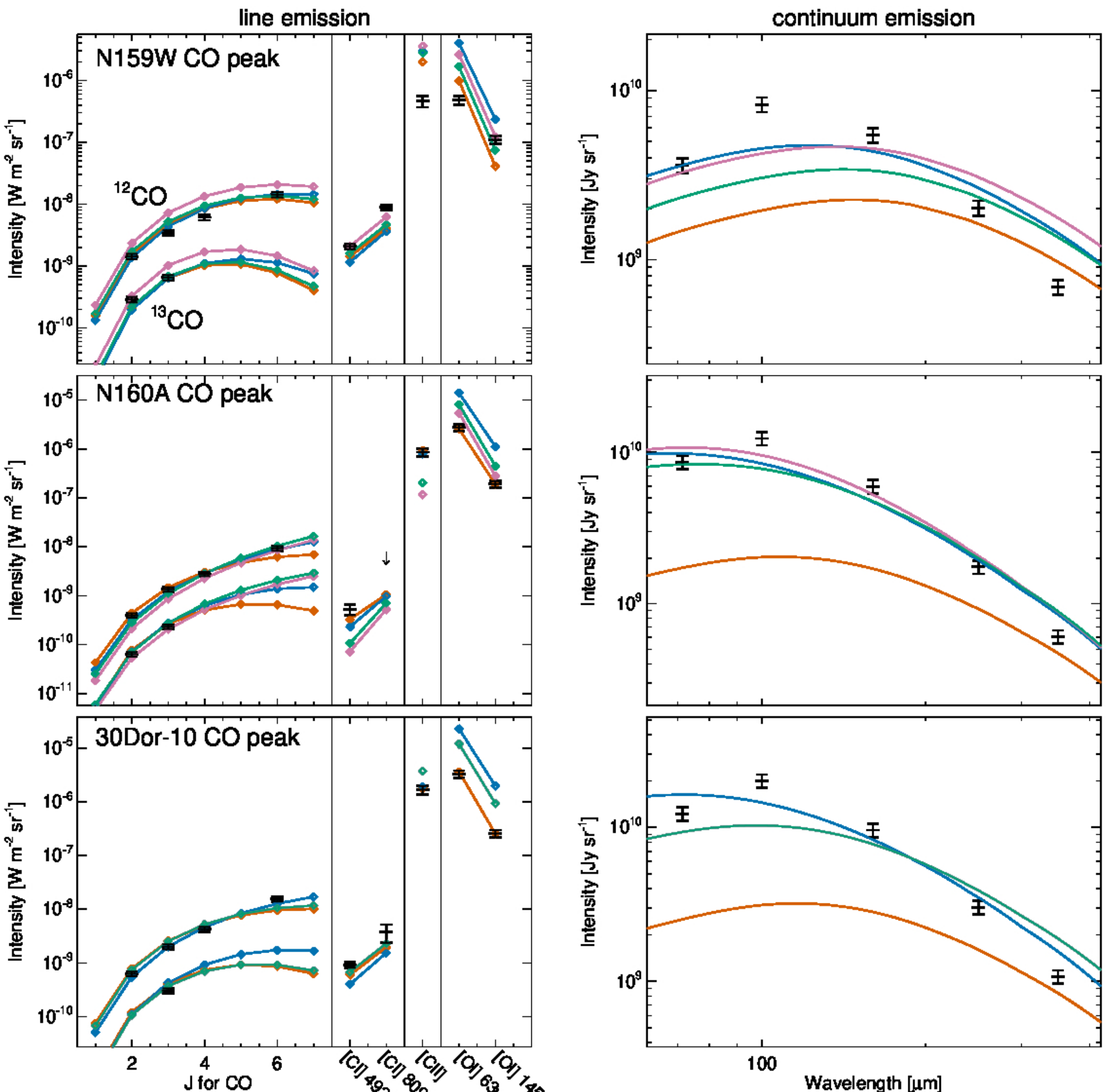
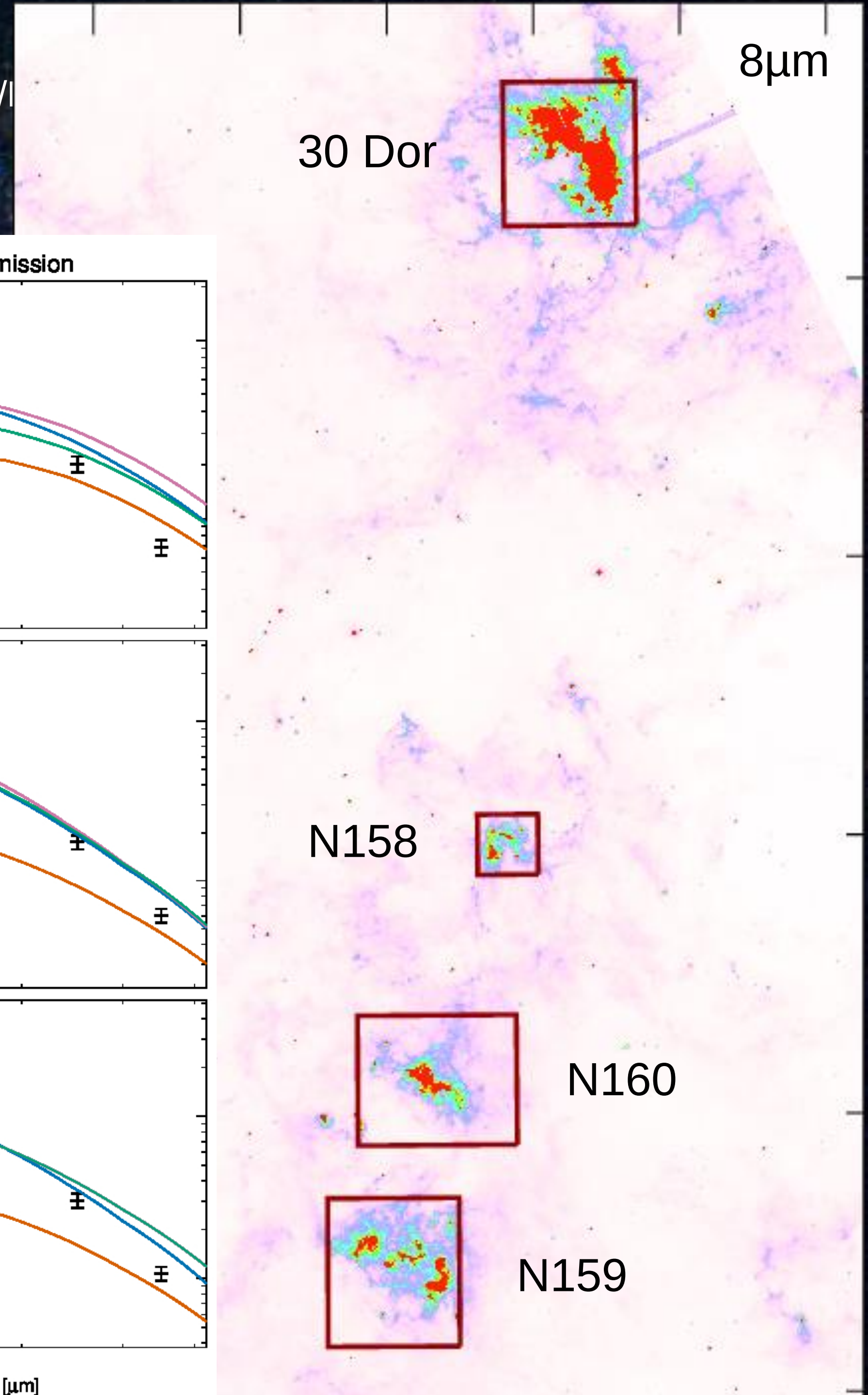

8μm
30 Dor
N158
N160
N159

LMC
©NASA/JPL-Caltech/

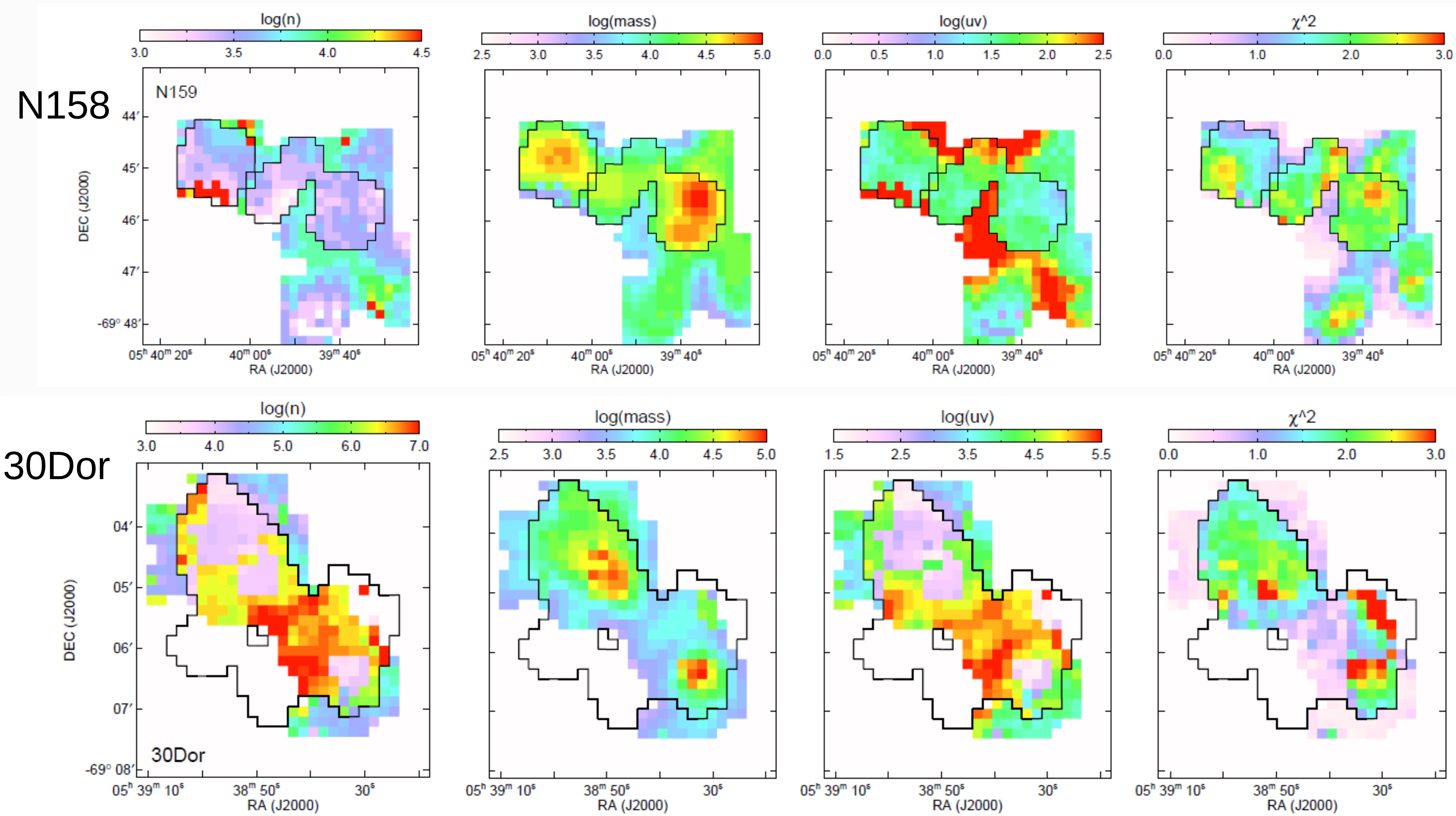
Fitting line **and** dust continuum emission





Map-based PDR Modelling

density mass UV



Current KOSMA-τ Developments

- Non-stationary PDR structure
  - t-dependent solution of chemistry (tests)
  - t-dependent parameters, e.g. FUV input
  - non-stationary particle transport , e.g. diffusion, advection, mass evaporation (PhD project A. Baby)
- KOSMA-τ 3D
  - inclusion of systematic velocities
  - full line & continuum radiative transfer (PhD projects C. Bruckmann & C. Yanitski)
  - performance improvements
- Microphysics/chemistry
  - chemical heating (tests)
  - surface chemistry (done)
  - full H2 excitation
    - IR quadrupole emission
    - UV fluorescent line emission
    - UV continuum emission
  - detailed PE heating
  - non-stationary PE heating
- Misc
  - Migration to modern FORTRAN standards
  - Coupling to MHD
  - stability improvements

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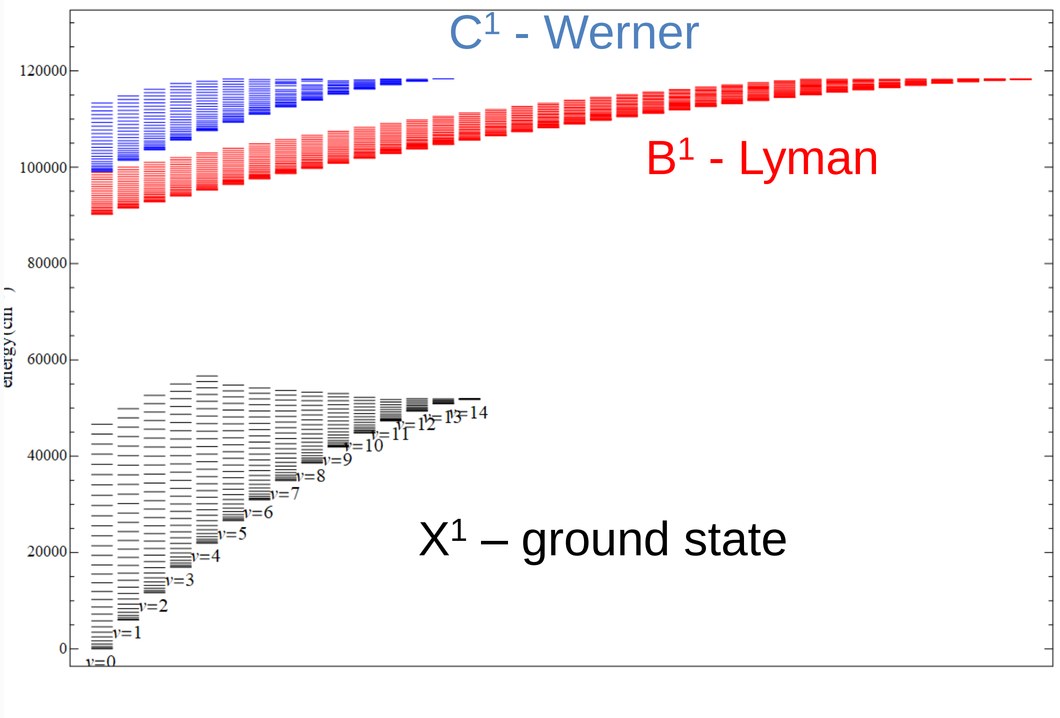
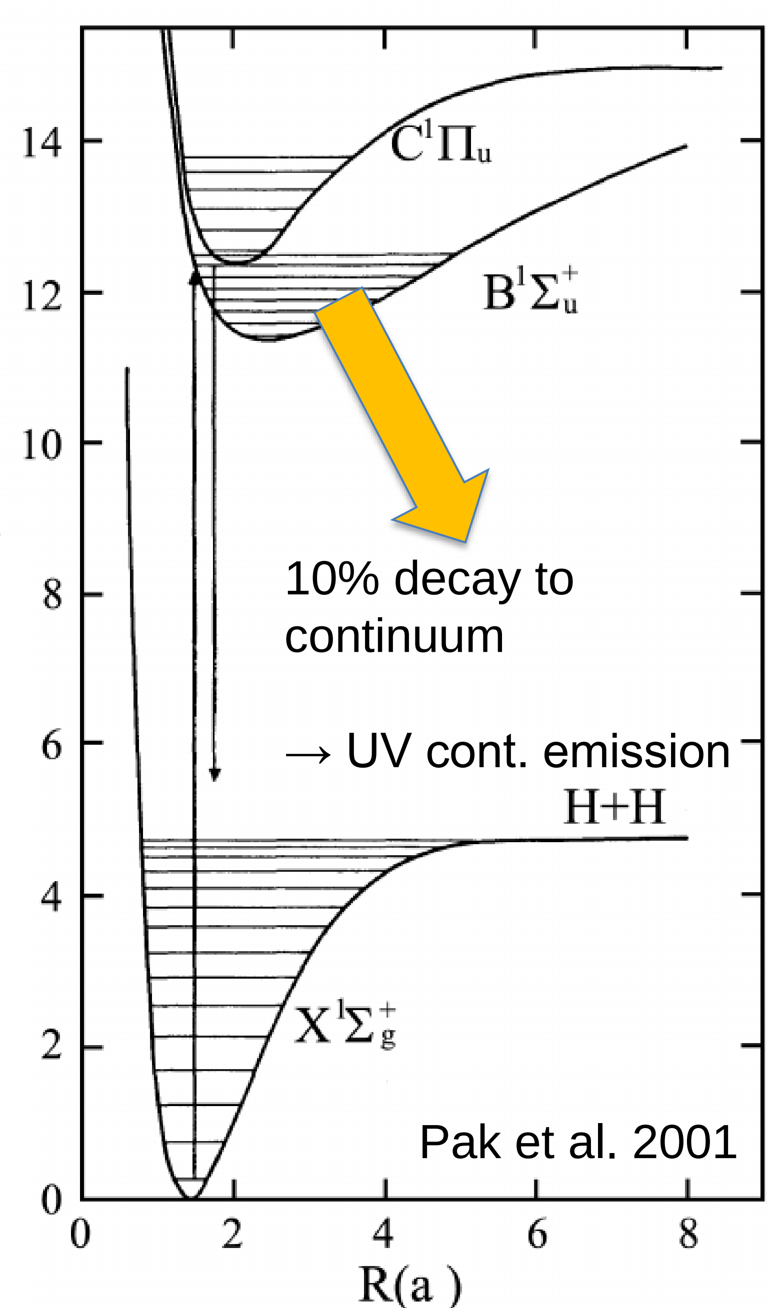
H_2 Excitation Problem

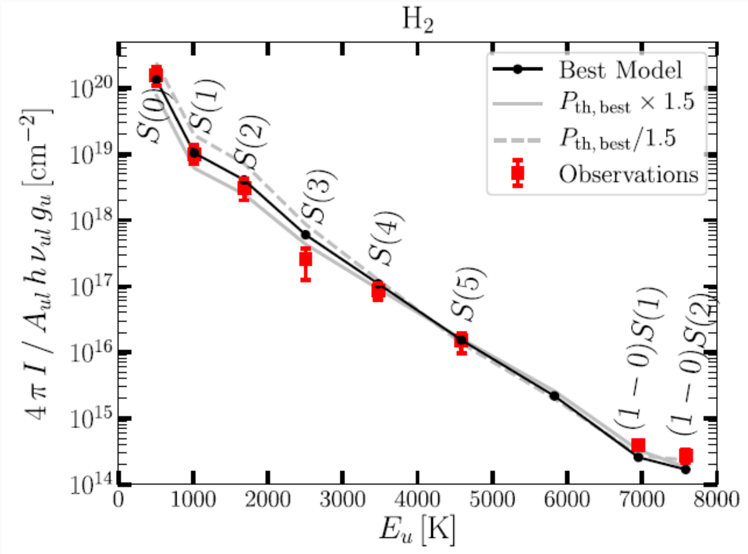
- H_2 dissociation via UV line absorption
- about 5000 quadrupole transitions
- about 15000 X-B and X-C dipole transitions



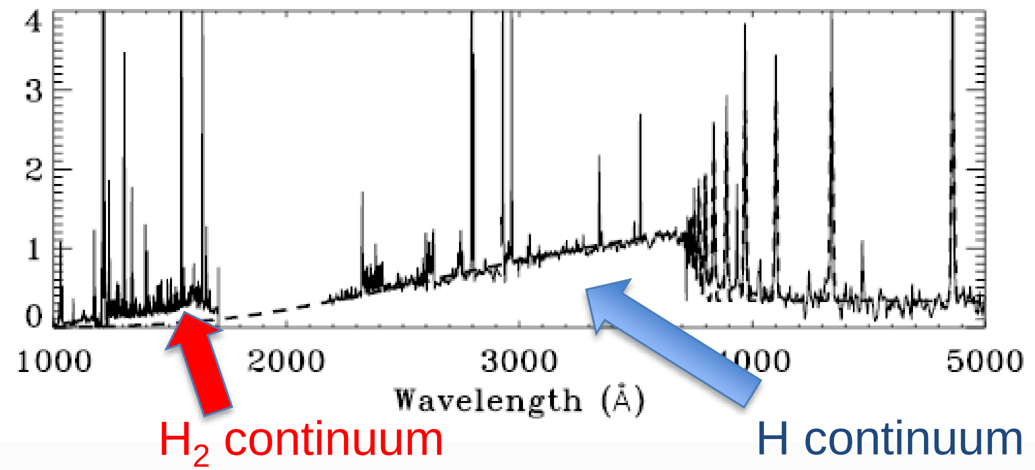


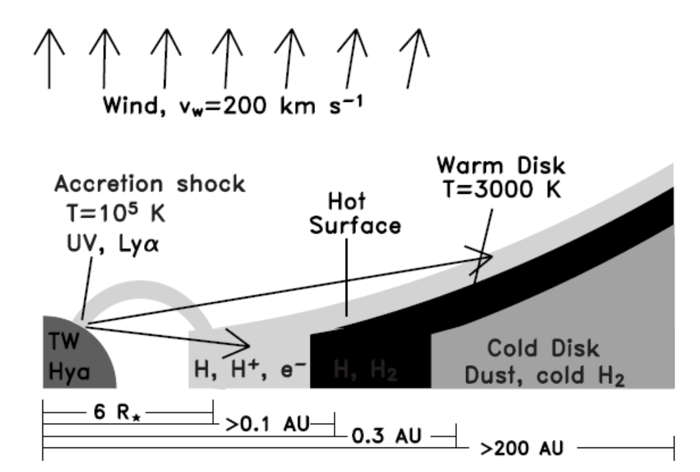
H_2 excitation problem

H_2 IR emission from PDRs
Joblin et al. 2018,
Habart et al. 2011



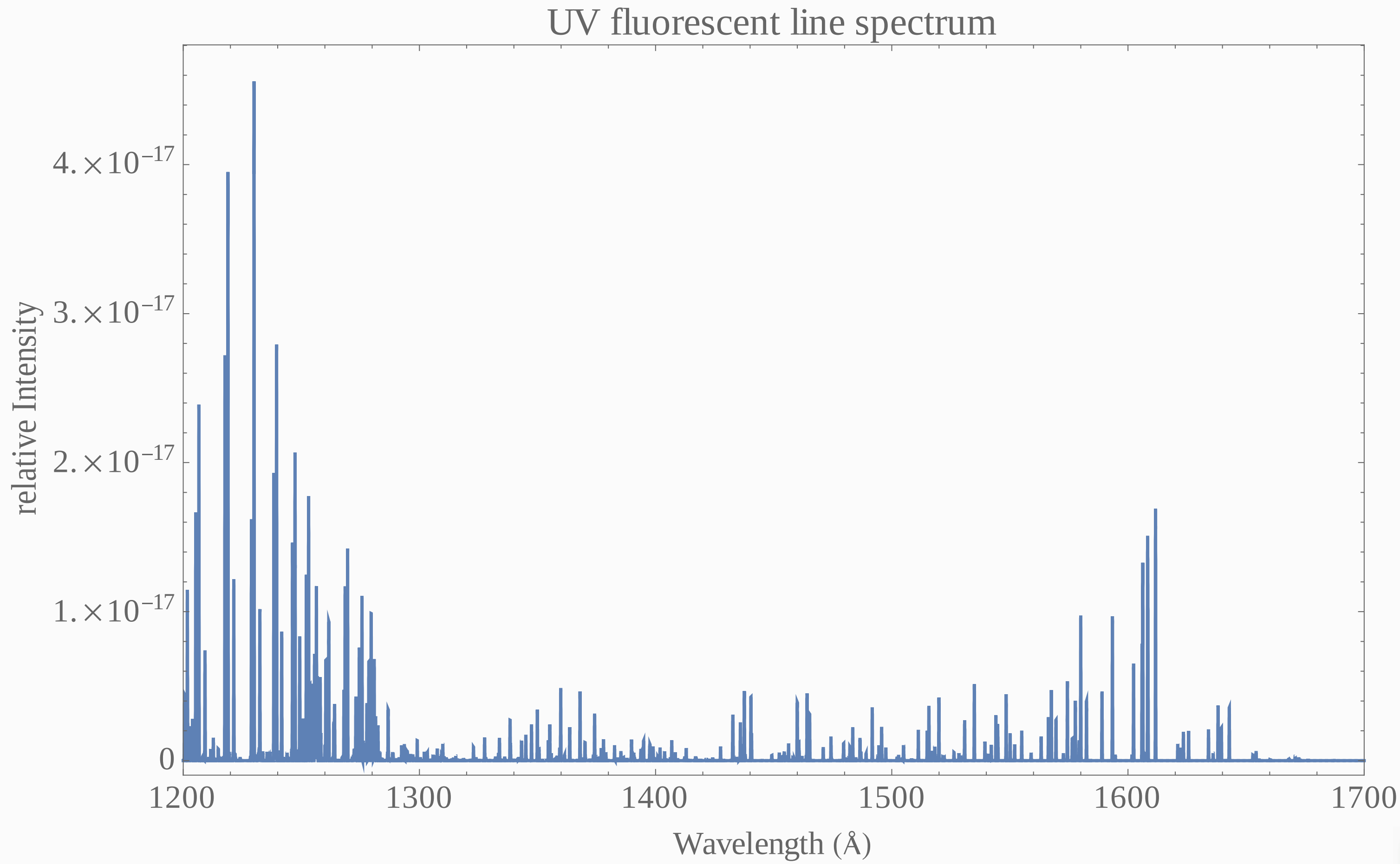
TW Hya spectrum, Herczeg et al. 2004



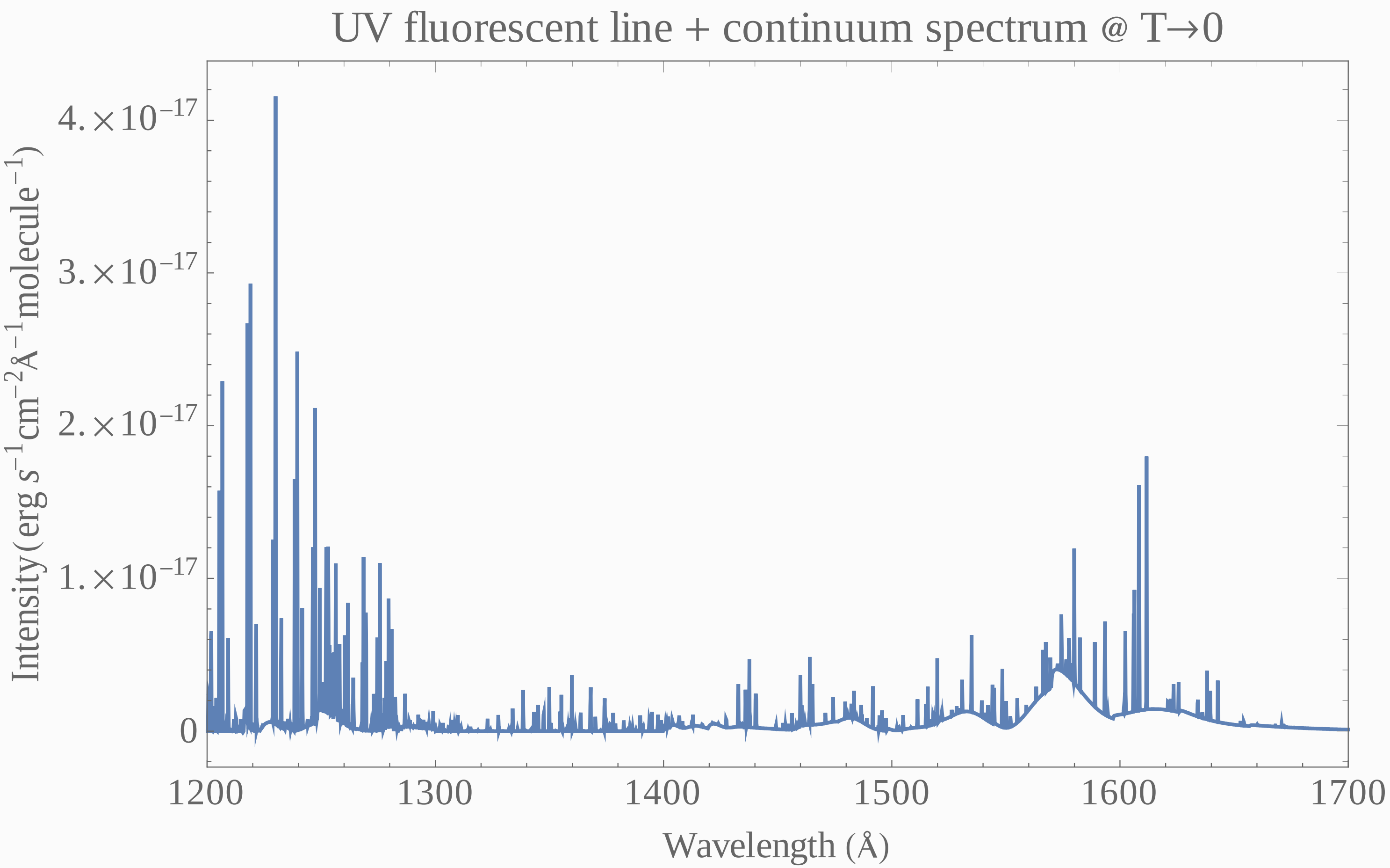


Preparing for JWST!

Fluorescent UV spectrum of H_2



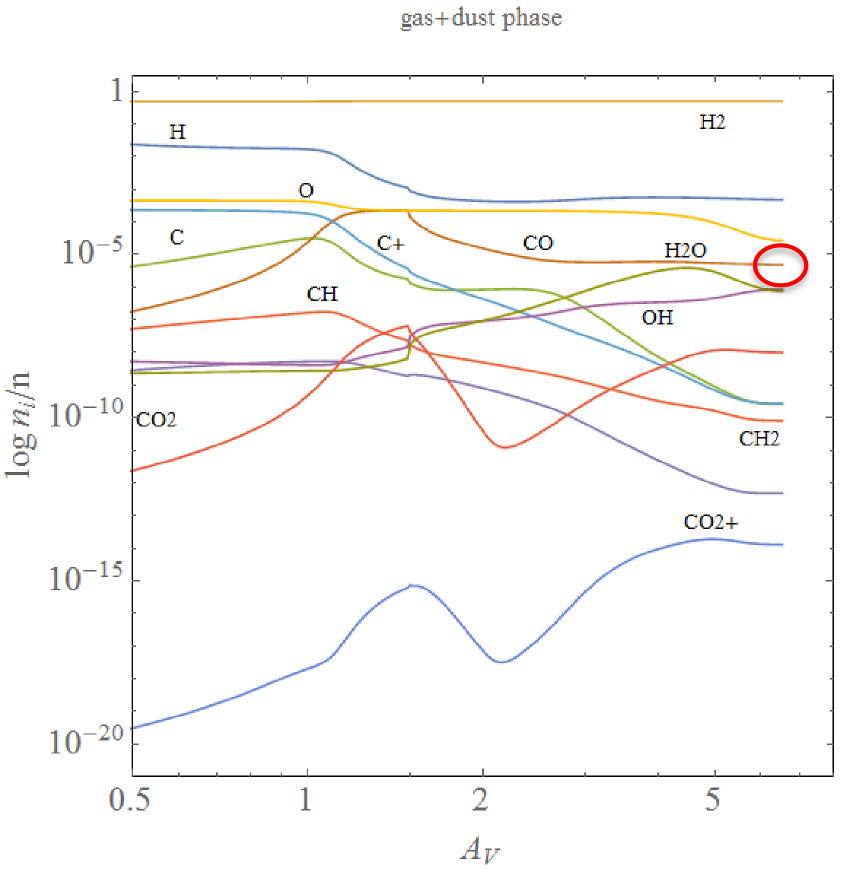
Fluorescent UV spectrum of H_2 + cont.

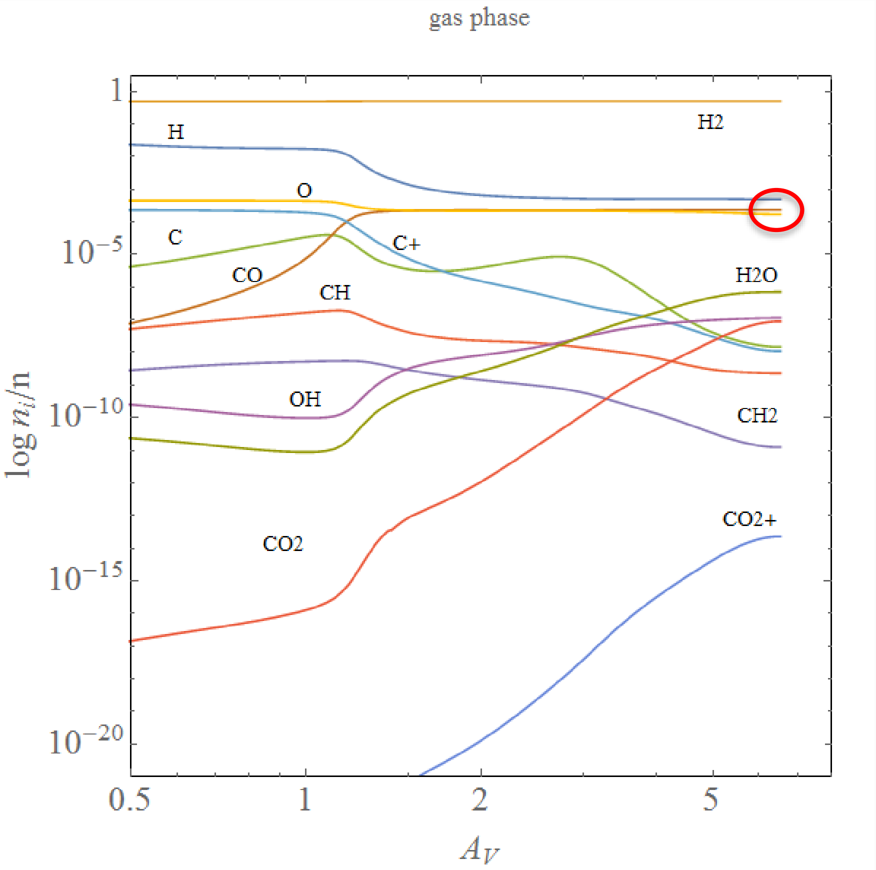


Thank you for the invitation!

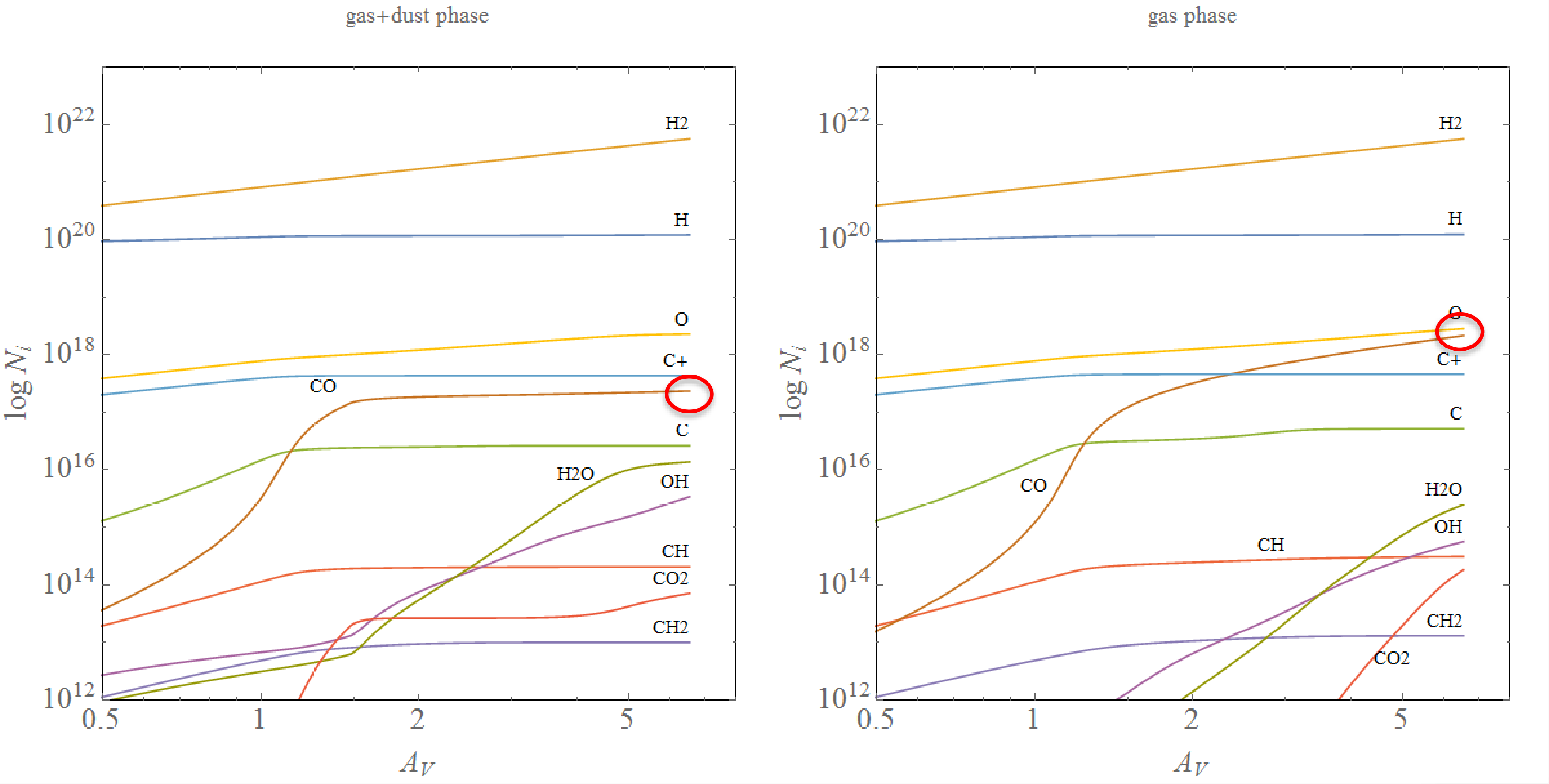
Thank you for your attention!

Density is no observable





Column density is no observable



Line intensities are observed

gas+dust phase

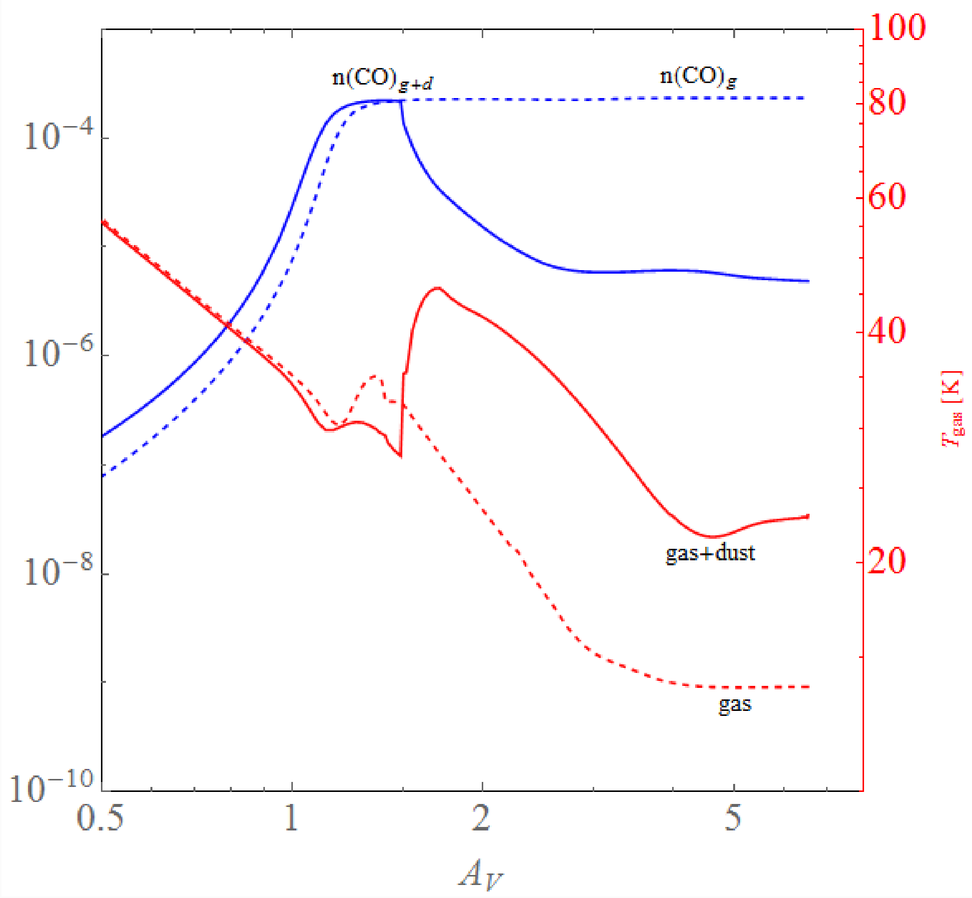
Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	5.8
CO J=2-1	7.3
CO J=3-2	4.3
CO J=4-3	1.4
[CII] 158µm	2.3
[CI] 609 µm	8.7
[CI] 370µm	2.3

gas phase

Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	0.66
CO J=2-1	0.55
CO J=3-2	0.14
CO J=4-3	0.016
[CII] 158µm	2.1
[CI] 609 µm	9.5
[CI] 370µm	2.6

lower column densities
higher intensities !

Excitation matters



gas cooling is significantly reduced in the absence of CO

→ gas temperatur increases