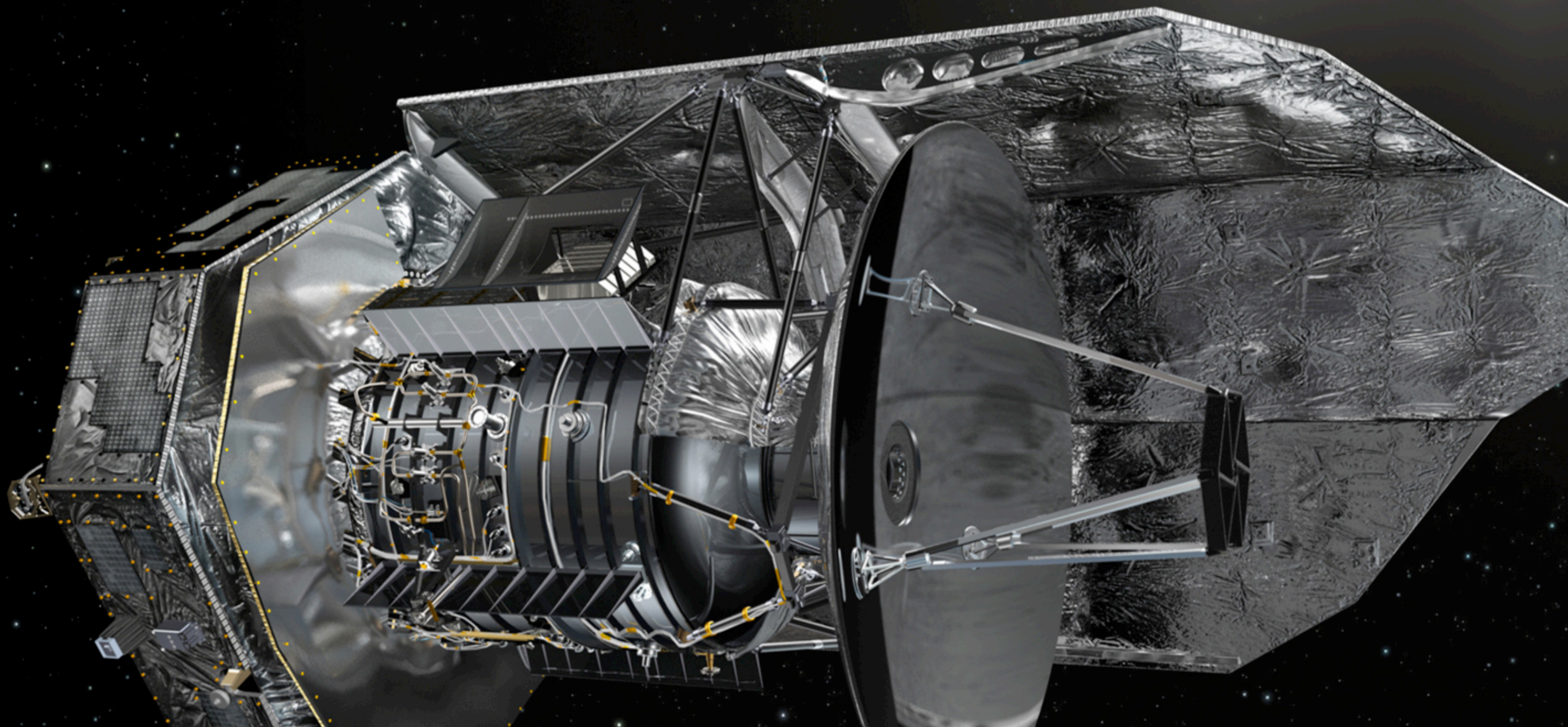
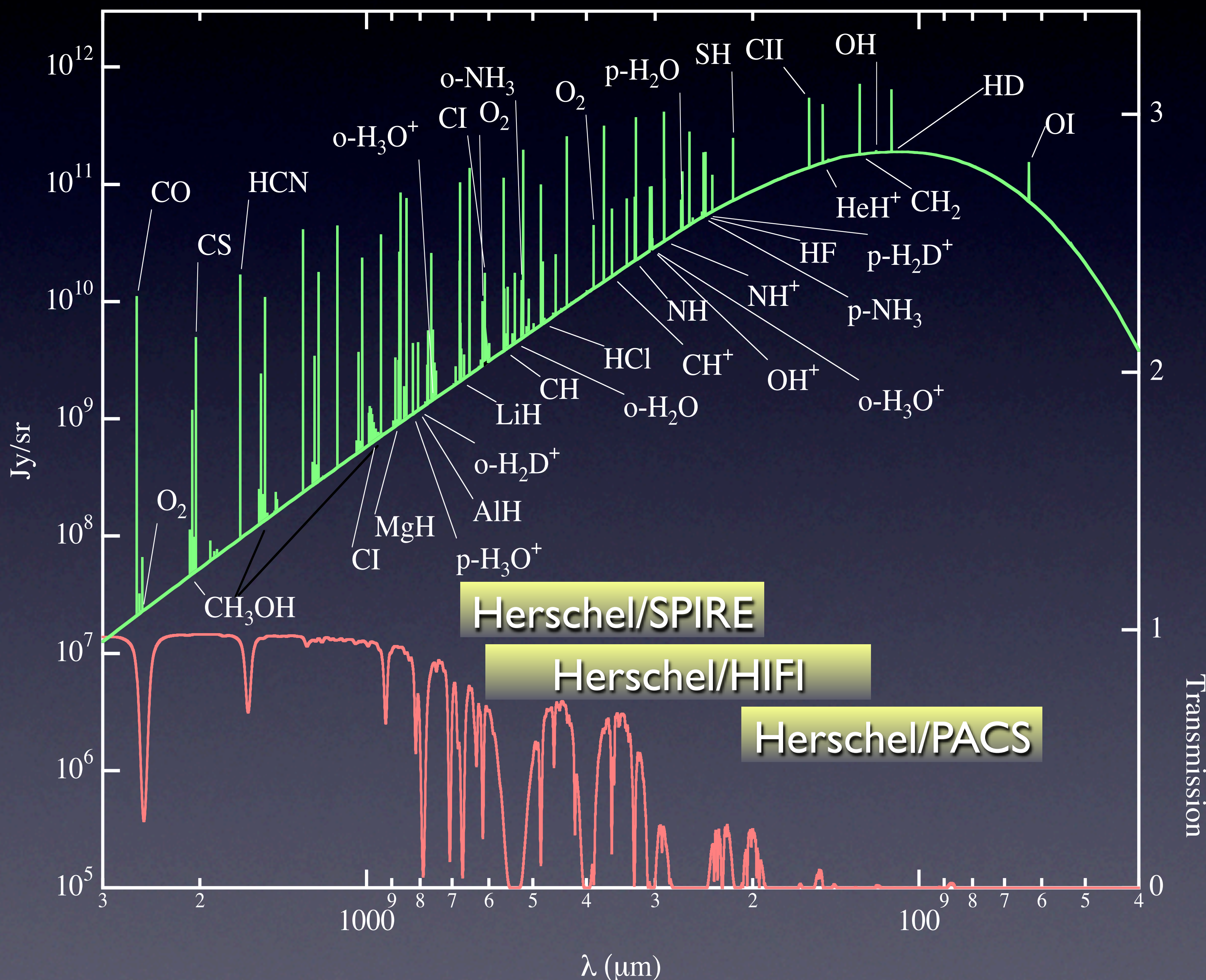
# Spectroscopy and Astrochemistry with Herschel



Darek Lis (Caltech)

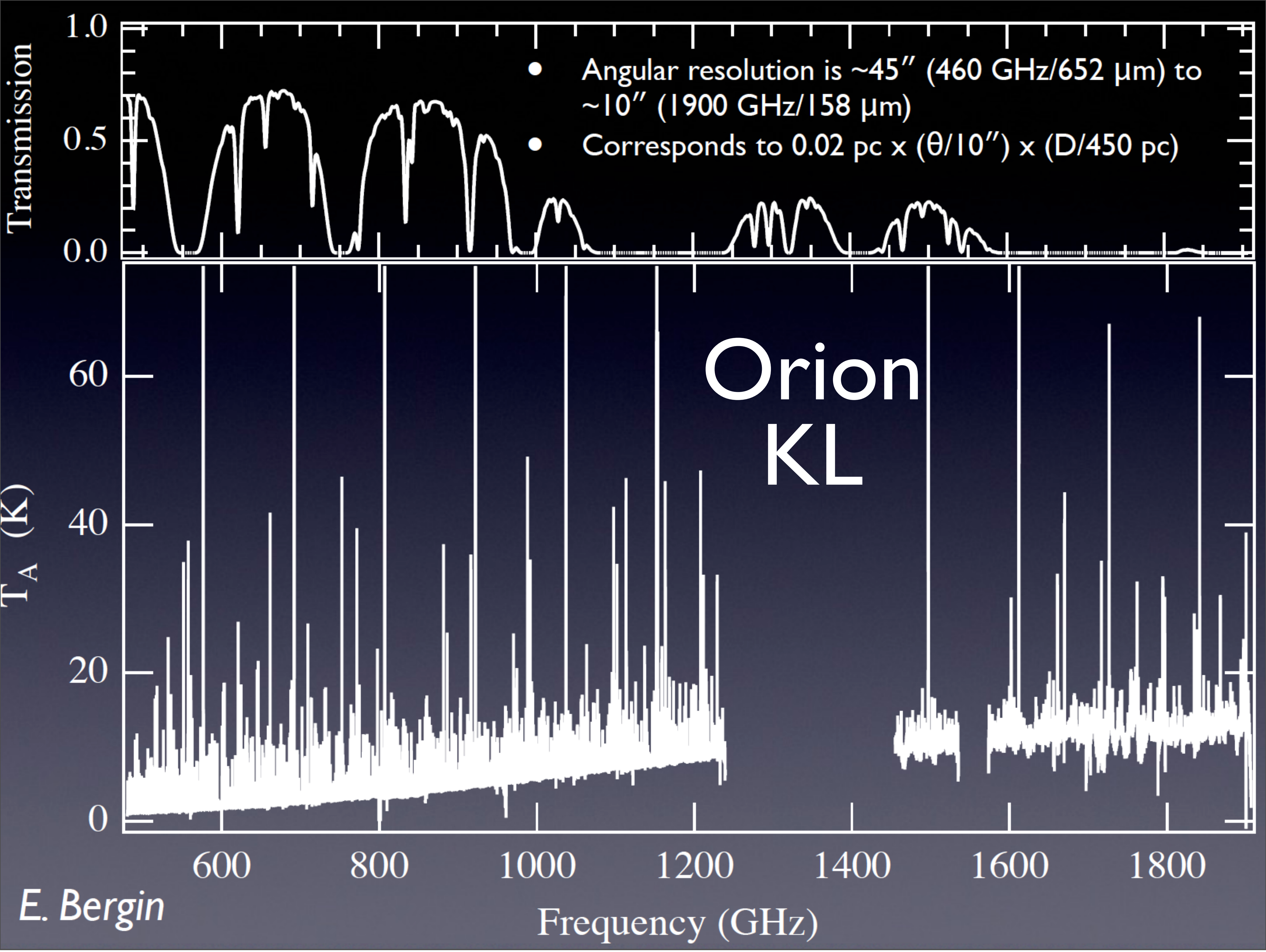
*Pasadena, August 26, 2013*

# Talk Outline



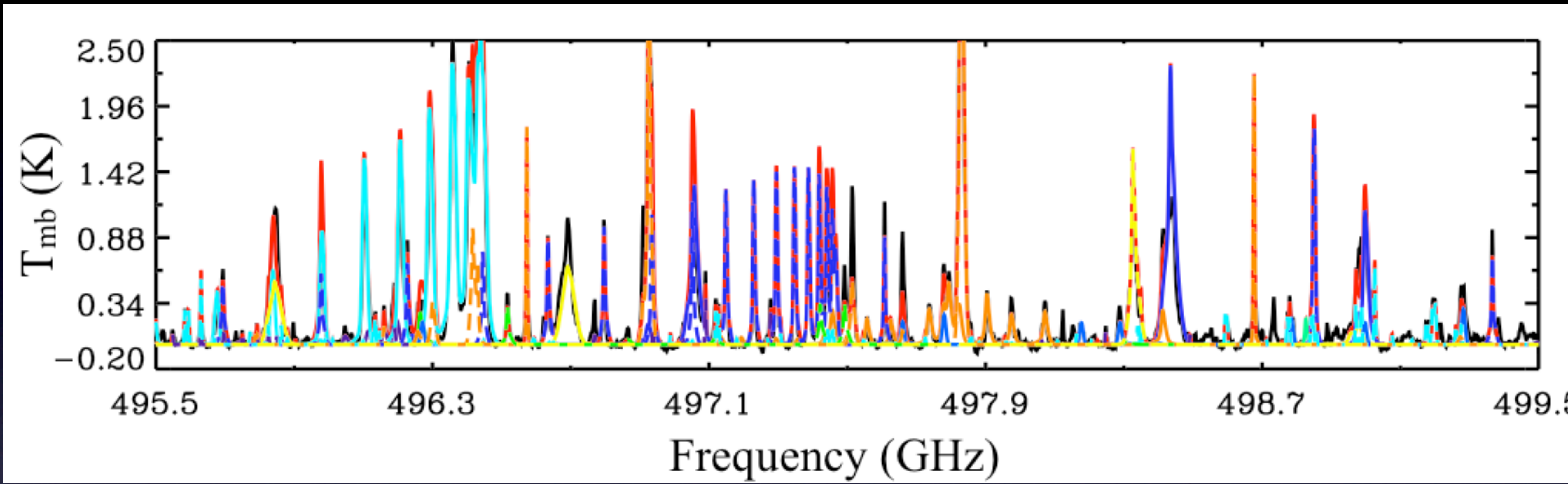

*E. Bergin*

- Goal: give a flavor of Herschel spectroscopic capabilities and the kind of spectroscopic data that can be found in the archive
- Focus on recent results (mostly 2012-13)
- Will cover a wide range of interstellar environments, from diffuse to dense galactic clouds, to ISM in nearby galaxies
- Spectral line surveys
- Water in cold environments
- PACS/SPIRE spectroscopy: Orion Bar and Sgr A*
- Absorption spectroscopy, new species: $H_2Cl^+$, $HCl^+$
- Formation pumping: $H_3O^+$
- PACS and SPIRE observations of nearby galaxies



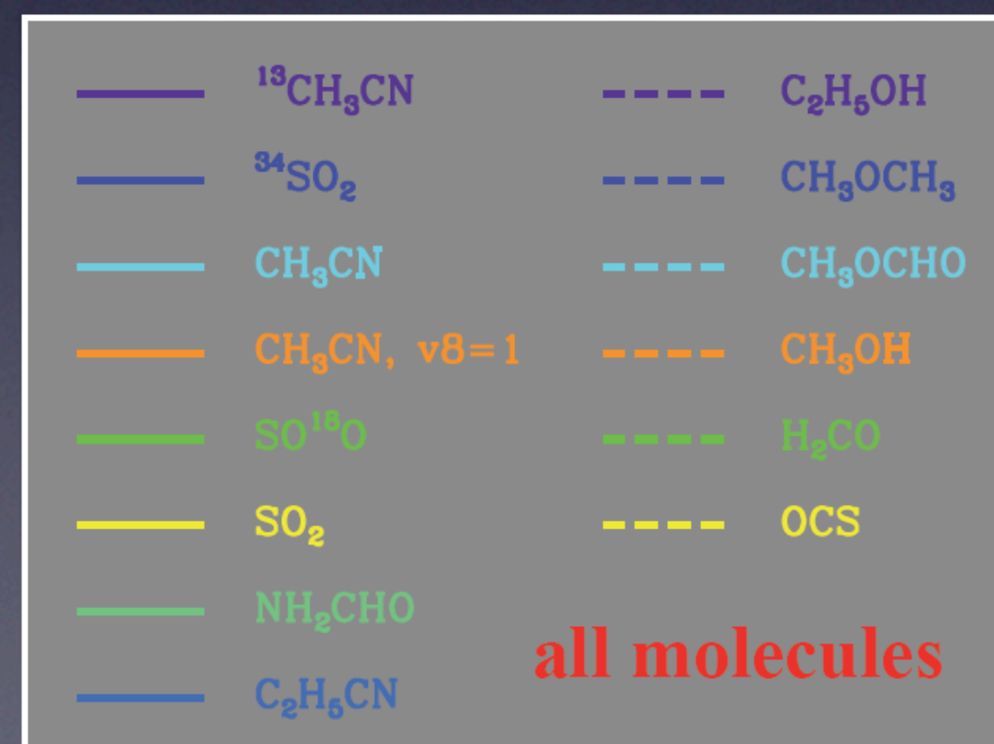
Angular resolution is ~45″ (460 GHz/652 μm) to ~10″ (1900 GHz/158 μm)
Corresponds to 0.02 pc x (θ/10″) x (D/450 pc)
Transmission
1.0
0.5
0.0
Orion KL
$T_A$ (K)
60
40
20
0
600
800
1000
1200
1400
1600
1800
Frequency (GHz)
E. Bergin

# Orion KL Full Band Analysis

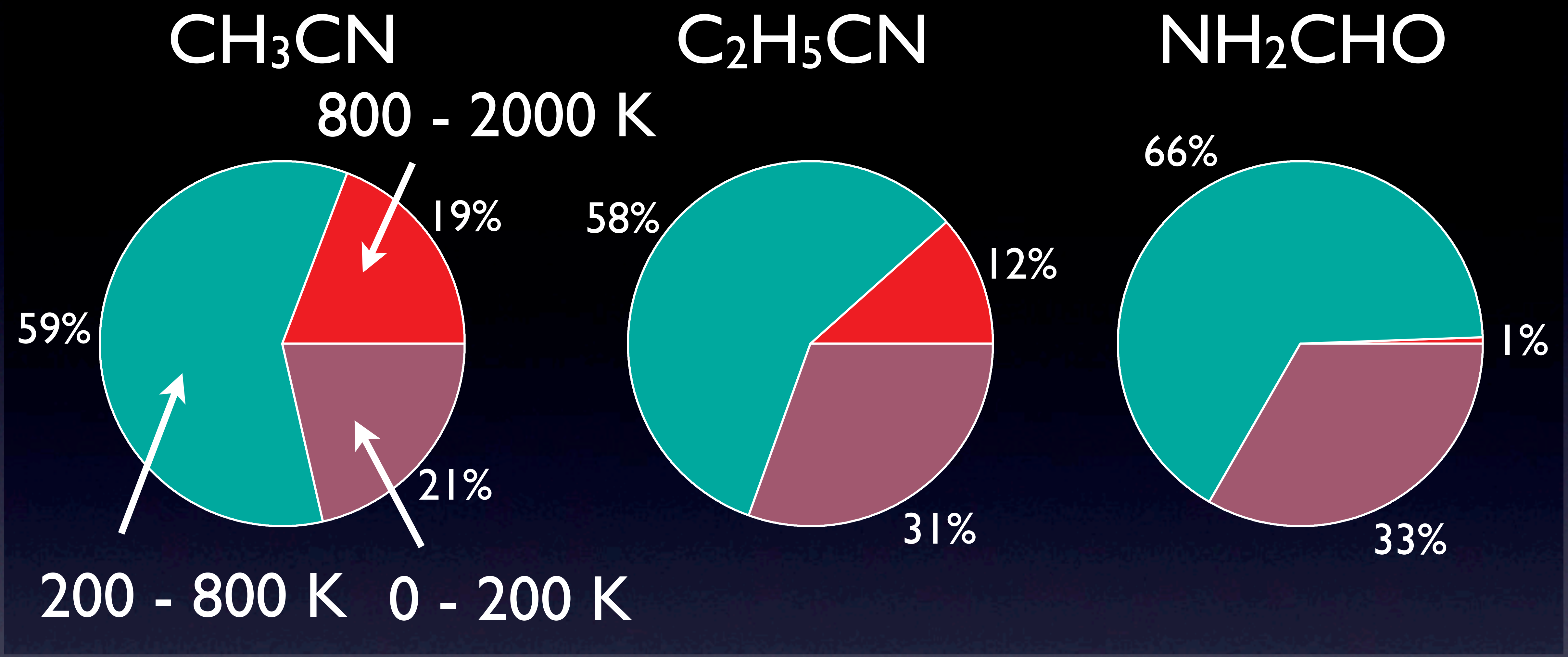



- One million independent data channels
- Over 60 species, including isotopologues, modeled by a team of ~20 people
- From residual fit: ~2500 U-lines out of 20,000 (~10%)

*N. Crockett*



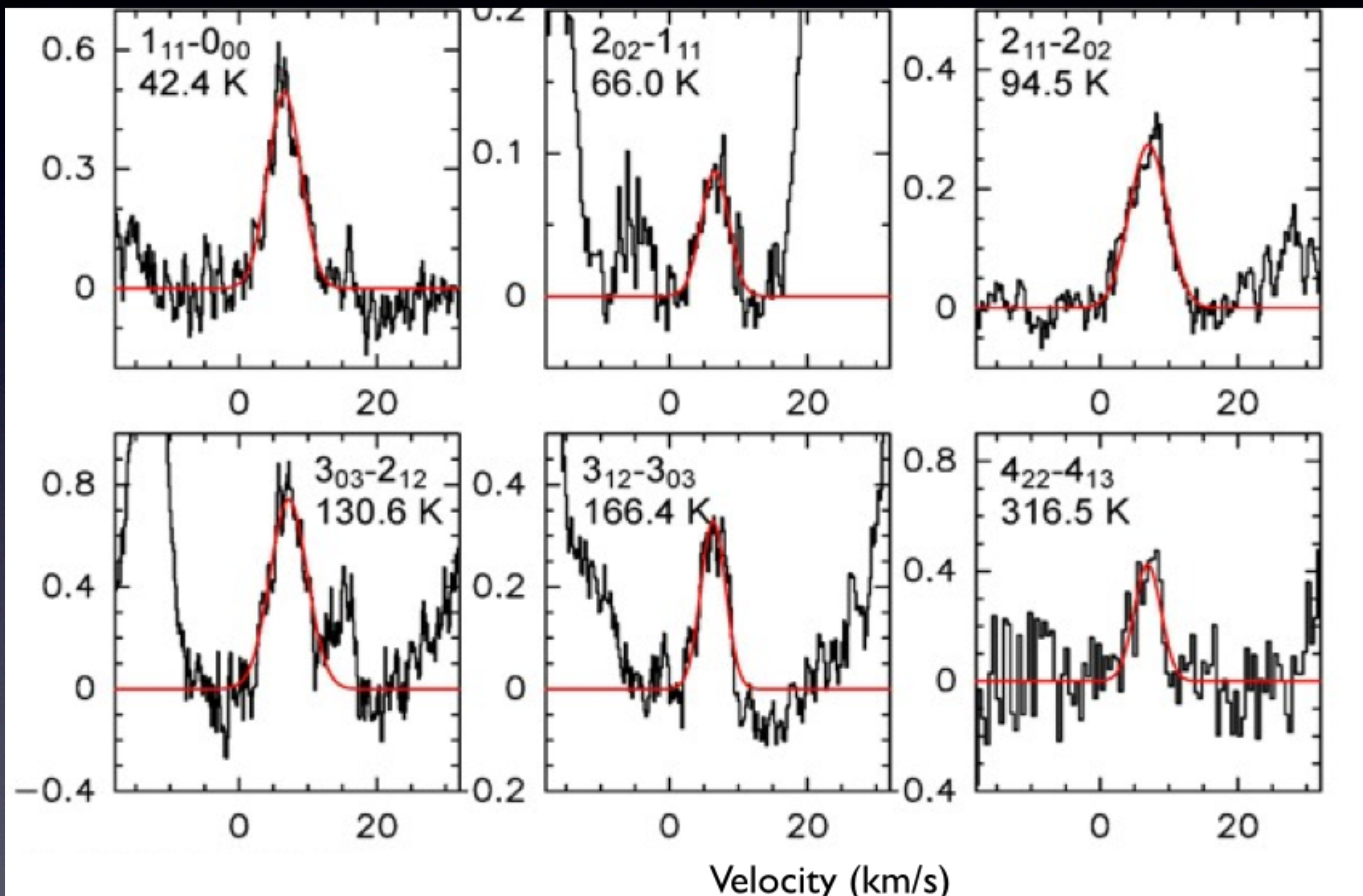
# Orion KL Organics




- LTE approximation generally works well for hot cores, can constrain excitation
- Column densities and abundances well determined—*assuming a source size*
- Methyl and ethyl cyanide show significant emission from energy levels > 800 K
- Harder to evaporate off the grains?
- Compare with models of organic synthesis

*N. Crockett*

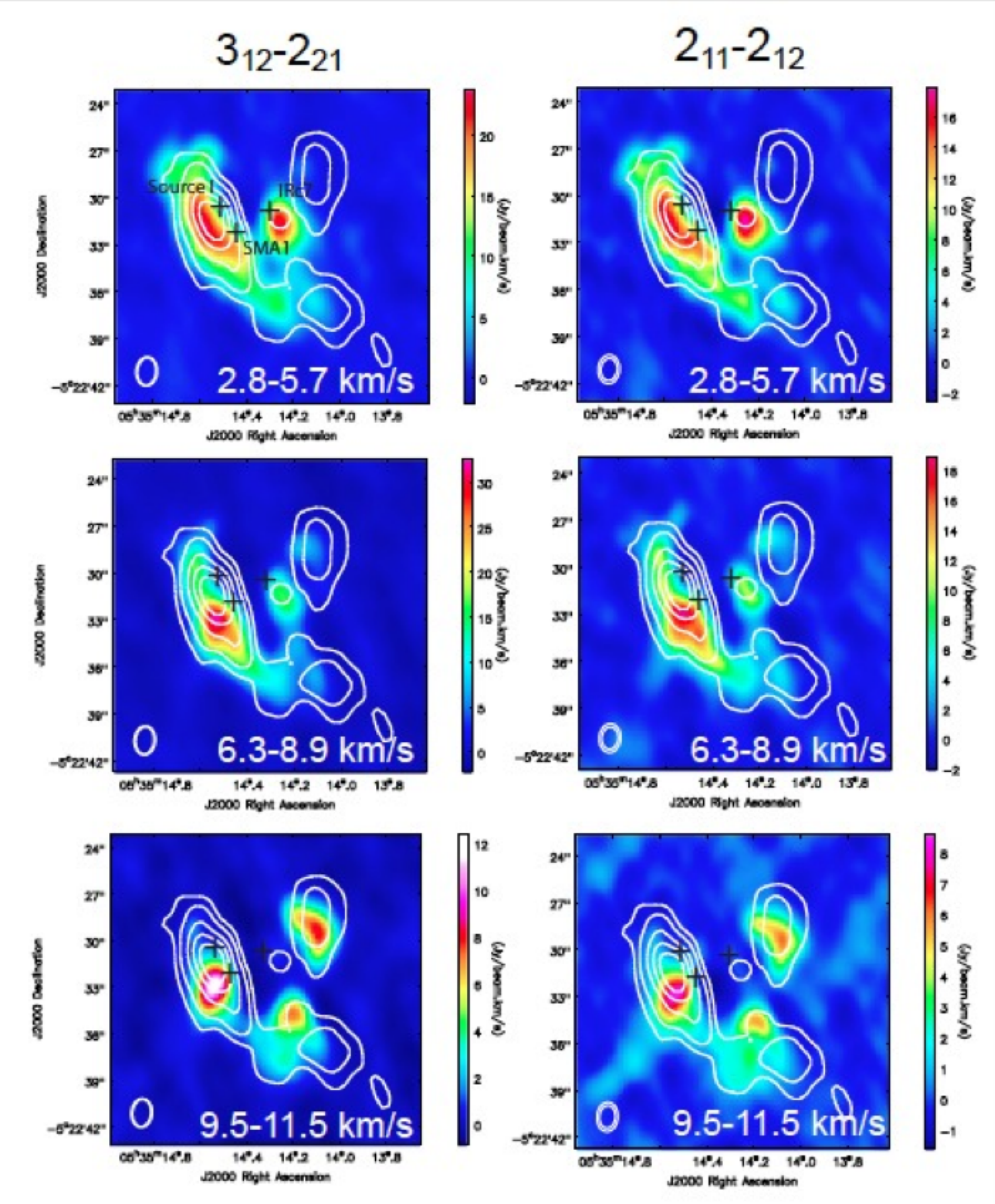
# Detection of $HD^{18}O$ in Orion




- Six $HD^{18}O$ lines detected with a $V_{LSR}$ ~ 6.5 km/s (does not exactly match the hot core velocity)
- Implies either very high D/H ratio or very high $H_2O$ column density in some component
- Need accurate source size to model the emission
- ALMA SV data provide spatially resolved images!

*J. Neill*

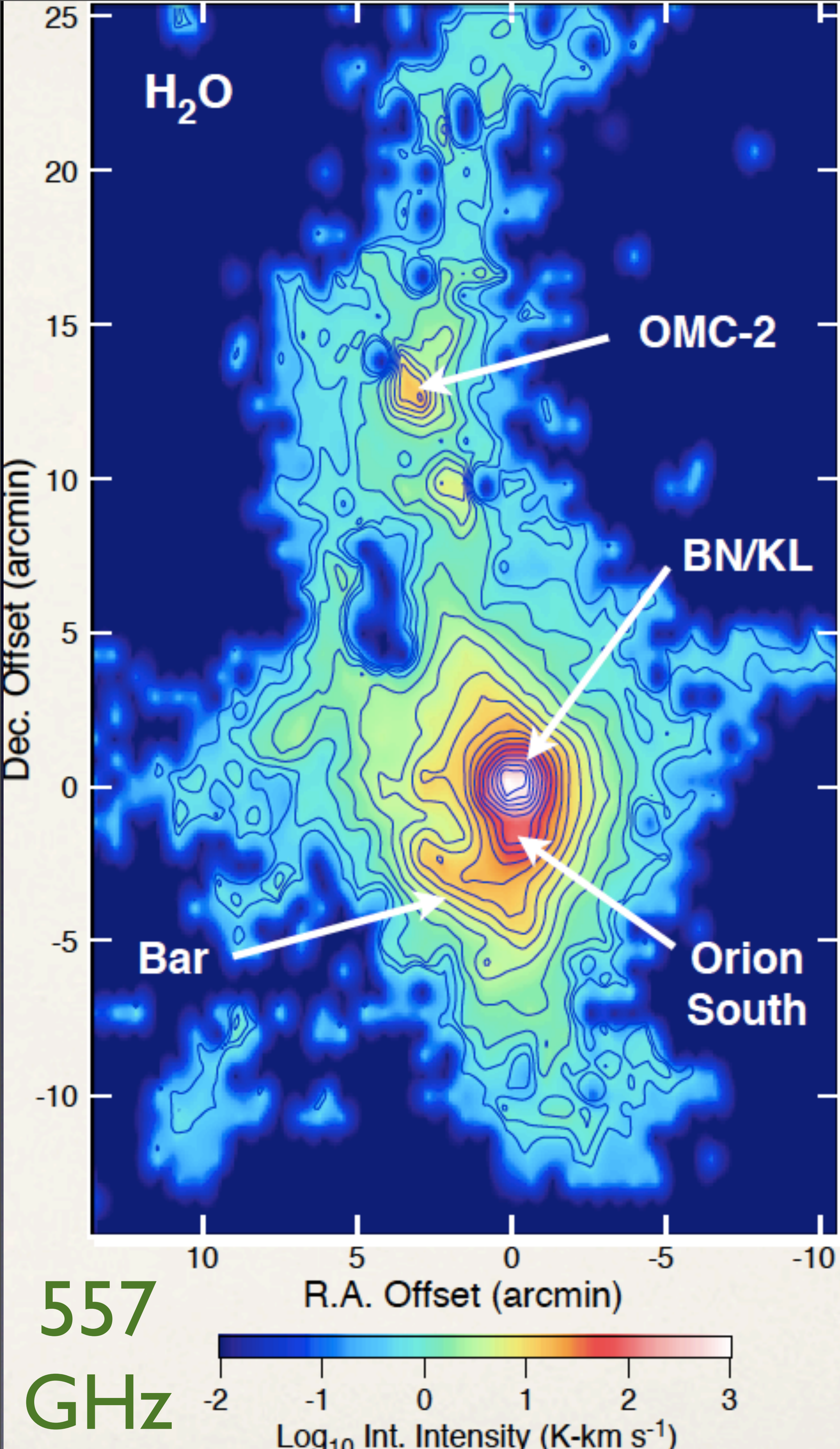
# HDO with ALMA




*Conturs 230 GHz continuum*
*Color HDO*

- Multiple spatial components
- Bright HDO emission in a small clump (2" in size) at ~7 km/s
- Agrees with $HD^{18}O$ velocities
- Analysis of water lines also consistent with emission from this small clump
- Additional components also contribute
- Revised $X(H_2O)$~6.5 $10^{-4}$; $HDO/H_2O$~0.003

*J. Neill*



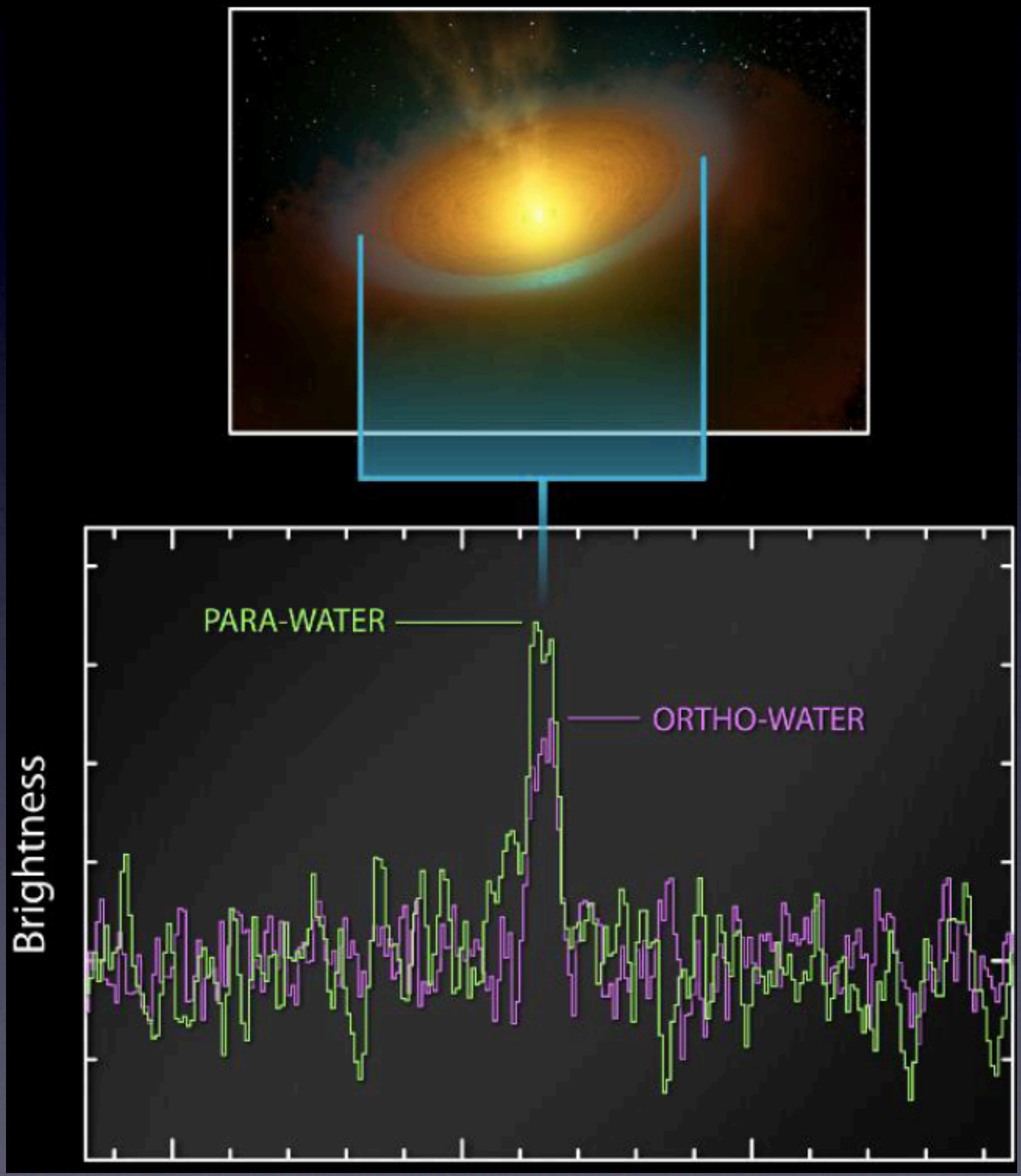

# Water

- Abundance enhanced in warm gas—outflows
- Derived hot core water abundances often lower than the canonical value of $10^{-4}$ (modeling deficiency?)
- Ortho-para ratio generally consistent with the high-temperature value of 3, but with some exceptions (e.g., Galactic Center)
- Spectacular detections of gas-phase water in disks and a prestellar core in very long HIFI integrations

*G. Melnick, V. Tolls*

# Water in Disks

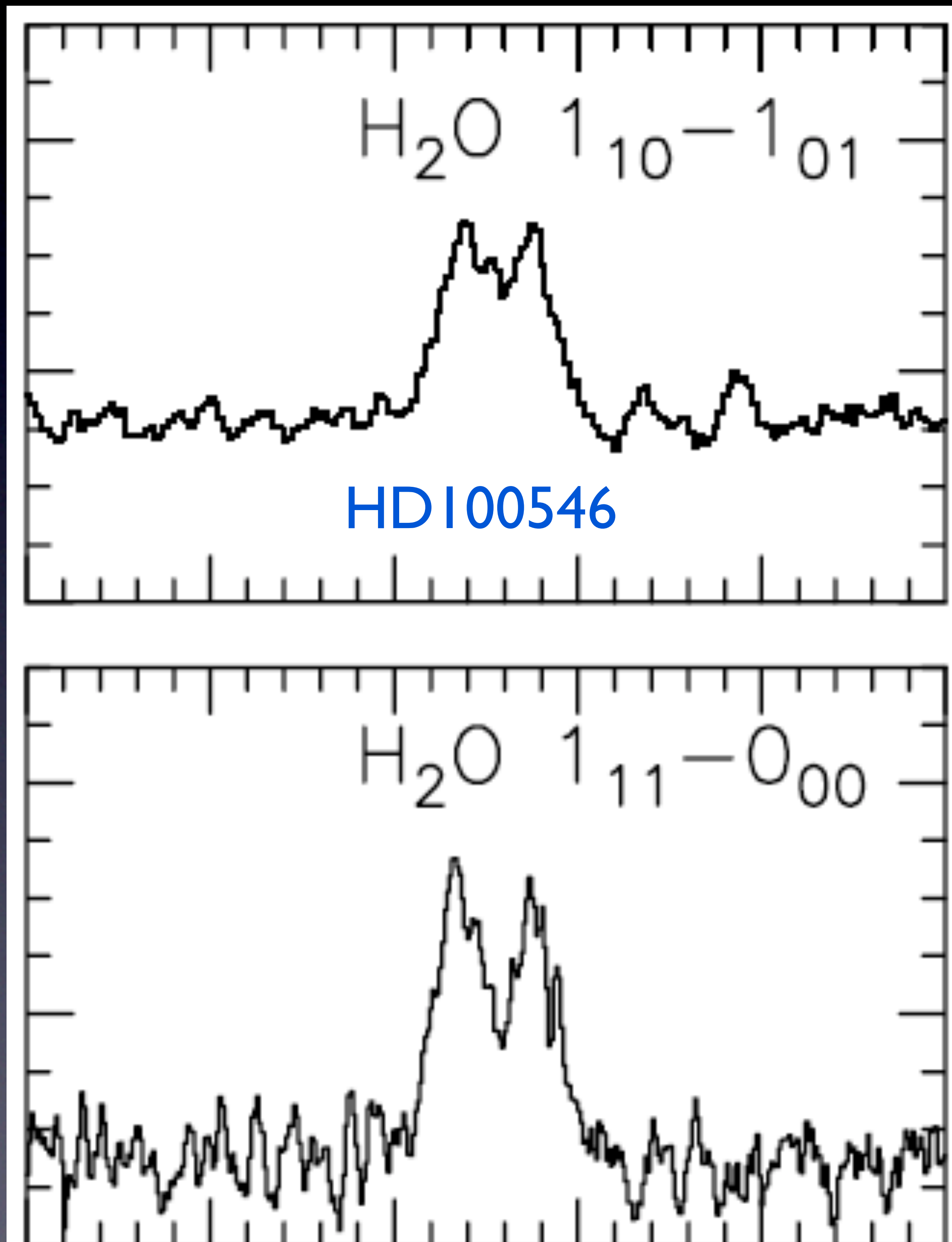
TW Hya




*M. Hogerheijde*

- Lines of ortho and para water detected for the first time with Herschel/HIFI in TW Hydrae
- 10 mln years old T Tauri star, 0.6 $M_\odot$ at 54 pc
- Several thousand oceans worth of *water ice*, at 100–200 AU from the star
- If other disks are similar to TW Hydrae, ample water exists in the outer disk, where comets form

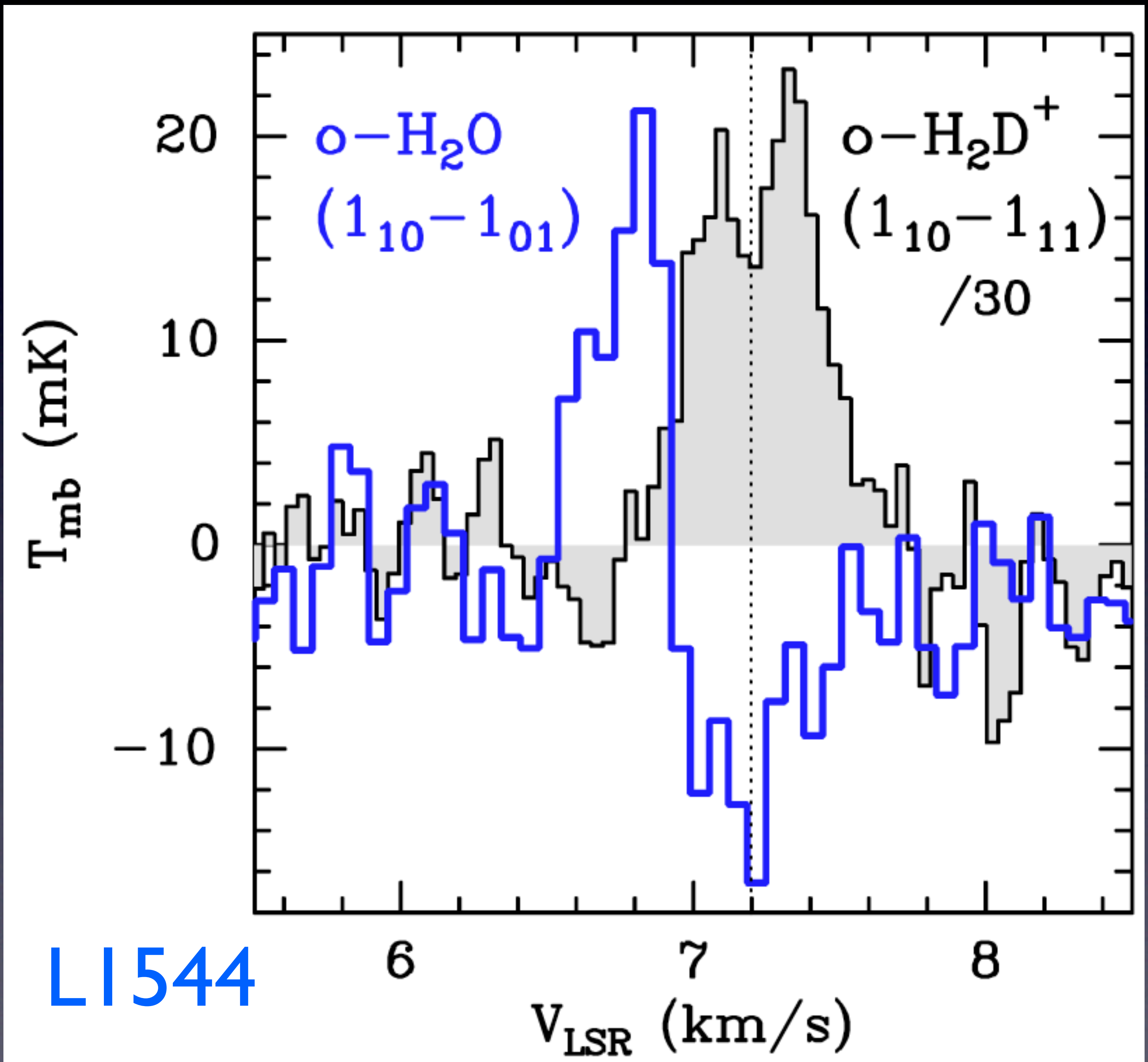
# Water in Disks




*M. Hogerheijde*

- New detection in HD100546 (plus several upper limits)
- Water-covered planets like Earth may be common

# Water in Prestellar Cores



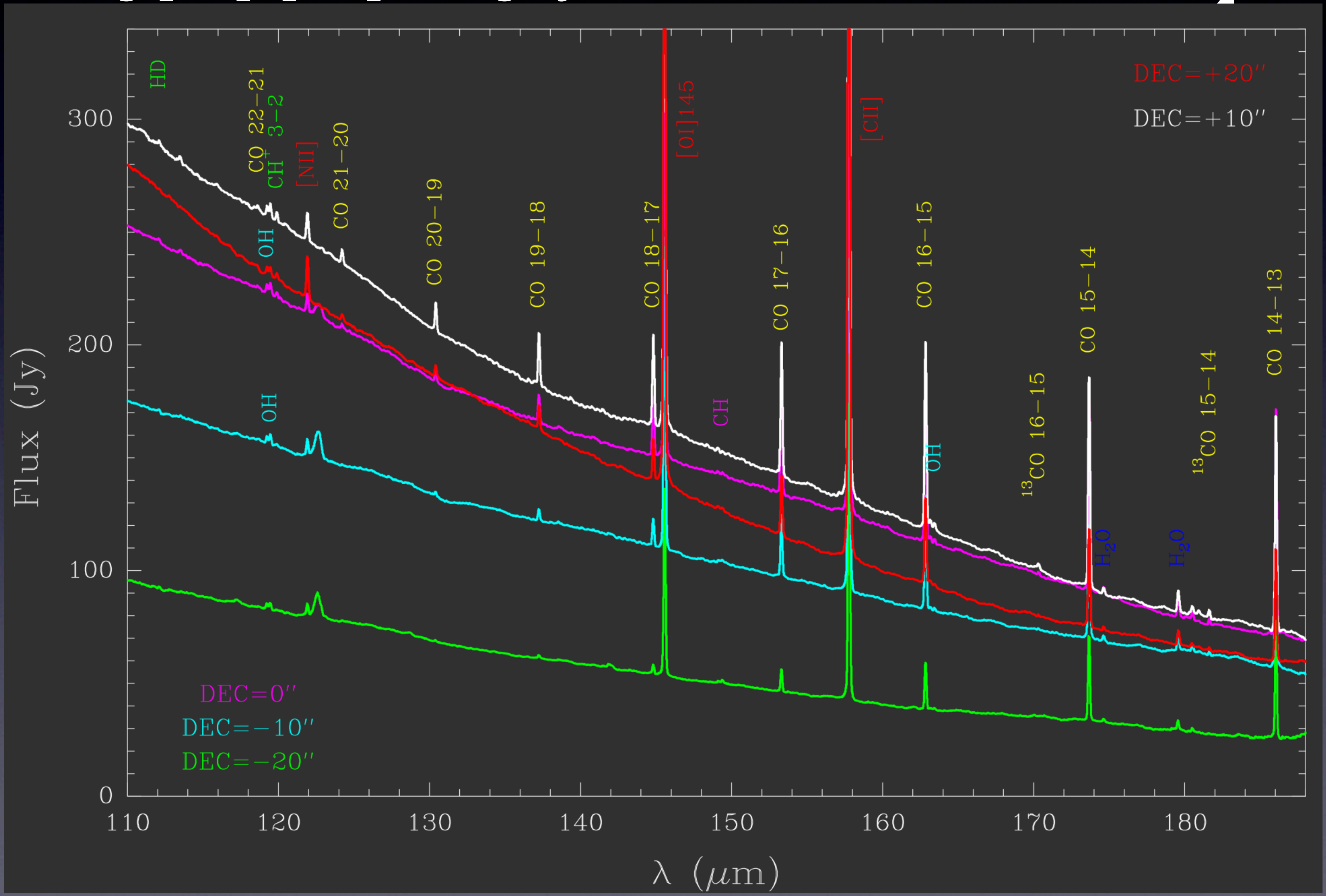

*P. Caselli*

- L1544, 13.6 hours
- Inverse P-Cygni profile indicative of infall
- Water has to be present in the central few 1000 AUs
- Water abundance (>$10^{-9}$) maintained by FUV photons locally produced by interaction of CRs with $H_2$
- FUV photons then irradiate icy mantles and release water molecules into the gas phase
- Complex interplay between gas and solids
- $H_2$ OPR>1
- The simple "onion" structure of prestellar cores has to be carefully re-evaluated (ALMA)

# PACS Orion Bar

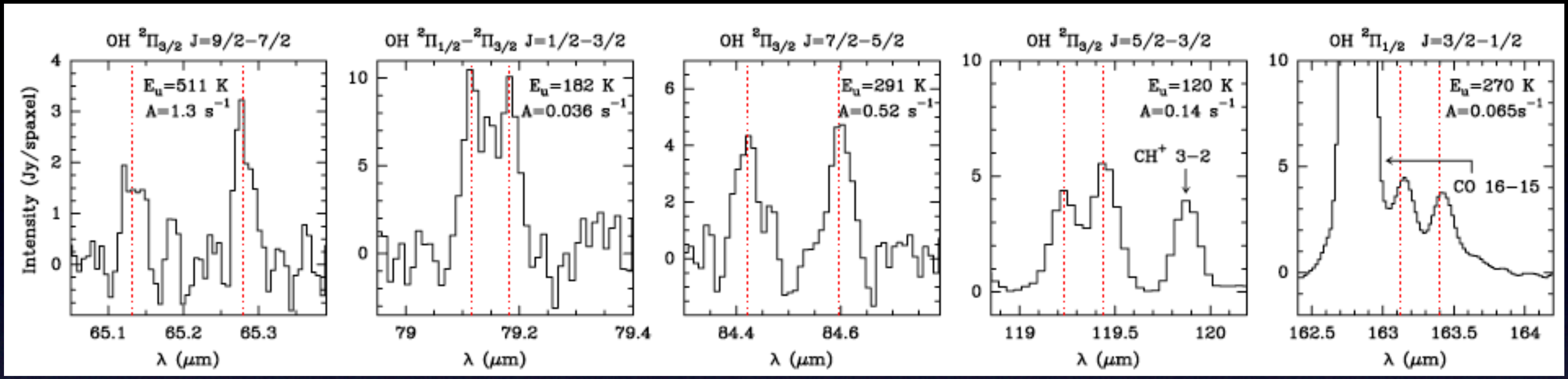
## Cooling and PDR Chemistry

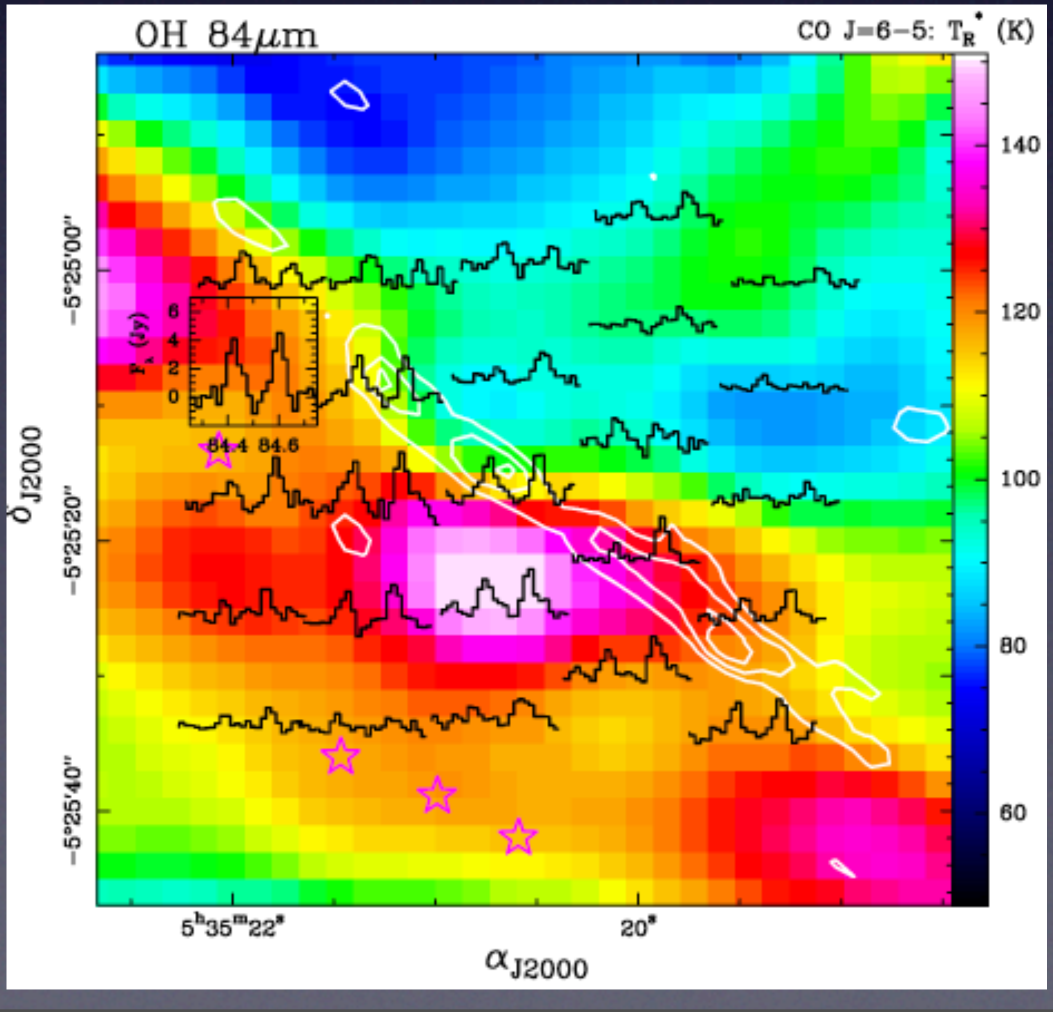
Strong [OI], [CII] + high-*J* CO + excited OH, $CH^+$, $H_2O$…




*C. Joblin, J. Goicoechea, A. Contursi*

# OH in Orion Bar

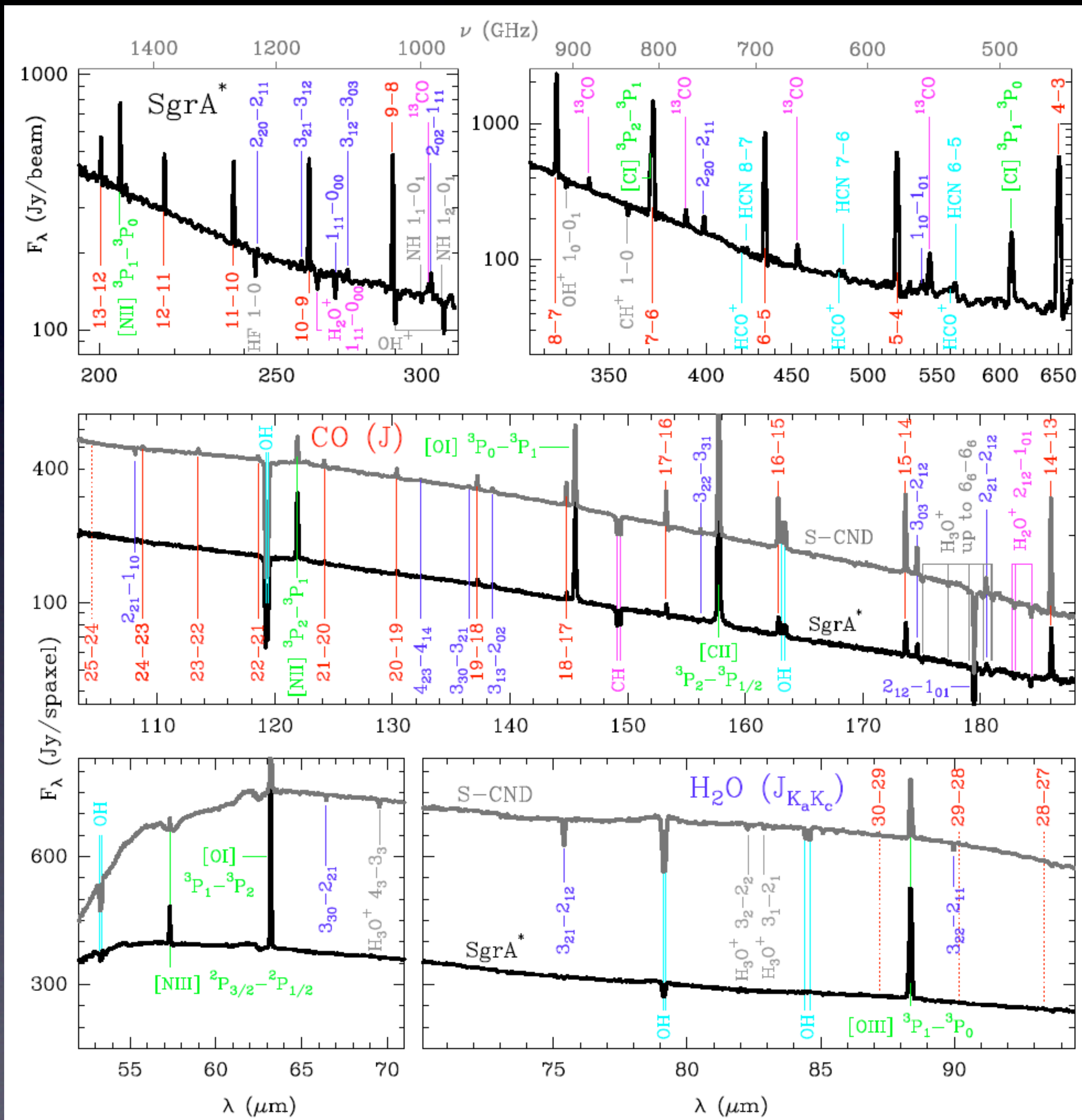


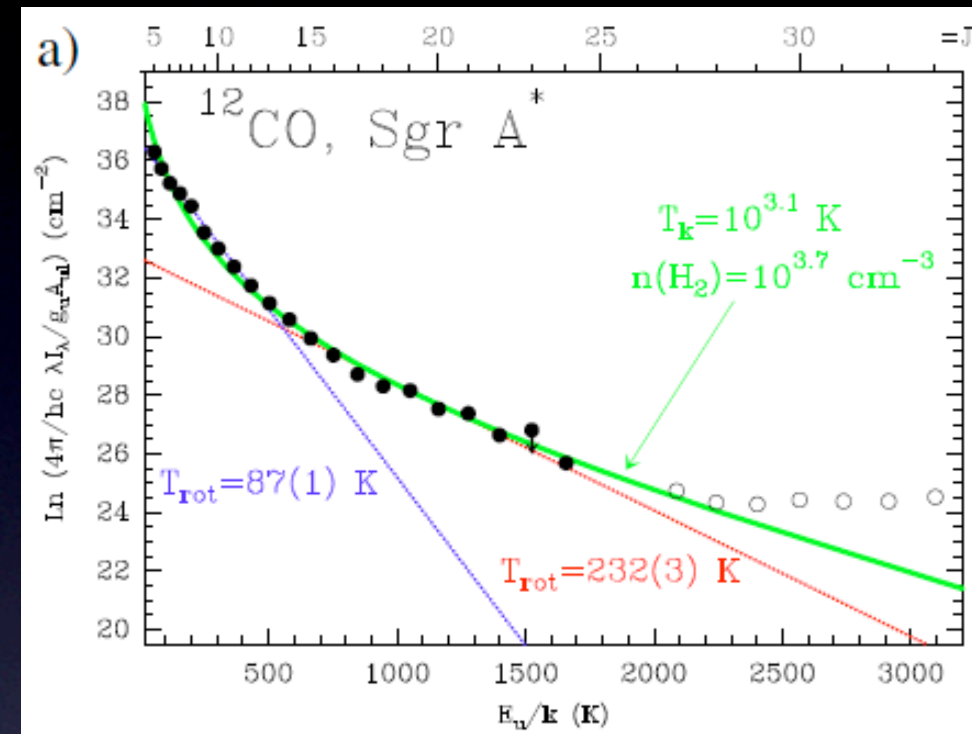




- Five rotational Λ–doublets up to 510 K
- Emission extended, correlates with high-J CO and $CH^+$, but not $H_2O$
- Warm (160–220 K), dense ($10^{6-7}$ cm$^{-3}$) gas; unresolved clumps exposed to FUV radiation (O + vib $H_2$)

*J. Goicoechea*

# PACS/SPIRE Sgr A*

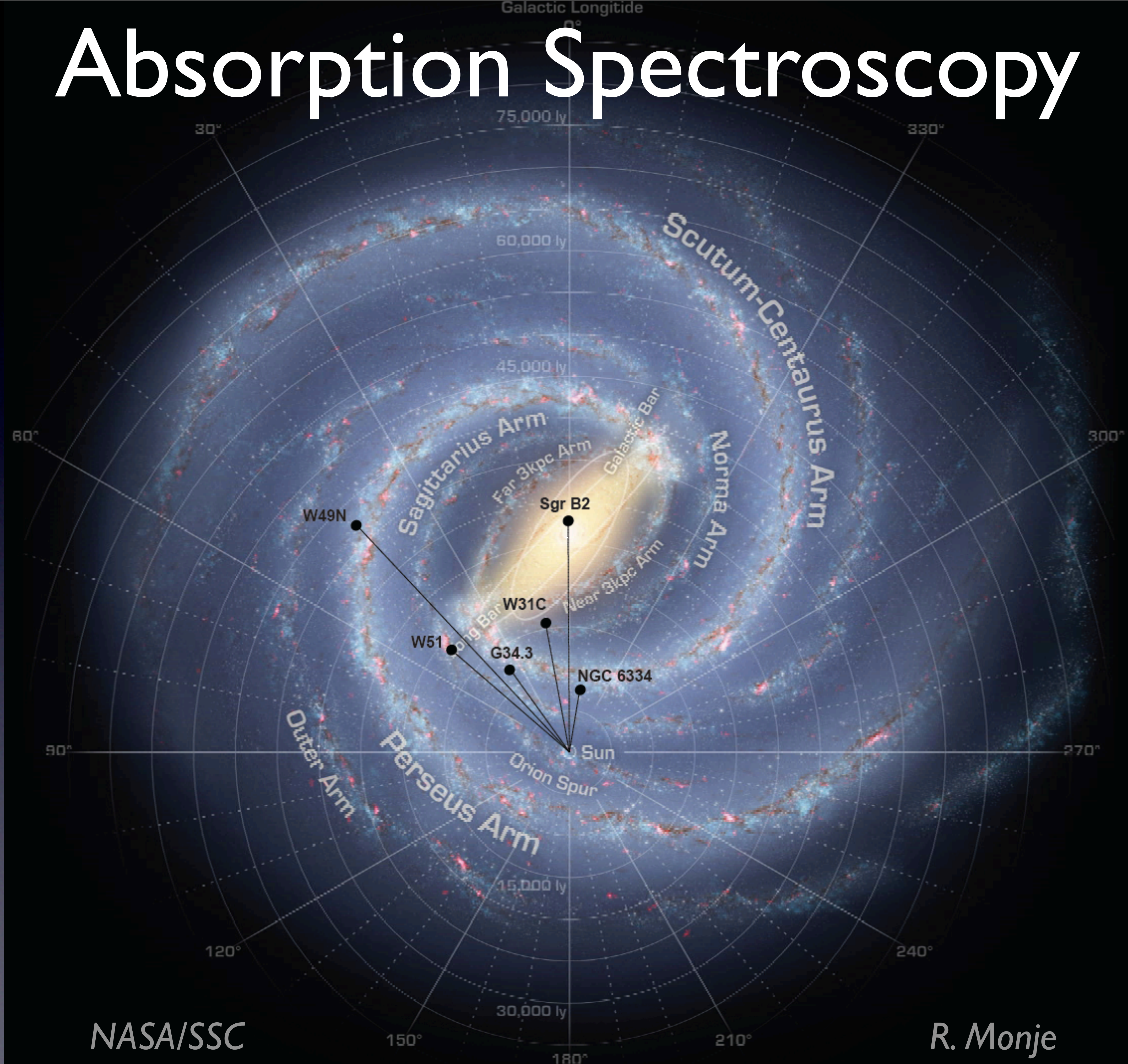


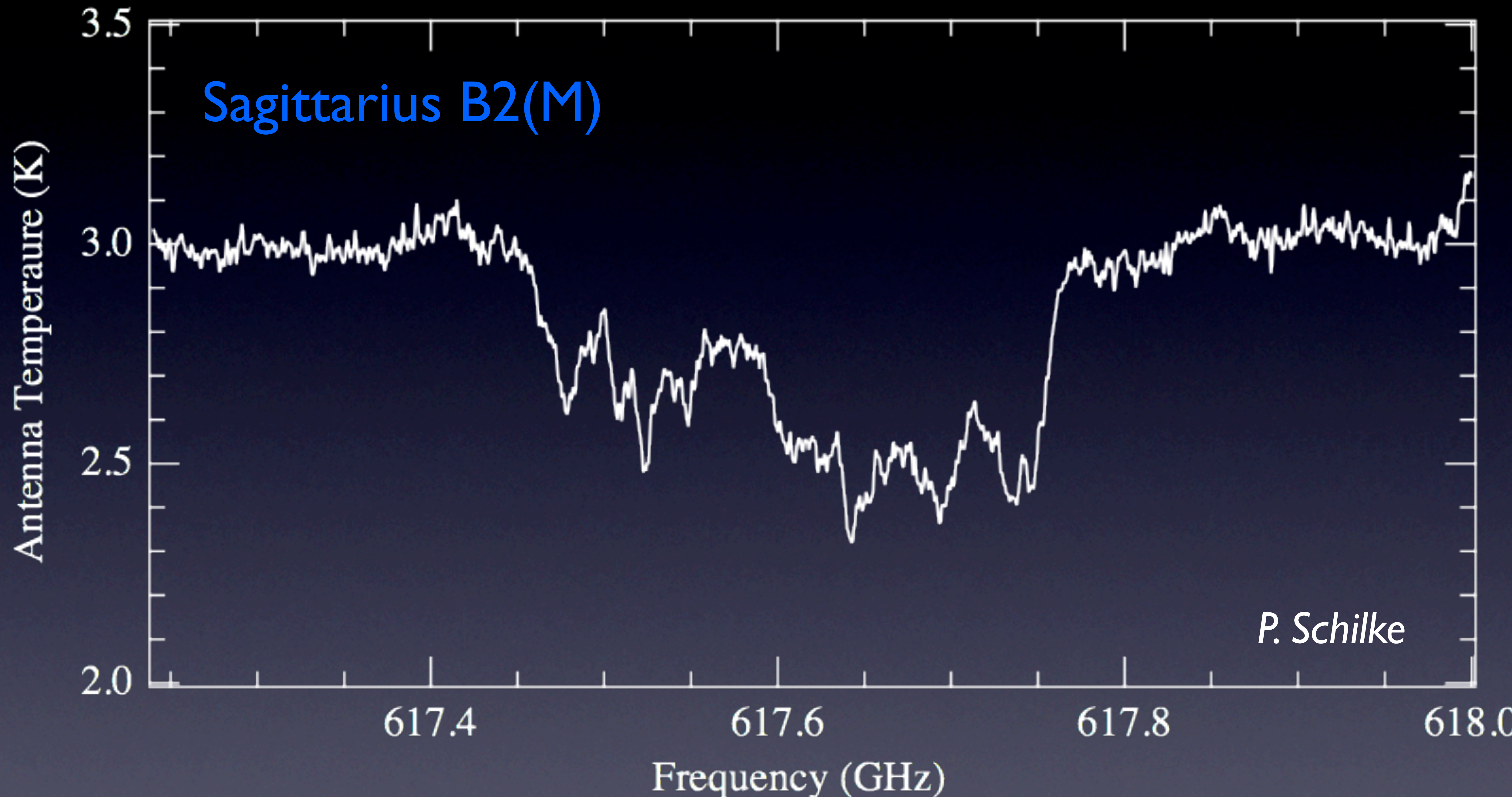

*J. Goicoechea*

- Separate emission from the central cavity and the CND
- X-rays or CRs do not play a dominant role in the energetics of the hot molecular gas
- Shocks or the related supersonic turbulence dissipation and magnetic viscous heating dominate

# Absorption Spectroscopy

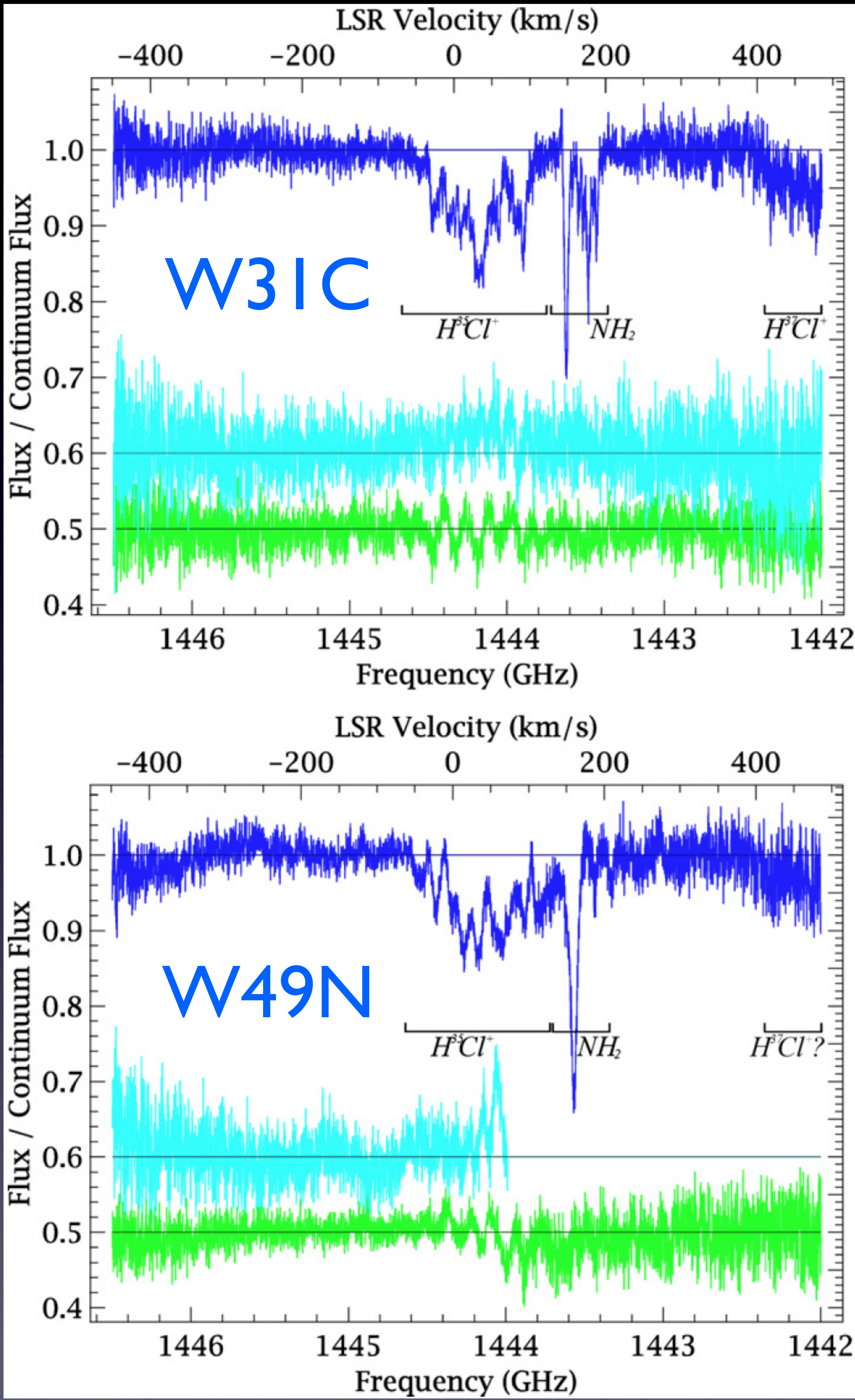


# First FIR DIB Analog?




- Molecule present in *all* spiral arm clouds between us and the galactic center, but not the Sgr B2 envelope (difficult to get precise frequency)

# $H_2Cl^+$ and $HCl^+$



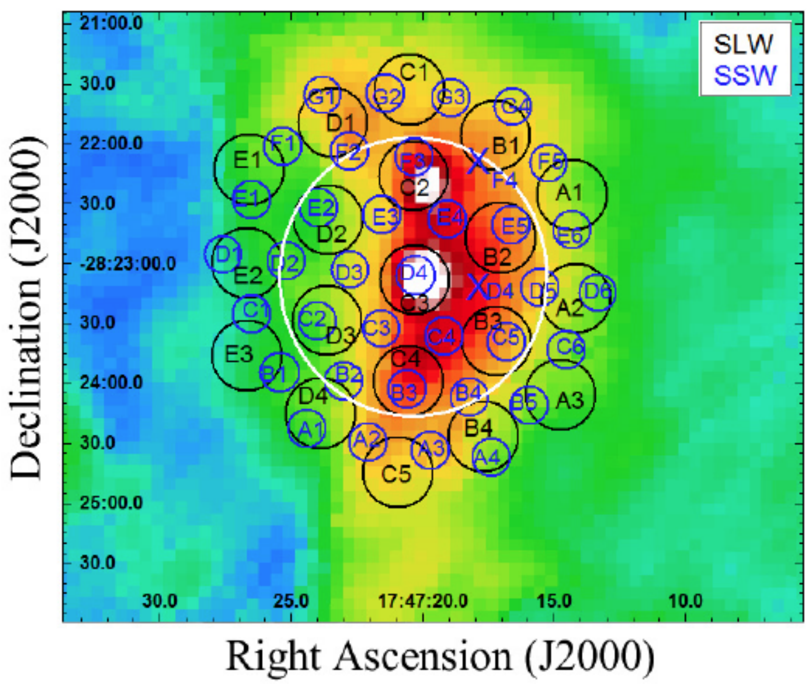

*M. De Luca*

- Chlorine chemistry in diffuse clouds is simple:

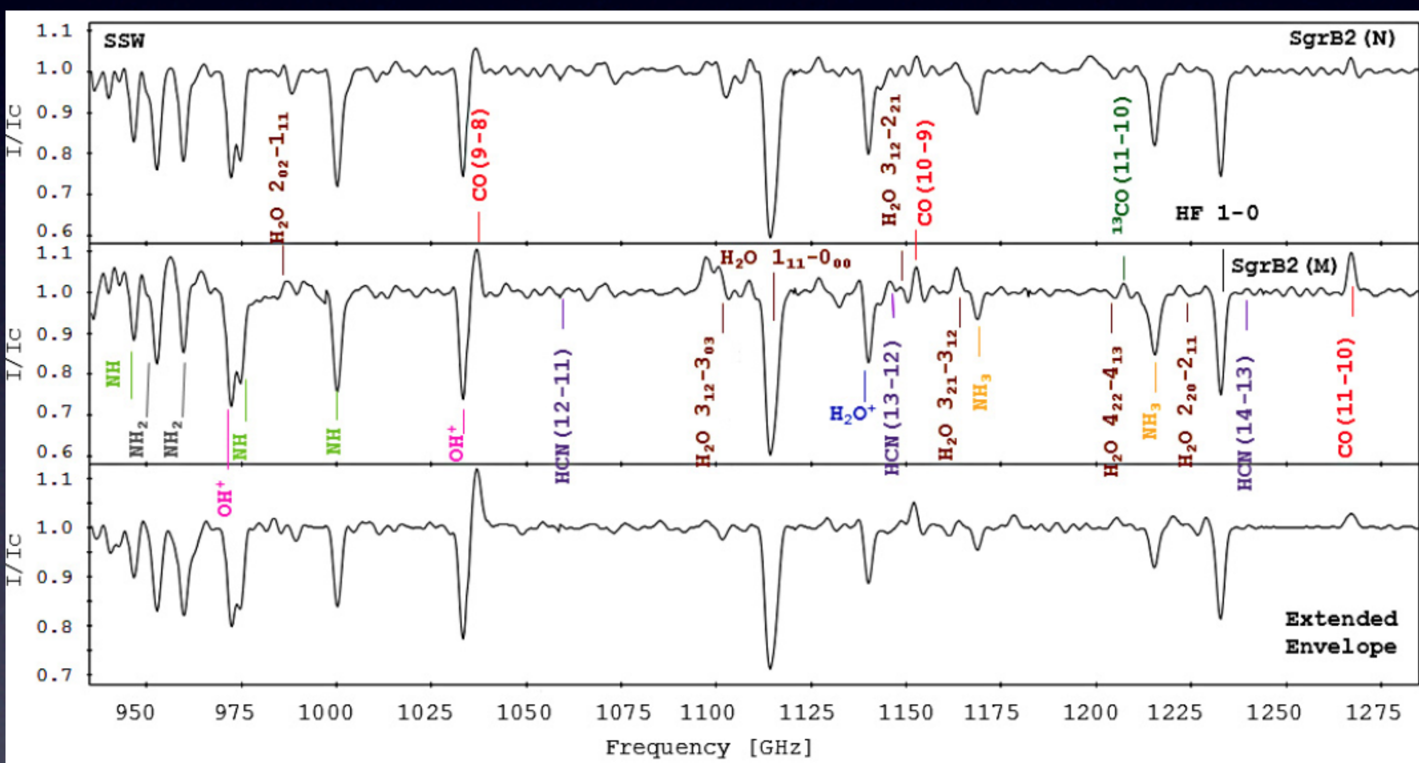
  $Cl^+ + H_2 \rightarrow HCl^+ + H$ $\quad$ $HCl^+ + H_2 \rightarrow H_2Cl^+ + H$

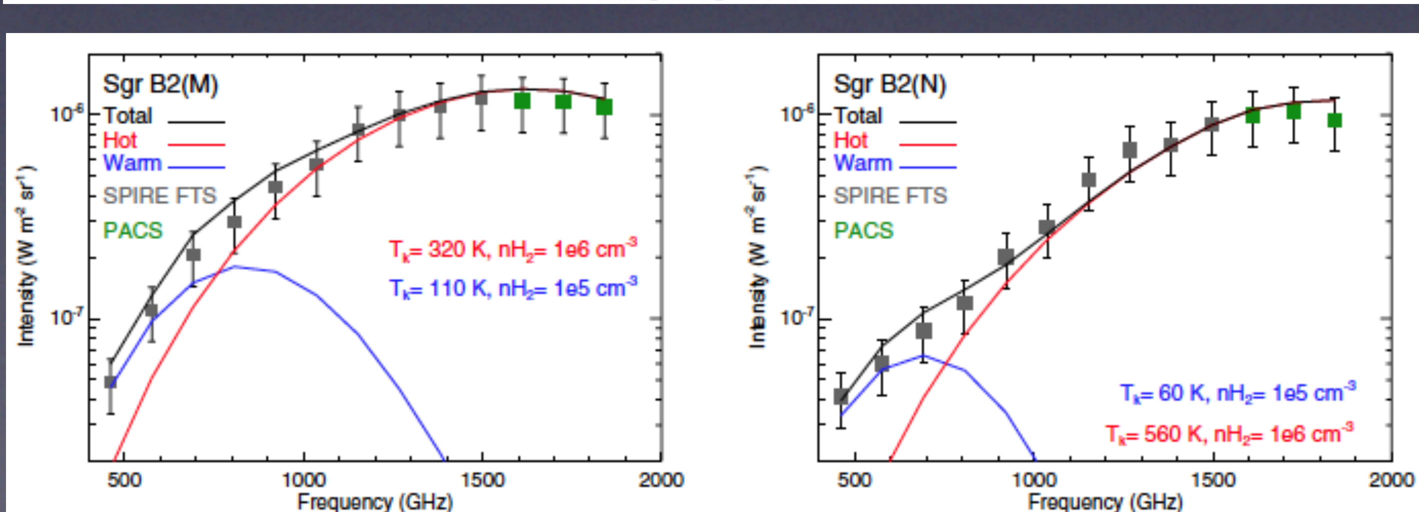
  $H_2Cl^+ + e \rightarrow HCl + H$ $\quad$ (10%)

  $\rightarrow Cl + \text{products}$ (90%)
- Dense clouds: proton transfer from $H_3^+$ to Cl can also initiate formation of Cl-bearing molecules
- $H_2Cl^+$ detected early on by HIFI, but $HCl^+$ has been a long struggle (needed precise lab frequencies—H. Gupta)
- $HCl^+/H_2Cl^+/HCl \sim 1$
- The two ions ions overabundant by a factor of a few compared to chemical model predictions
- ISM chlorine chemistry still a mystery
- $H_2Cl^+$ and HCl accessible from the ground




# SPIRE-FTS/PACS Sagittarius B2

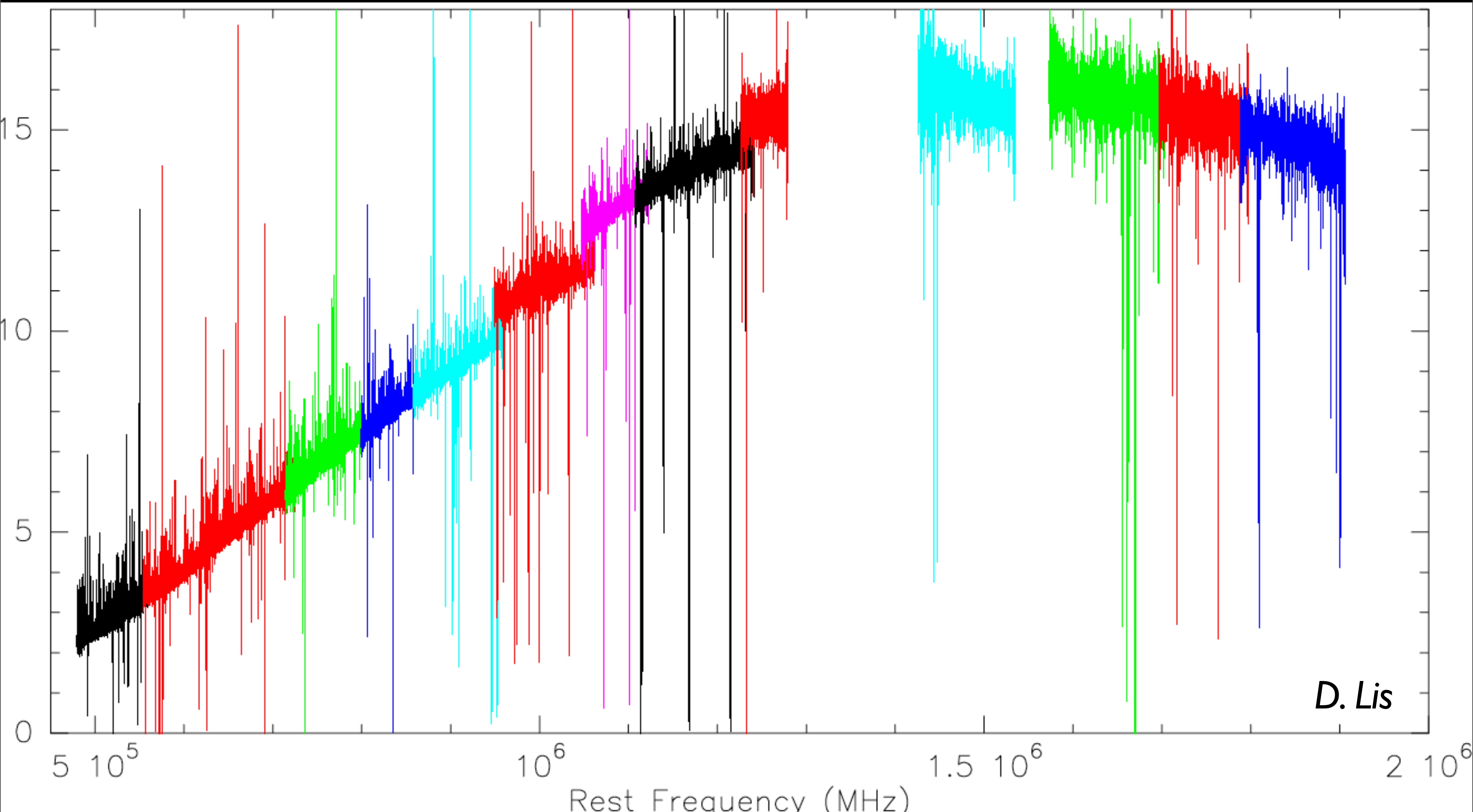



- Strong CO line emission (J=4 to 16)
- Extended warm component (50-100 K), hotter component toward N/M, heated by UV and shocks (dust only 20-30 K)
- High-density tracers (HCN, $HCO^+$...)
- Absorption lines of light hydrides
- Uniform luminosity ratio, CO/FIR~(1-3)$10^{-4}$, across the extended envelope; same heating mechanism on all scales

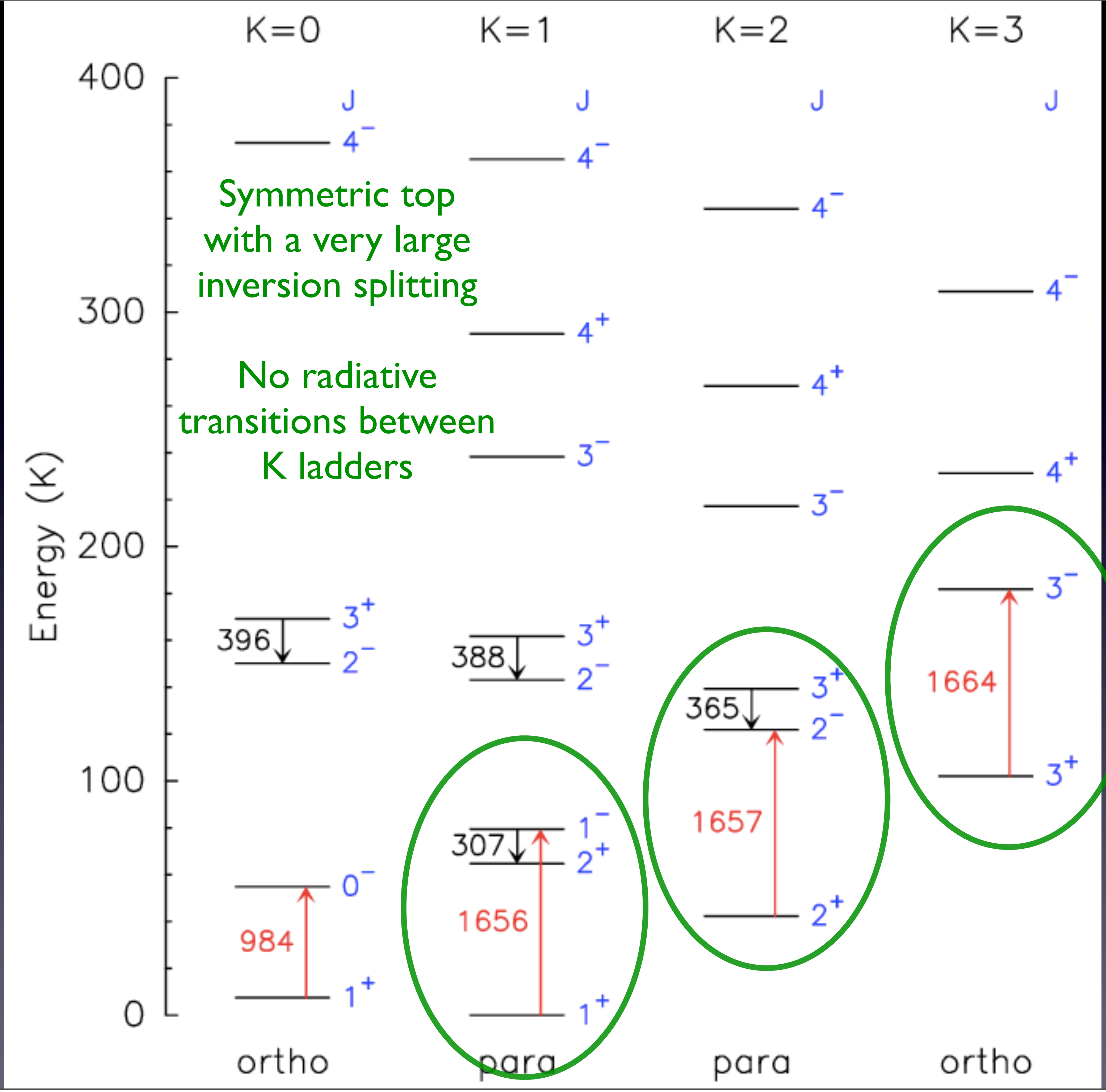
*M. Etxaluze*

# HIFI Sagittarius B2(N)



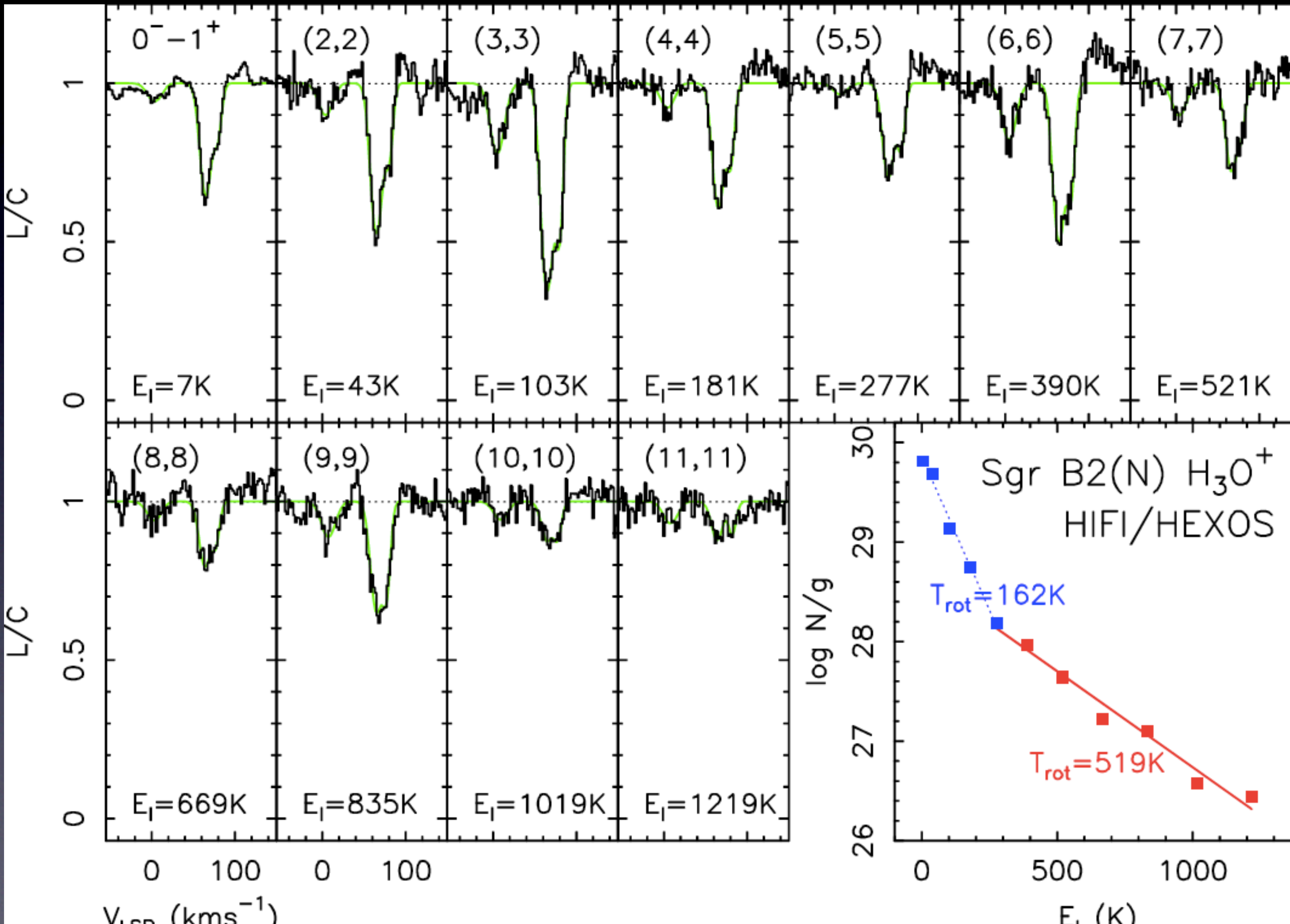

- HEB bands dominated by absorption lines—water isotopologues, low-energy ammonia lines, $C_3$, $C^+$…

# $H_3O^+$



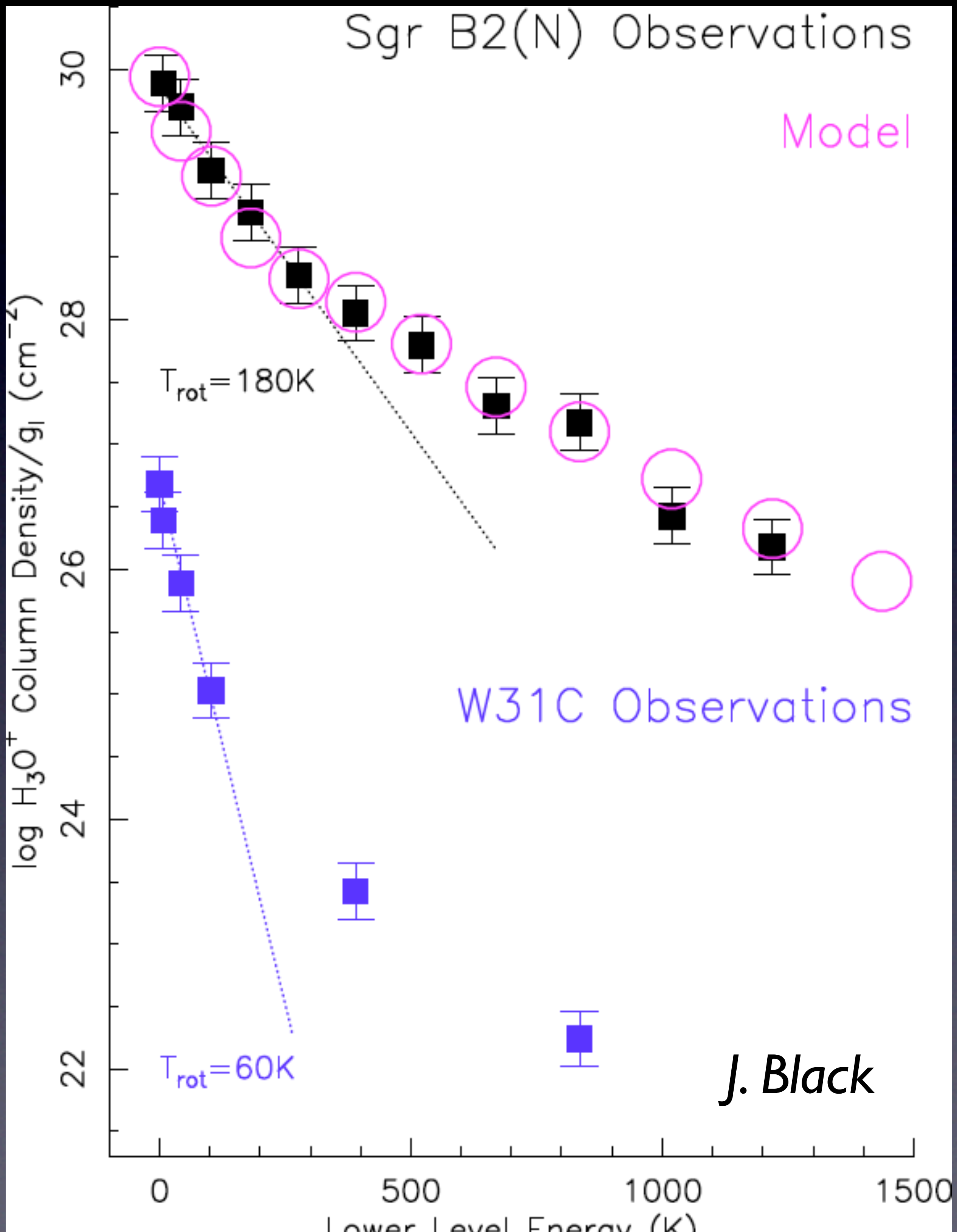
K=0
K=1
K=2
K=3
Energy (K)
400
300
200
100
0
J
4−
4+
3−
3+
2−
2+
1−
1+
0−
Symmetric top with a very large inversion splitting
No radiative transitions between K ladders
396
388
365
307
984
1656
1657
1664
ortho
para
para
ortho

# Metastable $H_3O^+$ in Sgr B2(N)



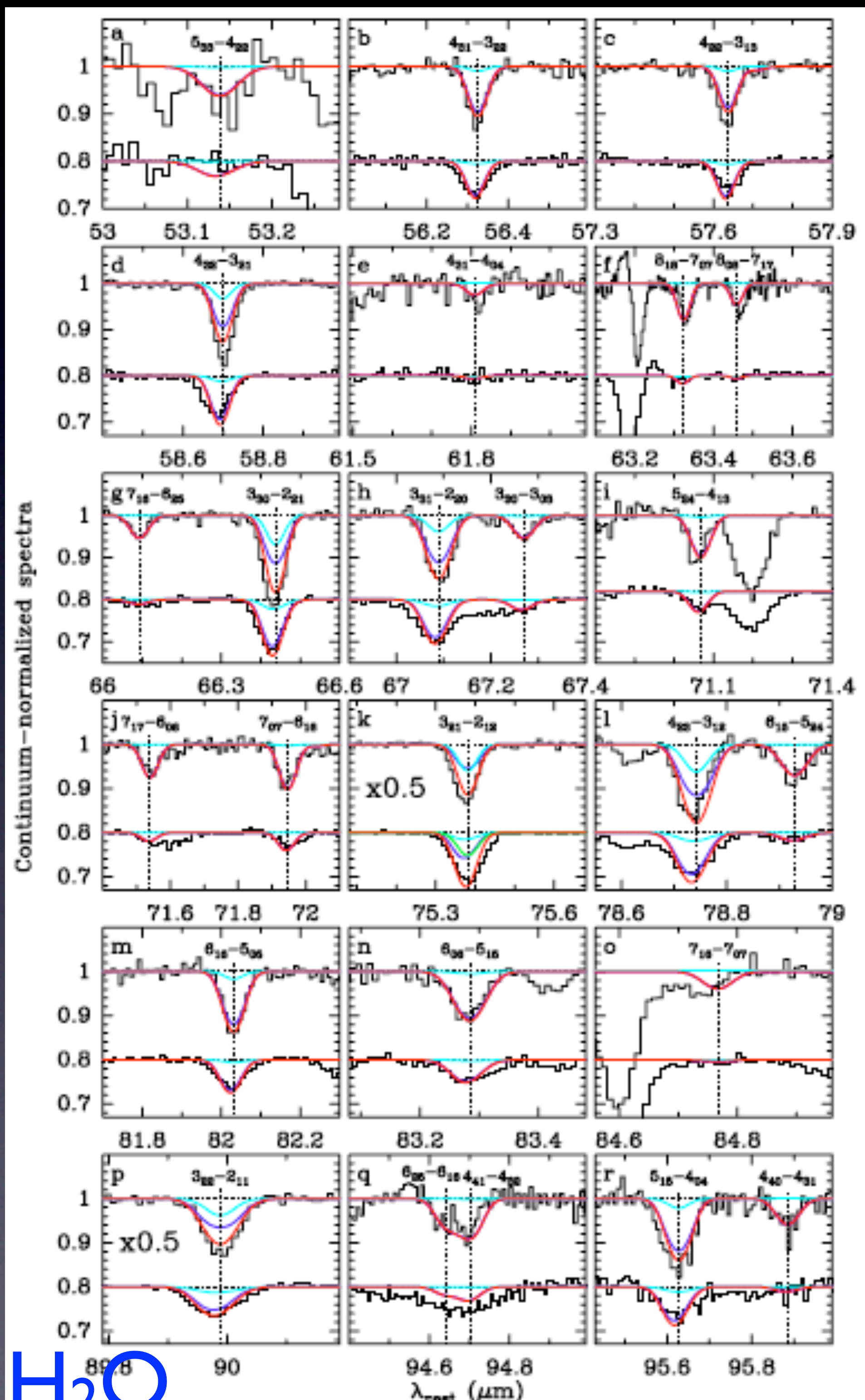

*D. Lis*

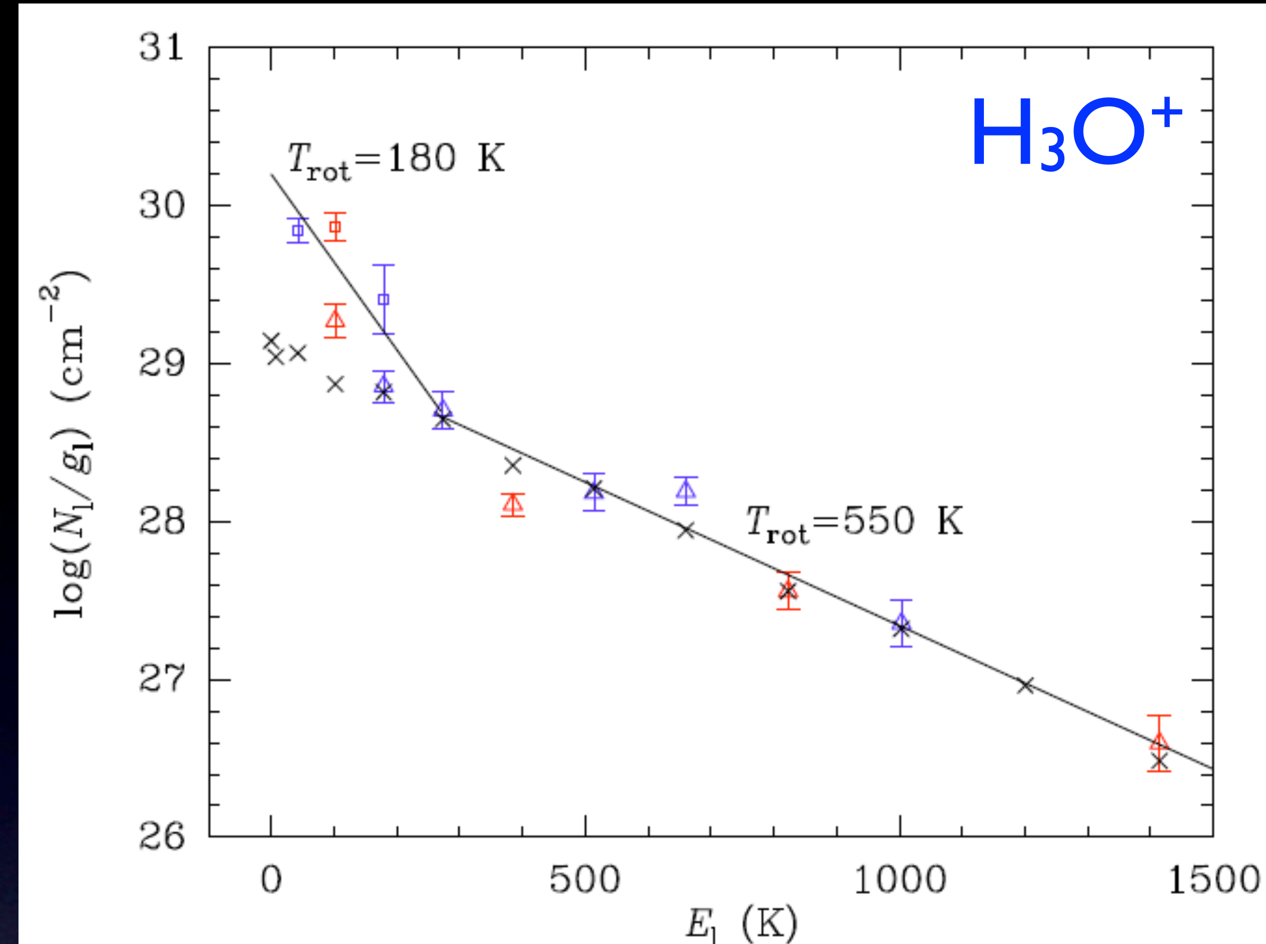
# Formation Pumping




- Cosmic/X-ray + $H_2$ → $H_3^+$ (widespread in the Galactic Center region)
  - $H_3^+ + O \rightarrow OH^+ + H_2$
  - $OH^+ + H_2 \rightarrow H_2O^+ + H$
  - $H_2O^+ + H_2 \rightarrow H_3O^+ + H +$ 1.69 eV
- Also
  - $H_3^+ + H_2O \rightarrow H_3O^+ + H_2 +$ 2.81 eV
- Collisional relaxation time has to be long compared to recombination/ reformation of $H_3O^+$ molecules to maintain the population
- Can the hot ammonia also be explained by formation pumping? (More stable, long lived—more time to relax through collisions?)

# PACS NGC4418 and Arp 220

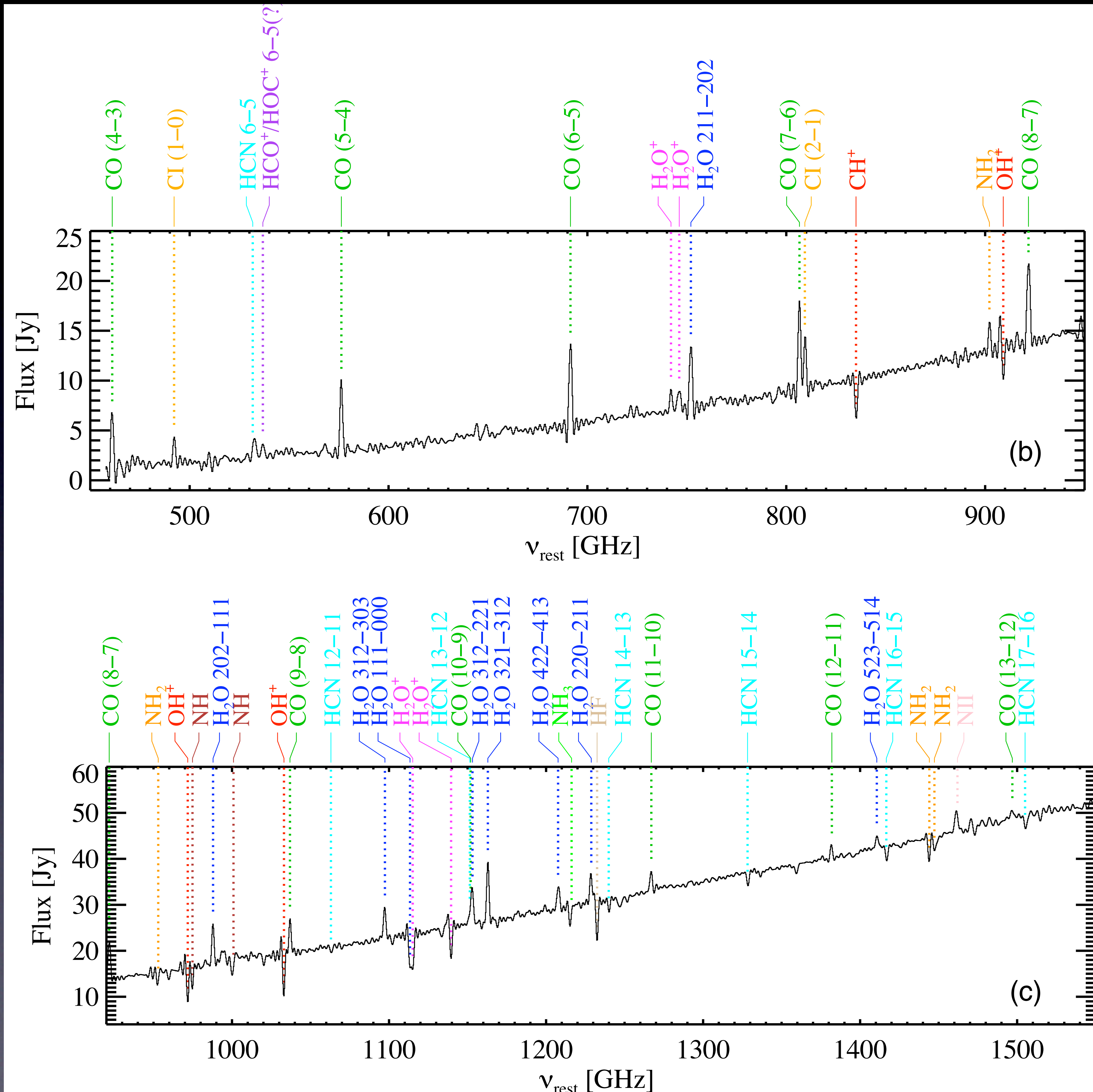


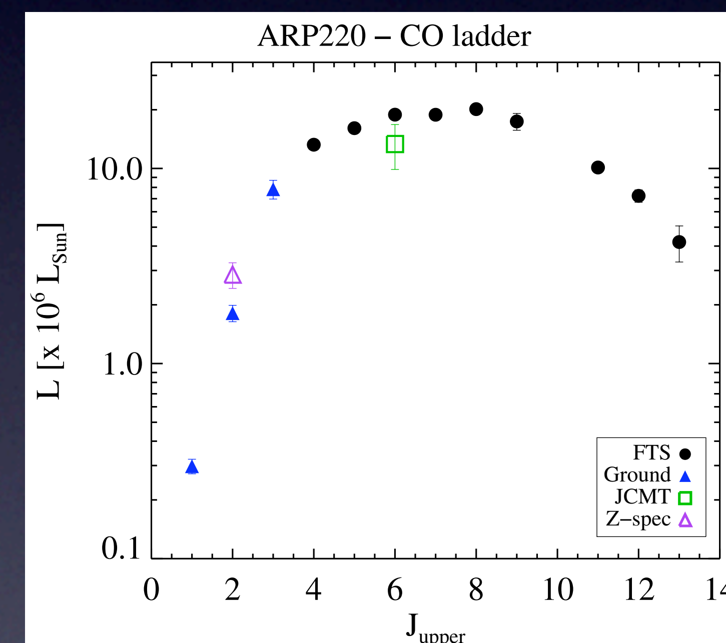




- Nuclear regions have high water abundances ~$10^{-5}$
- Chemistry typical of evolved hot cores, where grain mantle evaporation has occurred
- $OH/H_2O$~0.5 indicates effects of X-rays or CRs
- $H_3O^+$ rotational temperature ~500K in Arp 220, similar to Sagittarius B2
- Lines arise in a relatively low density (~$10^4$ cm$^{-3}$) interclump medium with a very high ionization rate (>$10^{-13}$ s$^{-1}$)

*E. Gonzalez-Alfonso*

# SPIRE FTS Arp 220




- ALMA will carry out similar studies in high-redshift universe

*N. Rangwala*

# Lesson 1— Spectral Scans

- Main goal of the GT teams was to characterize the far-infrared spectrum and identify the lines
- This has been done--reduced and calibrated data either already publicly available or will be soon
- A range of sources from low-mass to high-mass starforming regions observed--comparative studies
- If you have supporting ground-based data (interferometry), you can do a much better job at modeling HIFI spectral scan data

- All HIFI spectra are 2x4 GHz-wide spectral scans; the "bonus lines" have largely not been analyzed at all

# Lesson 2 — Modeling

- For many species with complex non-LTE excitation (e.g., water), the abundances are very model dependent
- To interpret observations of warm water, need realistic 3-d models of the source structure, including, e.g., outflow cavities
- If you have access to state-of-the-art radiative transfer models, there is a lot of important work to be done
- Legacy aspect

- Same applies to chemical models, as abundances of some of the newly-detected species do not match model predictions