The Mid-infrared Molecular Inventory Towards Orion IRc2 and Hot Molecular Cores

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Bay Area Environmental Research Institute

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SOFIA

Stratospheric Observatory for Infrared Astronomy

SOFIA Tele-talk
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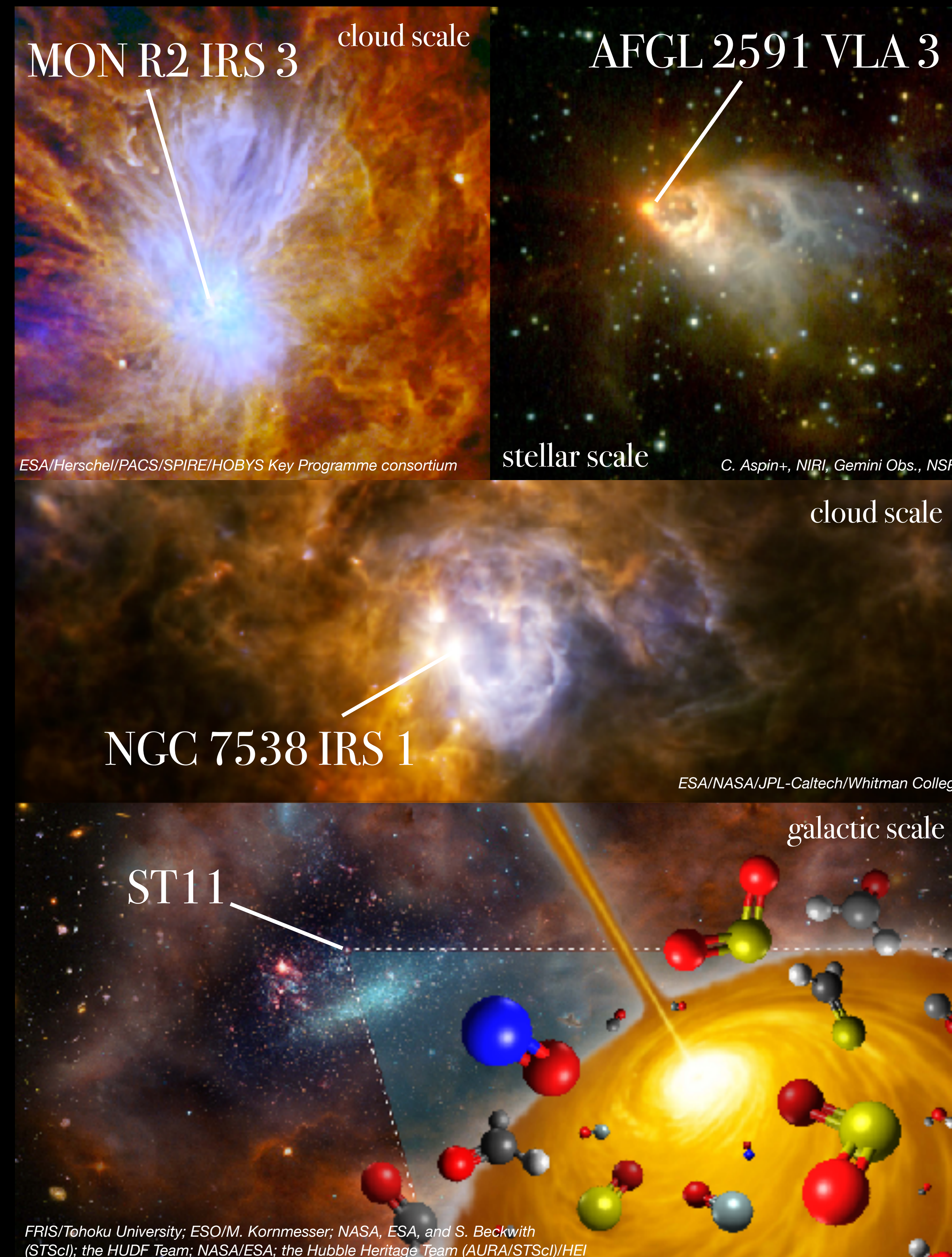
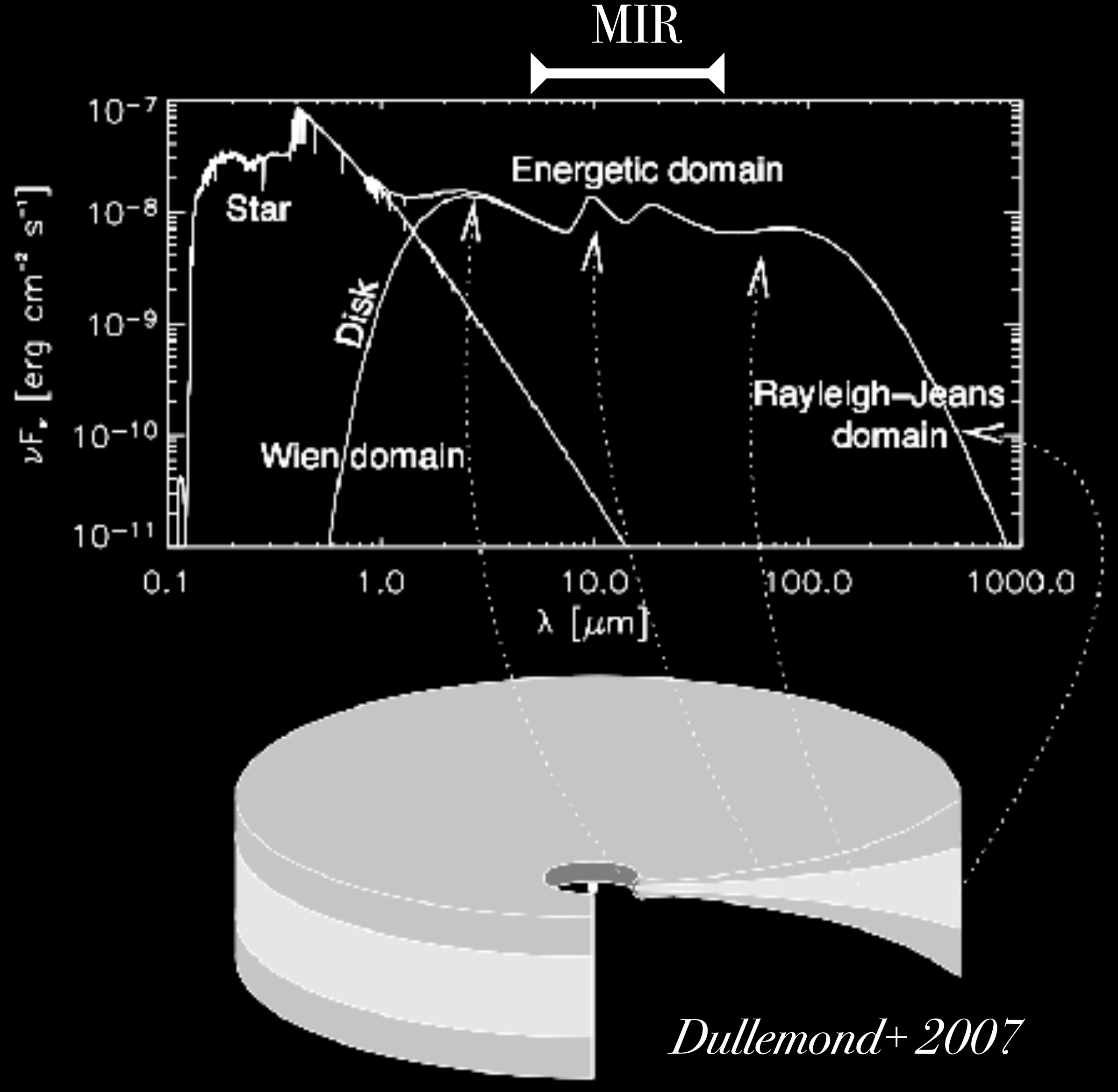
Hot Molecular Cores

- Warm (≥ 100 K), small (≤0.1 pc) and dense (10^5 to 10^8 cm^{-3}) gas near young, high mass protostars (Ohisi 1997)
- Stellar radiation evaporates ice on dust grains in molecular clouds
- Unlocks chemically rich reservoirs of complex and prebiotic molecules
- Abundant in rare molecular species (Kurtz+ 2000)
- Become the building blocks of planetary systems, such as our own Solar System
- Dozens discovered in the Milky Way, 4 total in the LMC



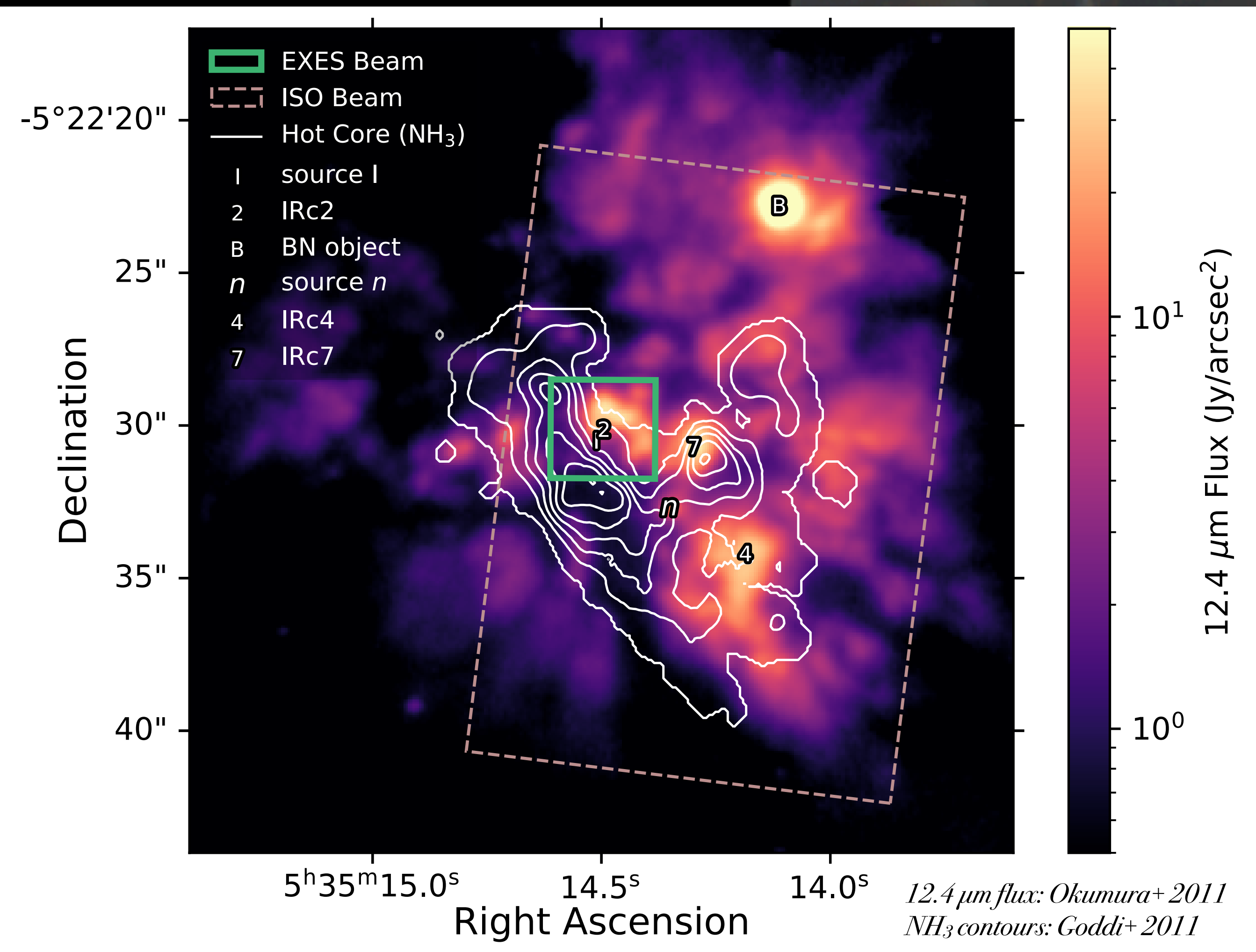
The Uniqueness of the MIR

- Previous high spectral resolution surveys limited to radio, sub-mm, mm, and far-infrared wavelengths
- These longer wavelengths capture rotational transitions of molecules with permanent dipole moments
- Easily accessible from the ground with facilities such as ALMA and SMA
- Only the mid-infrared (MIR) can observe rovibrational transitions and molecules with no permanent dipole moment (e.g. C_2H_2 and CH_4)
- Radio to FIR captures molecules in cooler, outer regions of discs while the MIR to NIR covers the inner regions (Dullemond+ 2007, Barr+ 2020)
- MIR difficult to access because of atmospheric interference
- Past space telescopes *ISO* and *Spitzer*, and present *JWST* cannot resolve individual lines of hots cores in the MIR

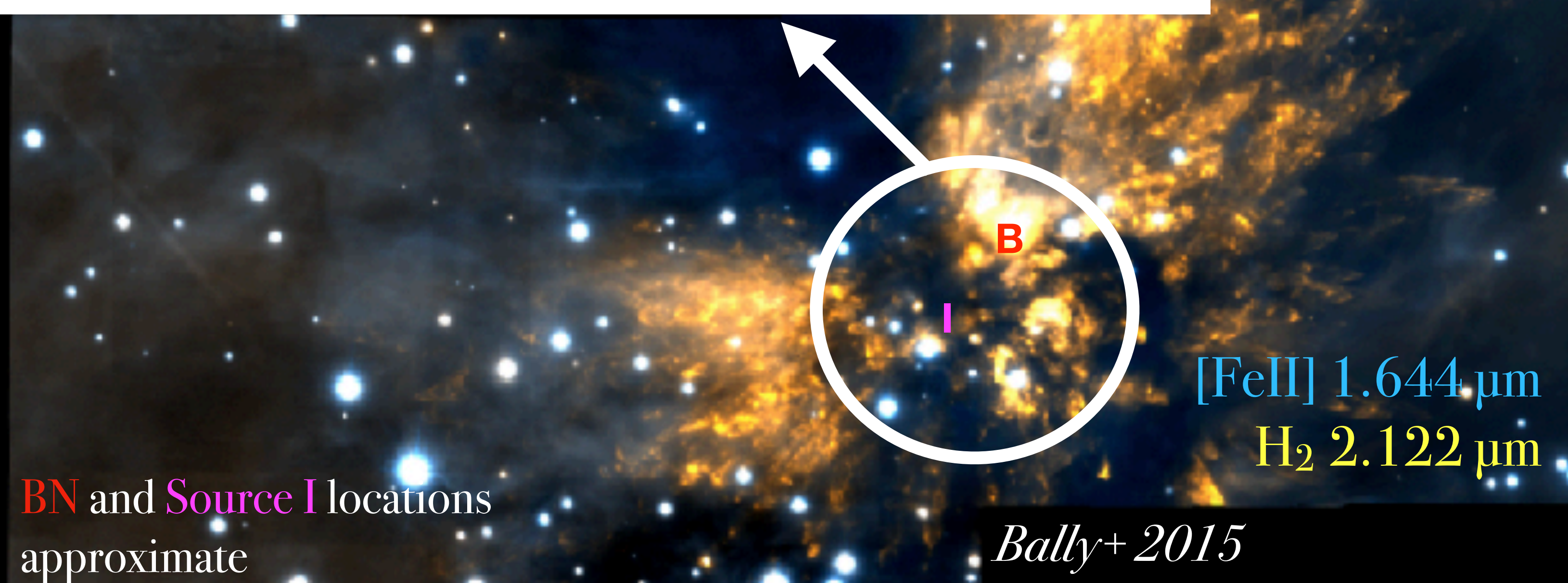


Schematic SED with origin of wavelength regimes emitted spatially along a protoplanetary disc

Atypical: The Orion Hot Core



12.4 μm flux: Okumura+ 2011
NH_3 contours: Goddi+ 2011

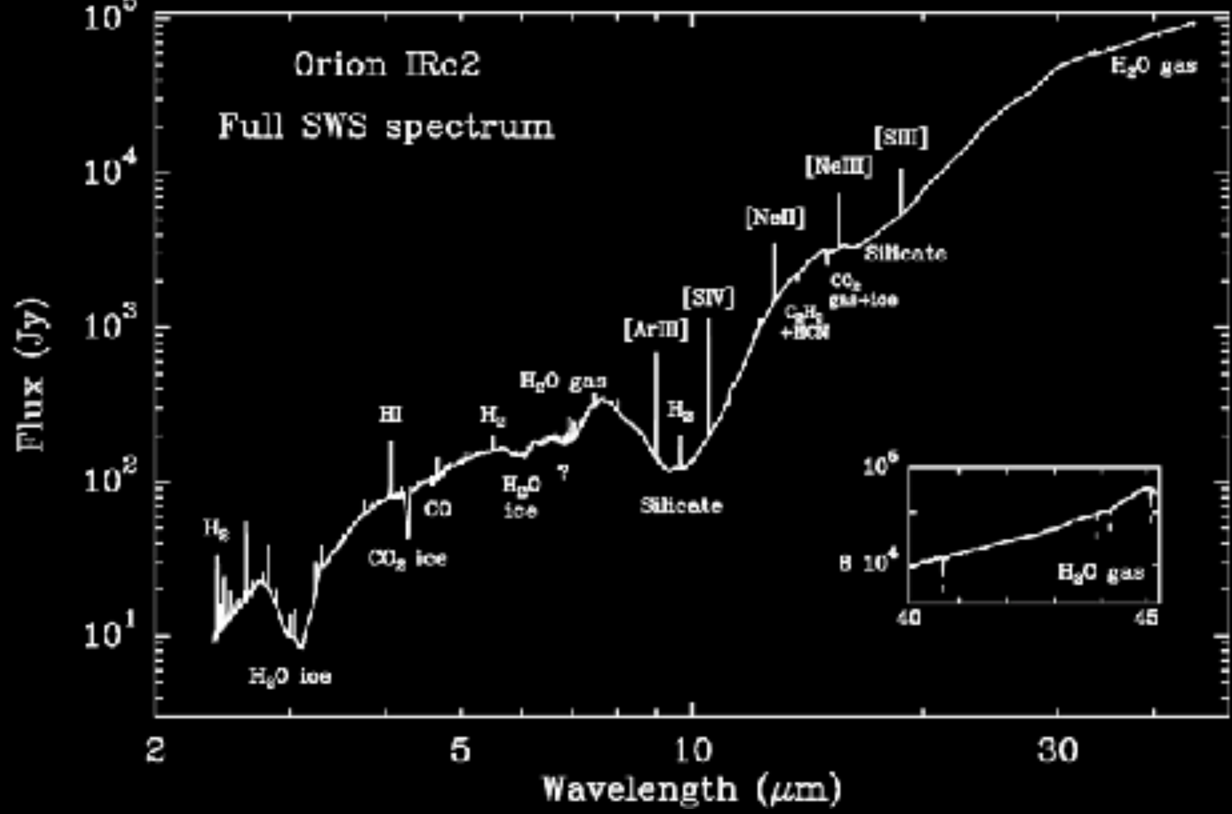


Bally+ 2015

- Orion BN/KL within closest and most studied massive star formation region
- Site of explosion ~500 years ago from multi-body encounter; pushed BN and source I apart (Bally+ 2015)
- Orion hot core was first hot molecular core discovered, via NH_3 emission (Ho+ 1979)
- Orion hot core: atypical, externally heated and has no embedded protostar
- The edge of the Orion hot core is illuminated in MIR by IRc2
- IRc2 is possibly scattered radiation from radio source I (Okumura+ 2011) or source *n* (Simpson+ 2006)
- IRc2 may be cavity in the Orion BN/KL nebula (Wynn-Williams+ 1984)

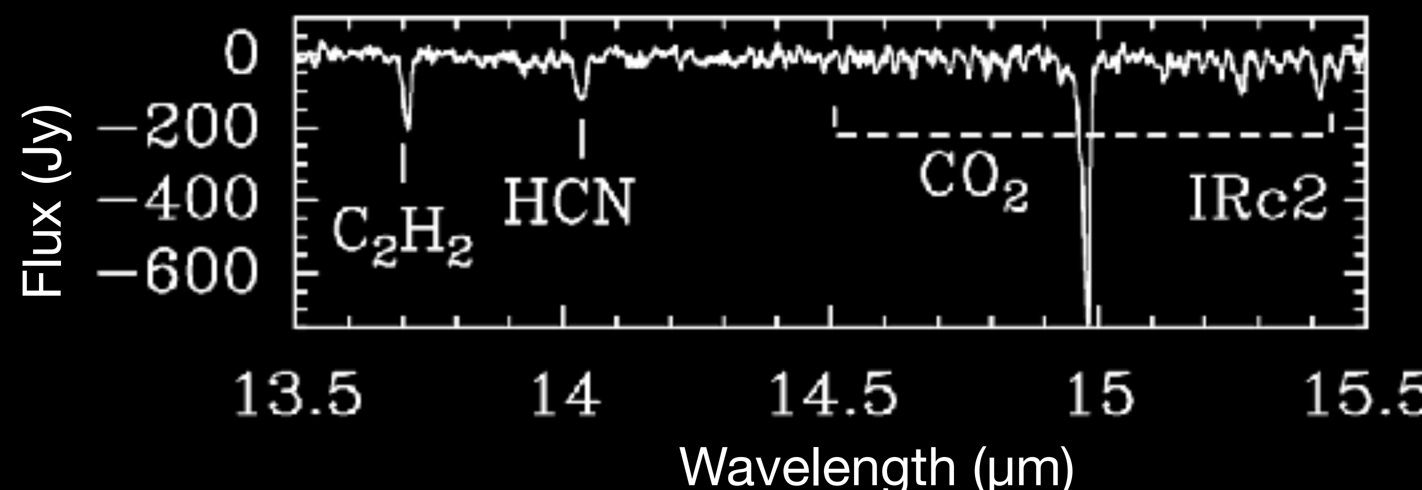
IRc2 in MIR

van Dishoeck+ 1998



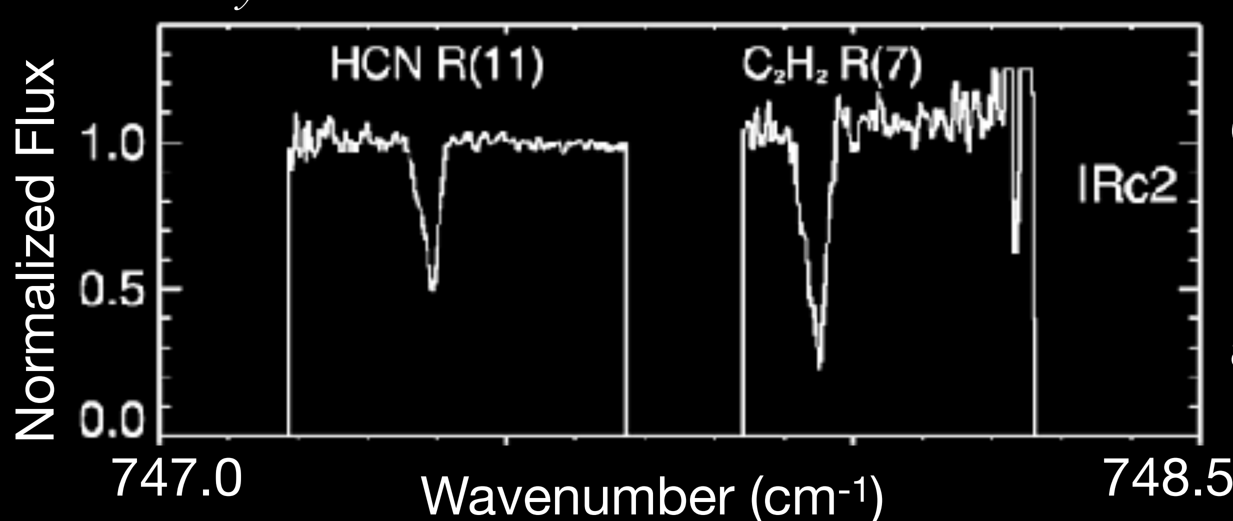
Previous survey in MIR with space-based telescope *ISO* 2.4 to 45.2 μm reveals rich molecular gas chemistry, species CO, H_2, C_2H_2, HCN, SO_2, and CO_2 (van Dishoeck+ 1998)

Boonman+ 2003



From 13.5 to 15.5 μm *ISO* only detects strongest absorption features (Boonman+ 2003); will be similar resolution to *JWST*

Lacy+ 2002



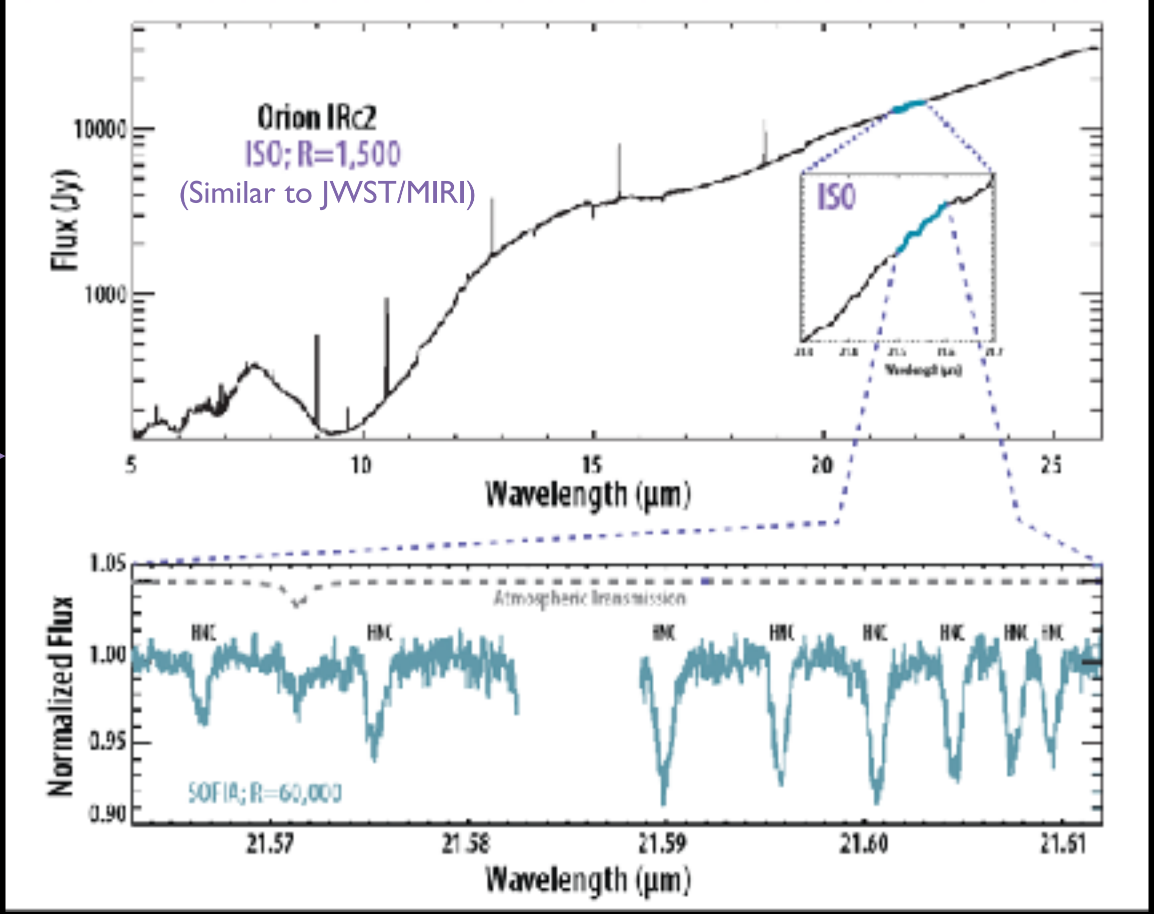
Ground-based TEXES can resolve individual lines of HCN and C_2H_2 in absorption, and SiO in emission but much of MIR is obscured by atmosphere (Lacy+ 2002, 2005)

SOFIA/EXES

- Stratospheric Observatory for Infrared Astronomy (SOFIA) had high spectral capability in the infrared
- Flew above most of the water vapour in the Earth's atmosphere ~40,000 ft
- EXES: Echelle spectrometer, 5–28 μm, resolution 10^3-10^5
- The only spectrograph with high enough resolution to identify individual molecules over the whole MIR
- We conducted an unbiased, MIR line survey at high resolution (R ~ 60,000) from 7.2 to 28.3 μm of Orion IRc2
- Complementary spectra from the ground with IRTF/TEXES

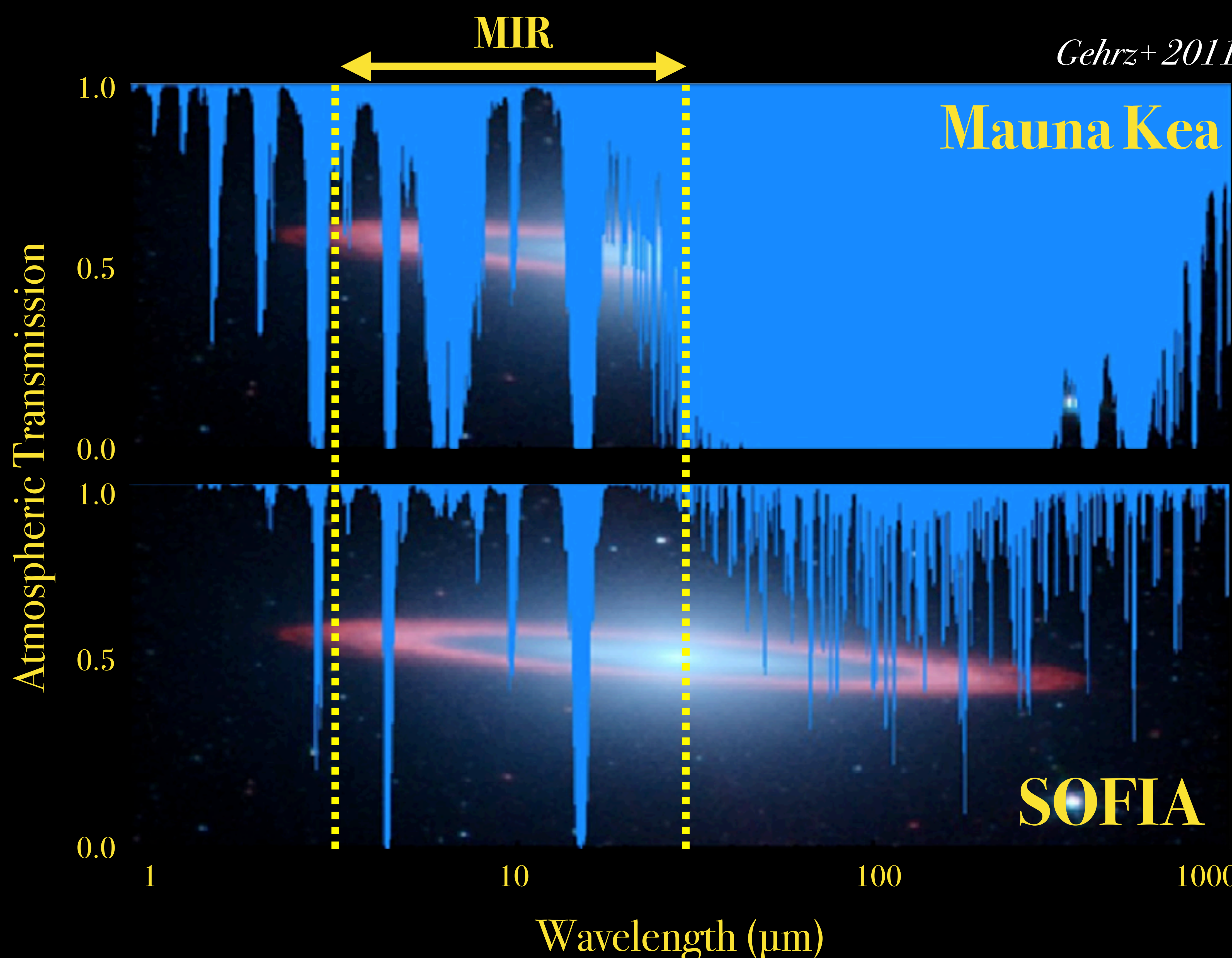
Compare resolution between MIR surveys towards Orion IRc2:

- Top: ISO/SWS, resolution ~1,500 (van Dishoeck et al. 1998), similar to JWST/MIRI
- Bottom: SOFIA/EXES, this survey, HNC absorption lines, resolution ~60,000
- With JWST/MIRI, these lines would be indiscernible from the continuum

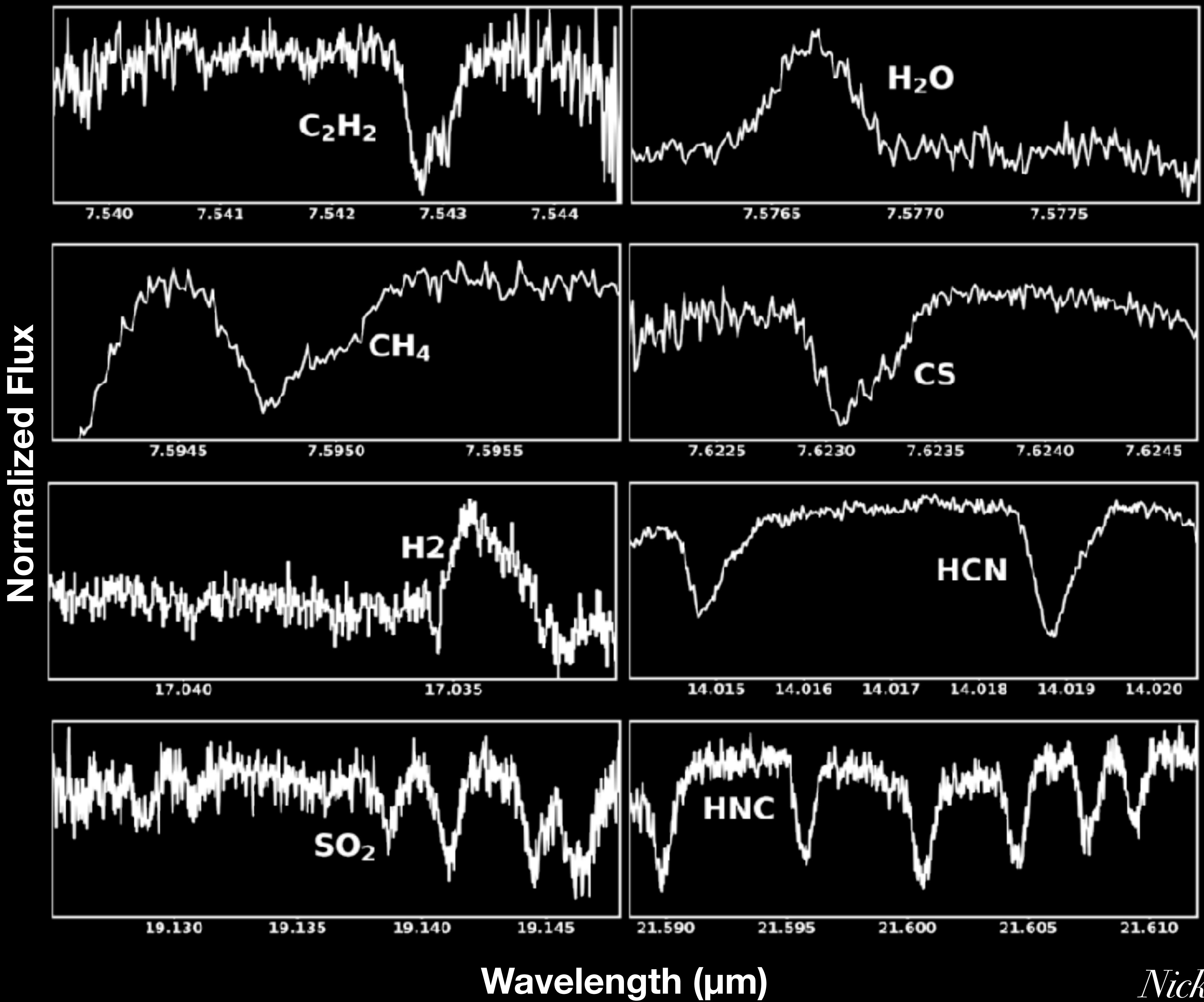


NASA/SOFIA/M. Rose/N. Rangwala

SOFIA versus Ground in MIR



EXES Spectra Towards Orion IRc2



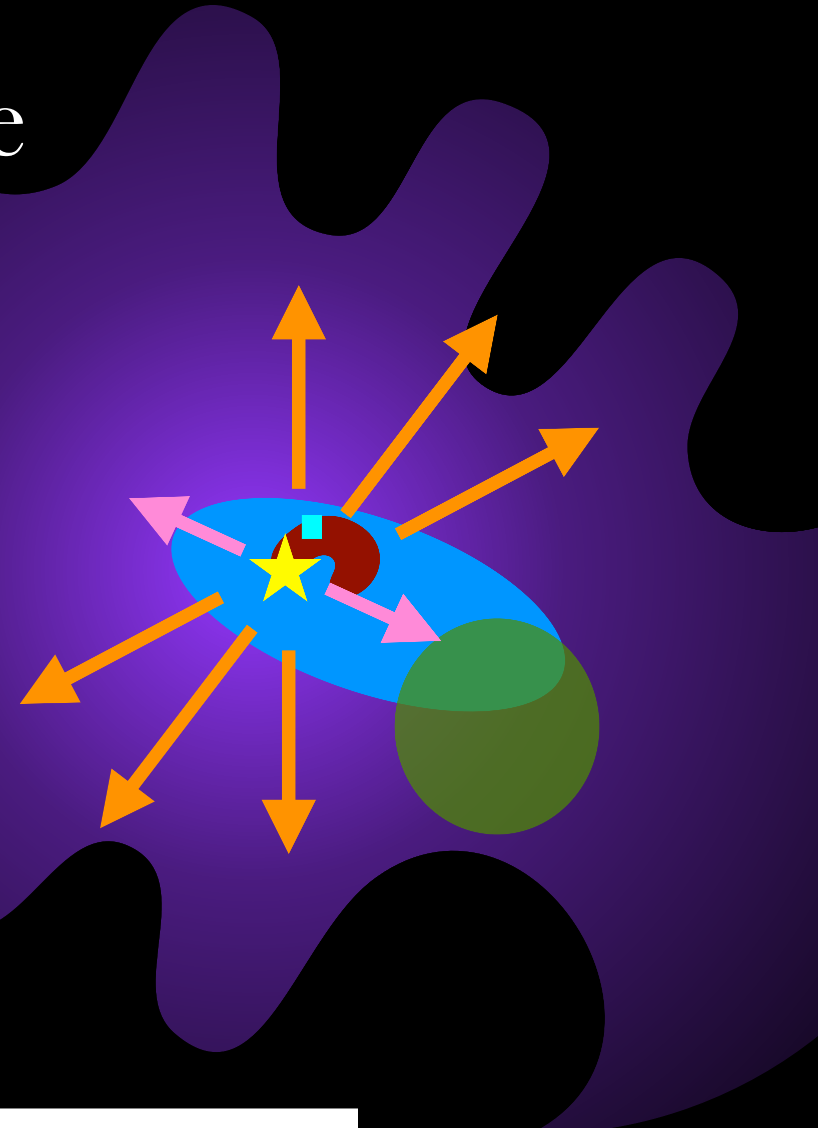
- Spectroscopic survey 7.2 to 28.3 µm
- Over 350 unique features
- Molecular species identified:
  - absorption: HCN, HNC, C_2H_2, H_2O, NH_3, CH_4, SO_2, CS, $H^{13}CN$ and $^{13}CCH_2$
  - emission: H_2, H_2O and SiO
- Detect two velocity components in some absorption species (e.g. C_2H_2, CH_4, and HCN) and H_2 emission
- These two components are newly identified in this work and unique to the MIR

Nickerson+ 2021, ApJ, 907, 51
Nickerson+ 2022, arXiv:2211.15707

Molecular Components of the Orion BN/KL Region

Classic components, from sub-mm to radio spectroscopy in emission:

- Hot Core: hot, dense, and molecular rich
- Extended Ridge: quiescent, ambient gas
- Plateau: outflow from Source I, split into low velocity and high velocity flows
- Compact Ridge: interface between plateau and extended ridge



Composite of maps from: Wright+ 1996, Greenhill+1998, Okumura+ 2011, Crockett+ 2014, and De Buizer + 2012

Diagram is highly schematic and not to scale

Overview of Kinematic Components in Orion BN/KL

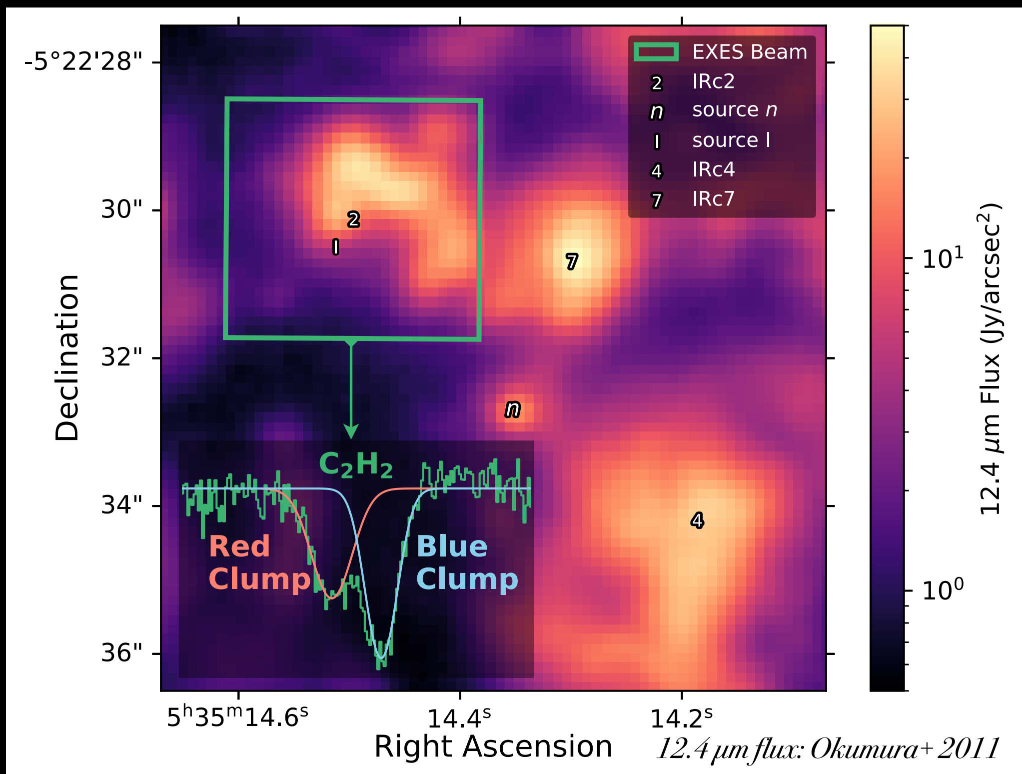
Component	v_{LSR} (km s^{-1})	v_{FWHM} (km s^{-1})	T (K)	Species Detected in This Work
MIR Components (This Work)				
Blue Clump	-7.1 ± 0.7	8.9 ± 1.8	135 ± 47	C_2H_2, $^{13}CCH_2$, CH_4, CS, HCN, $H^{13}CN$, HNC, H_2*, H_2O, NH_3, OH?, SO_2
Red Clump	1.4 ± 0.5	7.7 ± 0.5	146 ± 52	C_2H_2, $^{13}CCH_2$, CH_4, H_2*, HCN
[a]Classic Components (Sub-mm to Radio Surveys)				
Hot Core	[c]2.5–7.5	5–15	[b]150–400	—
Extended Ridge	[c]7–11	3–5	55–70	—
Compact Ridge	[c]7–9	3–5	80–150	—
Plateau	6–9	>20	95–150	—

NOTE—Columns are from left to right: central local standard of rest velocity, line full-width half-maximum, temperature, and species detected in this work only. Numbers are averages for this present work, and a typical range from other works. [a]Ranges are compiled from combing Blake et al. (1987); Genzel & Stutzki (1989); Tercero et al. (2010, 2011); Esplugues et al. (2013) with supplementary data from: [b]Wilson et al. (2000) and [c]Wright et al. (1996). H_2, H_2O, OH, and $2\nu_2$ HCN are not counted towards the average v_{LSR} and v_{FWHM} in this work due to only two or one lines analyzed per species. * denotes emission lines. ? denotes the tentative detection of OH.

- The two kinematic component in this survey detected in absorption lines and H_2 emission
- Have distinct properties from the classic components
- We name them the blue and red clumps for their v_{LSR}

Nickerson+ 2022, arXiv:2211.15707

The Blue and Red Clumps



- Uniquely identified with MIR spectroscopy
- Possibly distinct kinematic components unrelated to classic components
- Absorption species have same v_{LSR} as H_2 emission line in this survey
- Blue and red clumps may or may not be related to hot core, but high abundances suggest hot core-like chemistry regardless of their relationship

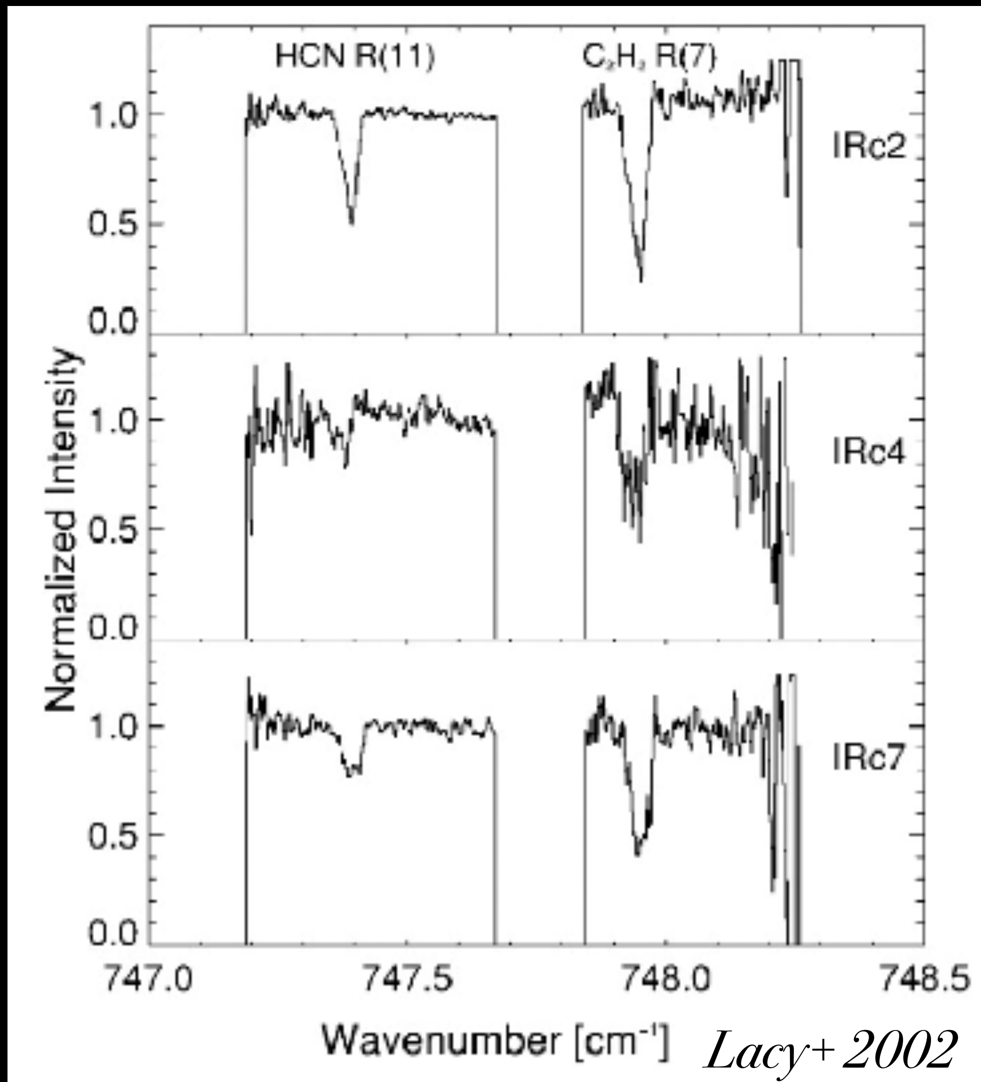
- Blue and red clumps have similar temperatures (~140 K), and FWHM (~8 km/s)
- Different v_{LSR} (-7.1 km/s for blue clump; 1.4 km/s for red clump)
- Blue clump has higher species abundances
- Every absorption species detected in this work is found in the blue clump; red clump contains a subset of these species

Column Density Ratio for Blue and Red Clumps

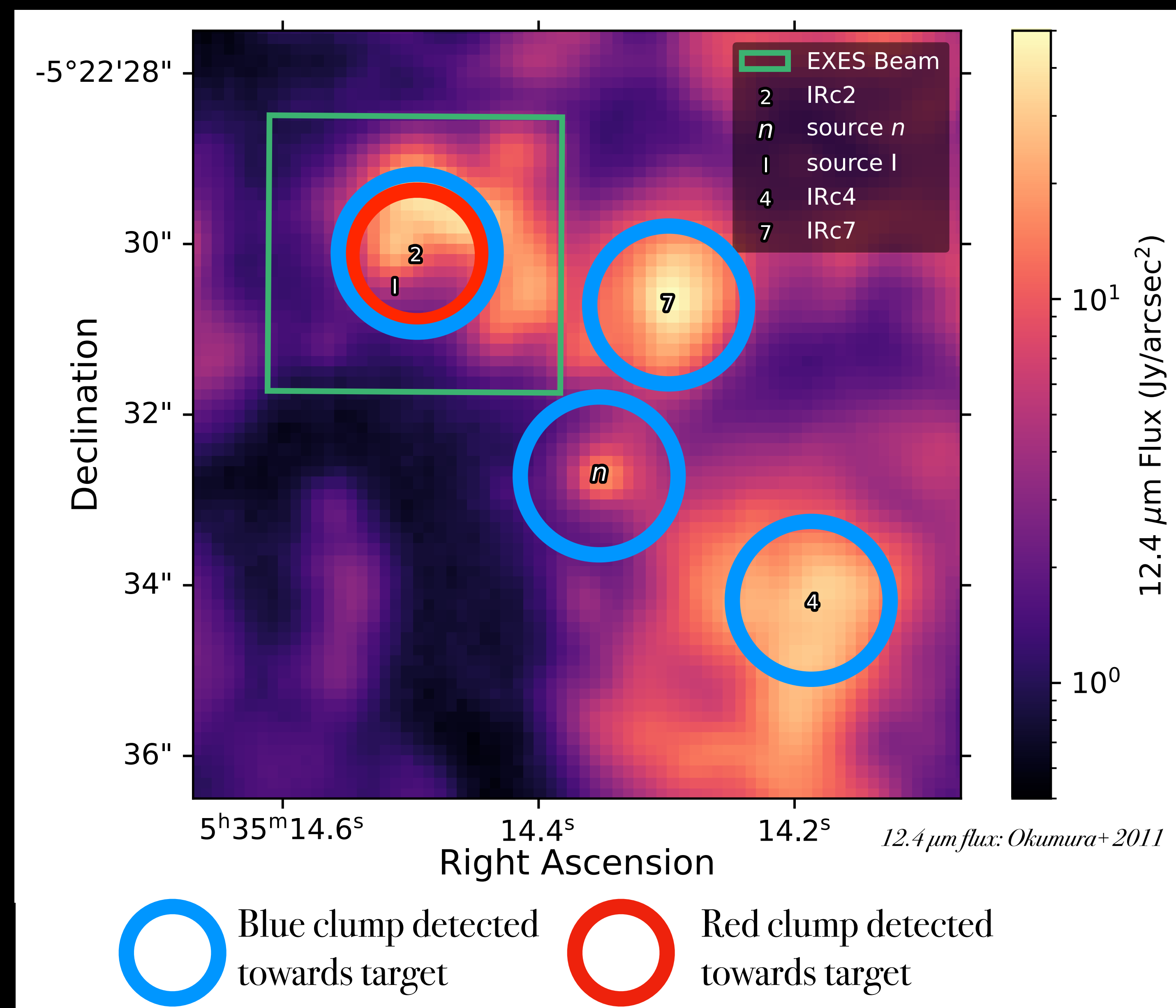
Species	Band	$N_{\text{blue clump}}/N_{\text{red clump}}$
ortho-C_2H_2	ν_5	4.19 ± 0.93
para-C_2H_2	ν_5	3.98 ± 0.88
$^{13}CCH_2$	ν_5	3.80 ± 0.45
ortho-C_2H_2	$\nu_4 + \nu_5$	1.77 ± 0.50
para-C_2H_2	$\nu_4 + \nu_5$	1.37 ± 0.31
CH_4	ν_4	2.26 ± 0.56
HCN	ν_2	2.91 ± 0.65

Nickerson+ 2022, arXiv:2211.15707

Extent of the Blue and Red Clumps



- Spectroscopy towards other targets shows that the blue clump is extended over IRc4, IRc7, and source *n* (Lacy+ 2002, Beuther+ 2010)
- Blue clump is not detected towards BN Object (Scoville+ 1983, Beuther + 2010, Indriolo+ 2018)
- Extent of the red clump is unknown



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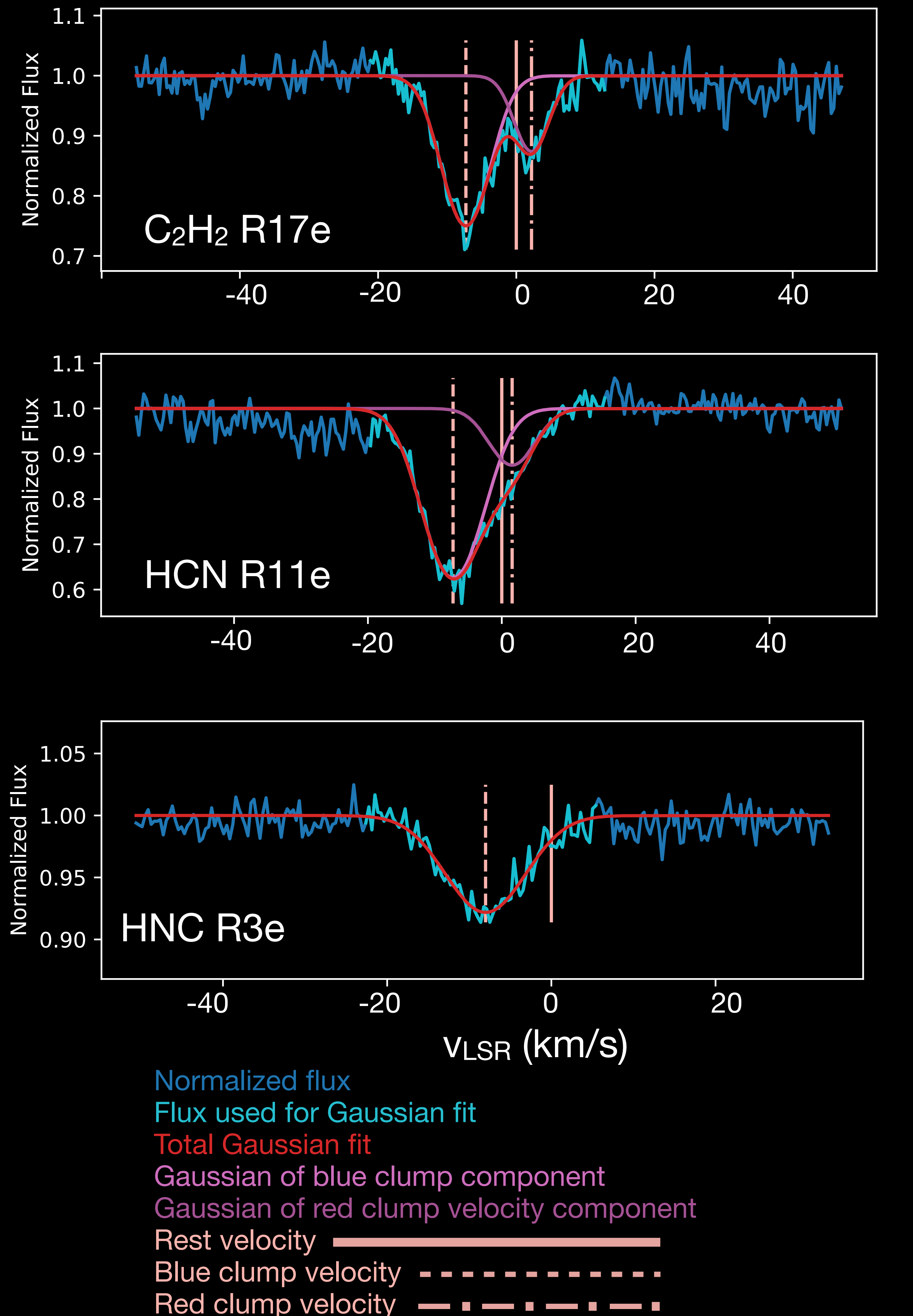
Analysis Recipe

1. Identify line of interest with databases HITRAN (Gordon+ 2017), GEISA (Jacquinet-Husson+ 2015), and ExoMol (Tennyson & Yurchenko 2012)
2. Normalize the baseline around line and atmospheric flux to 1
3. Divide out atmospheric flux
4. Fit line to a Gaussian, or two if second velocity component
5. Integrate under Gaussian for column density
6. Assuming local thermodynamic equilibrium, can fit to Boltzmann's equation (Goldsmith & Langer 1999) to obtain overall column density and excitation temperature of species:

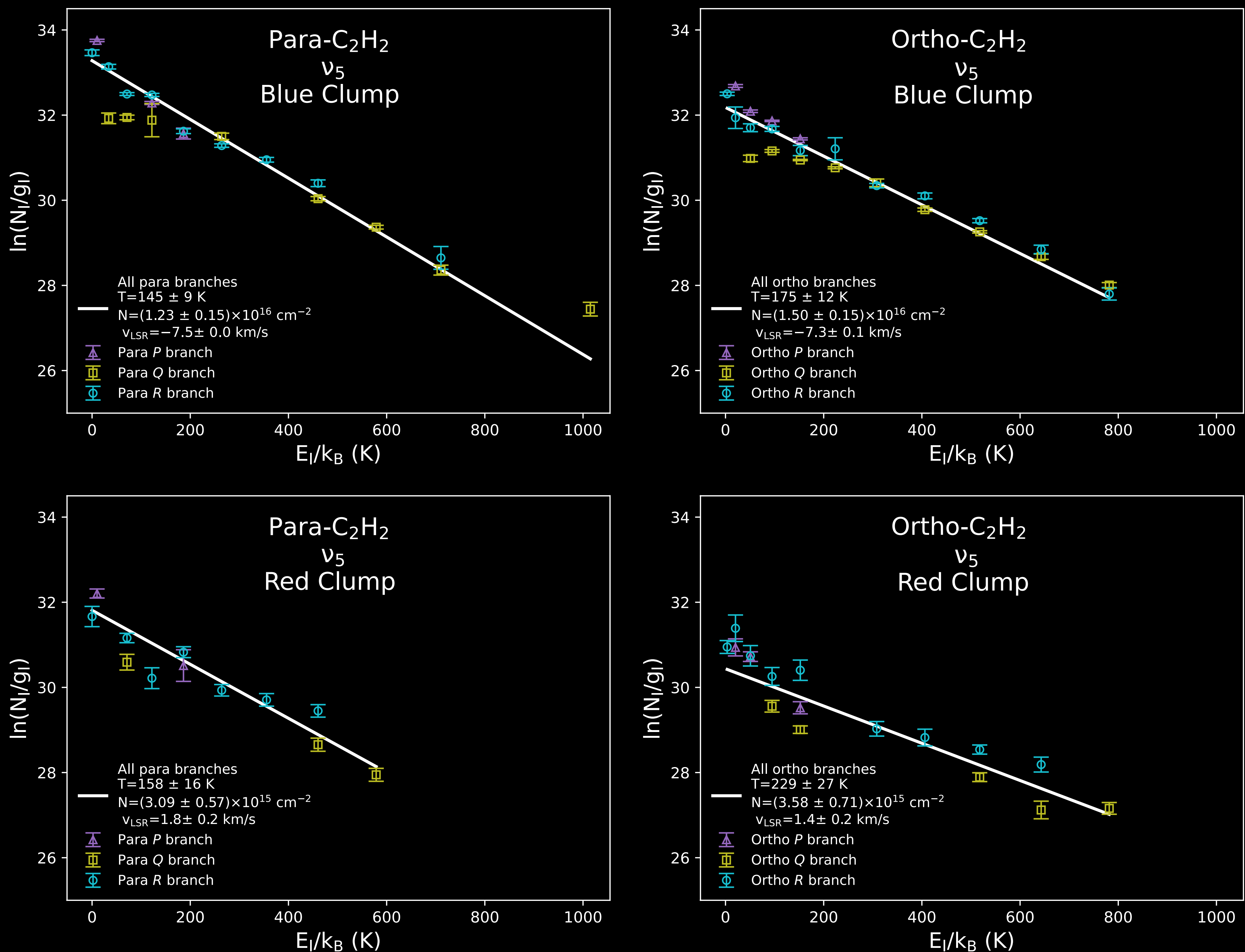
$$\ln \frac{N_j}{g_j} = \ln \frac{N}{Q_R(T_{ex})} - \frac{E}{kT_{ex}}$$

N_j: transition column density
g_j: transition statistical weight
N: total column density

T_{ex}: excitation temperature
$Q_R(T_{ex})$: partition function
E: energy of transition
k: Boltzmann constant



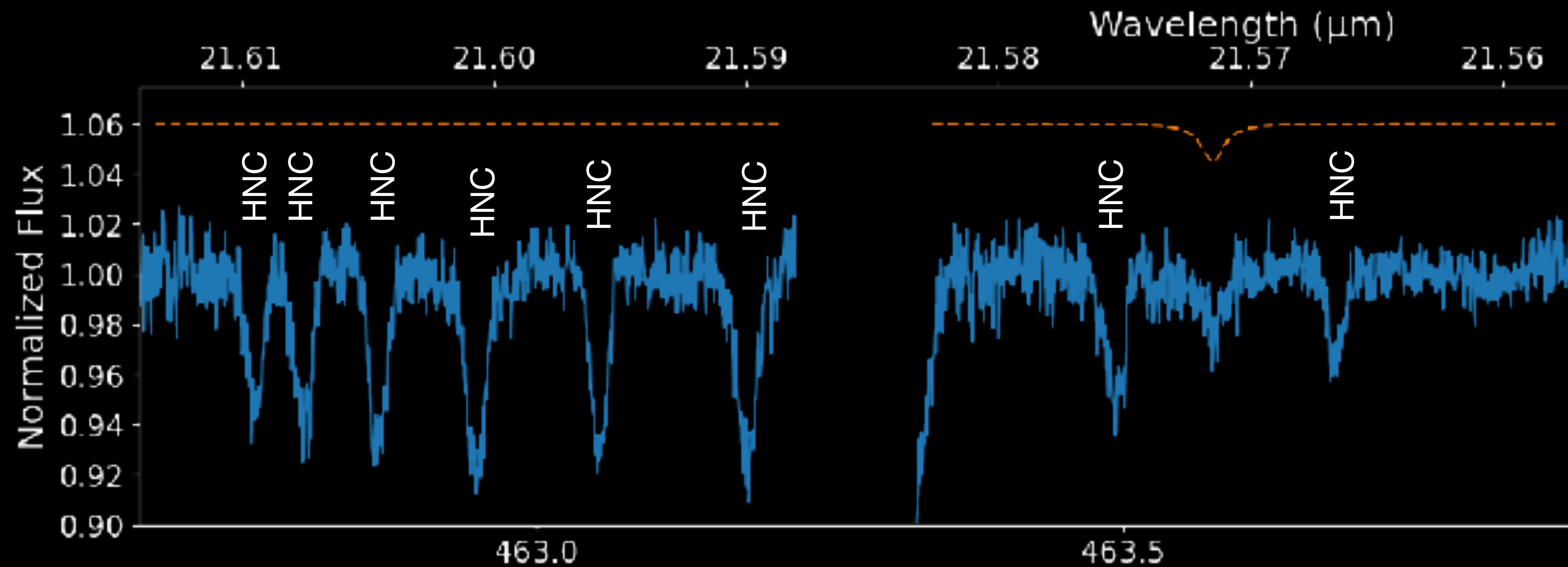
C_2H_2: History and Structure



- Two bands: ν_5 (shown) and ν_{4+5} at different wavelengths
- In both clumps and bands, ortho and para ladders not in equilibrium, trace separate temperatures and densities; ortho-to-para ratio (OPR)~1.2-2.5
- Upon formation on dust grains, H_2 OPR~3, while in cold pre-stellar cores OPR<0.001
- This shows that both clumps are closer to formation than cold gas
- Column densities are higher in both clumps for the ν_{4+5} band compared to the ν_5 band, suggesting that the the ν_{4+5} band probes material deeper into the clumps

Nickerson+ 2022, arXiv:2211.15707

HCN, HNC, and H^{13}CN: History and Mystery

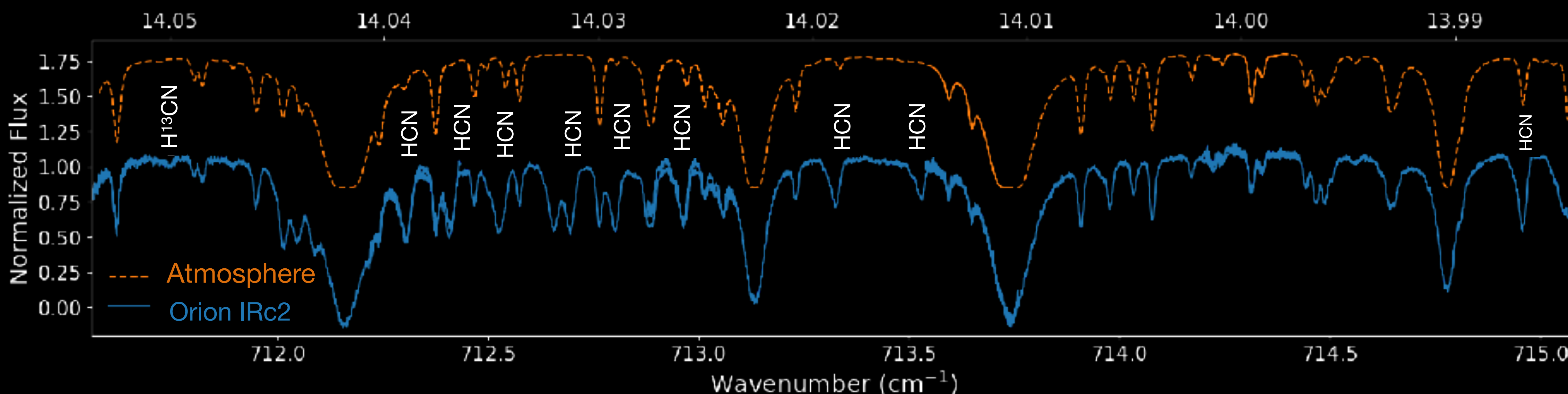


HNC, Blue Clump
T_{ex}~97 K
N~7.4x10^{14} cm^{-2}
V_{LSR}~-7.7 km/s

HCN, Blue Clump
T_{ex}~135 K
N~5.4x10^{16} cm^{-2}
V_{LSR}~-7.3 km/s

H^{13}CN, Blue Clump
T_{ex}=99 K
N=4.4x10^{15} cm^{-2}
V_{LSR}=-6.6 km/s

HCN, Red Clump
T_{ex}~182 K
N~1.9x10^{16} cm^{-2}
V_{LSR}~1.0 km/s



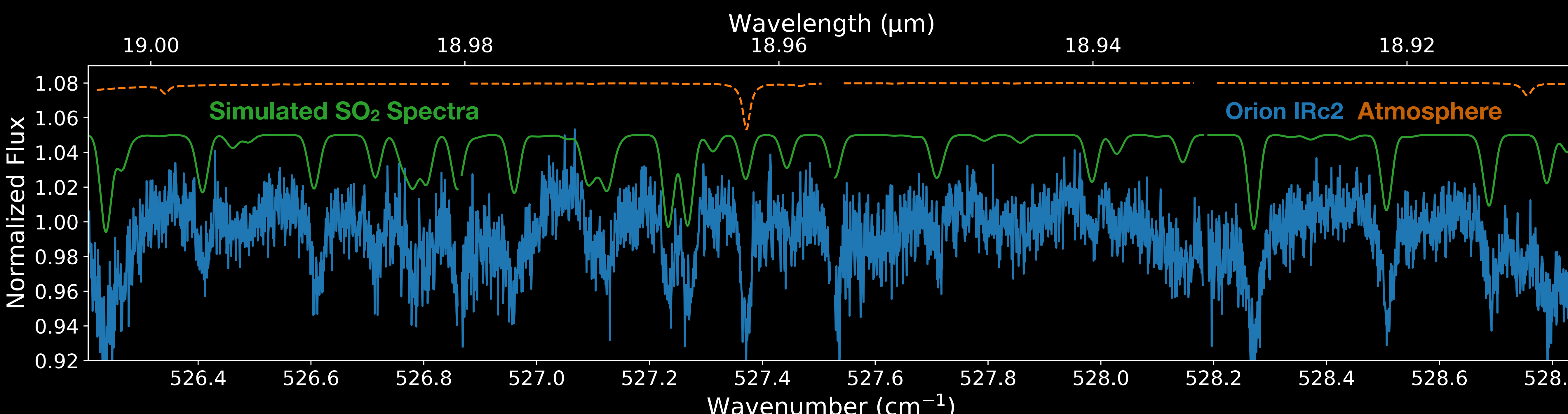
- First MIR detections of HNC and H^{13}CN in the ISM; complement the story of HCN
- HCN/HNC nearly equal at low temperatures (Schilke+ 1992) but HNC depletion increases with temperature (Hirota+ 1998)
- HCN/HNC=73 and with modelling pinpoint the gas's chemical age to ~10^6 years
- $^{12}C/^{13}C$=13 much lower than expected for Galactocentric distance; similar number found with C_2H_2; wider problem requires followup

Nickerson+ 2021

Crowded Lines: SO_2

- SO_2 transitions too numerous and close together to fit individual transitions to Gaussians
- Instead produce simulated spectra from the Boltzman equation, assuming LTE
- With a Markov chain Monte Carlo algorithm (Foreman-Mackey+ 2013) find the parameters that best fit the flux in Orion IRc2
- Similar temperature ~100 K to HNC, $H^{13}CN$, and $^{13}CCH_2$ in the blue clump

ν_2 SO_2
T_{ex}=94 K
N=6.17×10^{16} cm^{-2}
V_{LSR}=-6.1 km/s



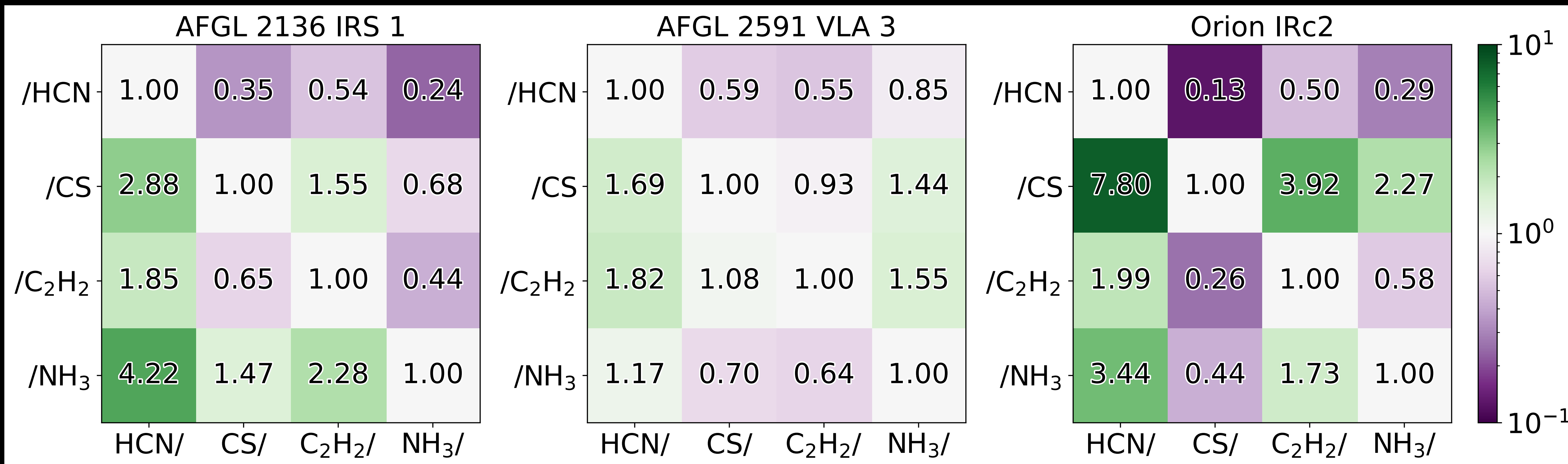
Nickerson+ 2022, arXiv:2211.15707

New Targets: Diverse Hot Cores

- MIR-bright hot cores identified as molecular-rich by *ISO*
- < 7 μm covered by publications and SOFIA archival data
- New EXES observations in 2022 extend coverage: 7 to 24 μm
- Analyzing new data, and complement with archival data and publications to construct the MIR inventory of these hot cores

All images: 2MASS in NIR (except Orion IRc2 in MIR, Okumura+ 2013)

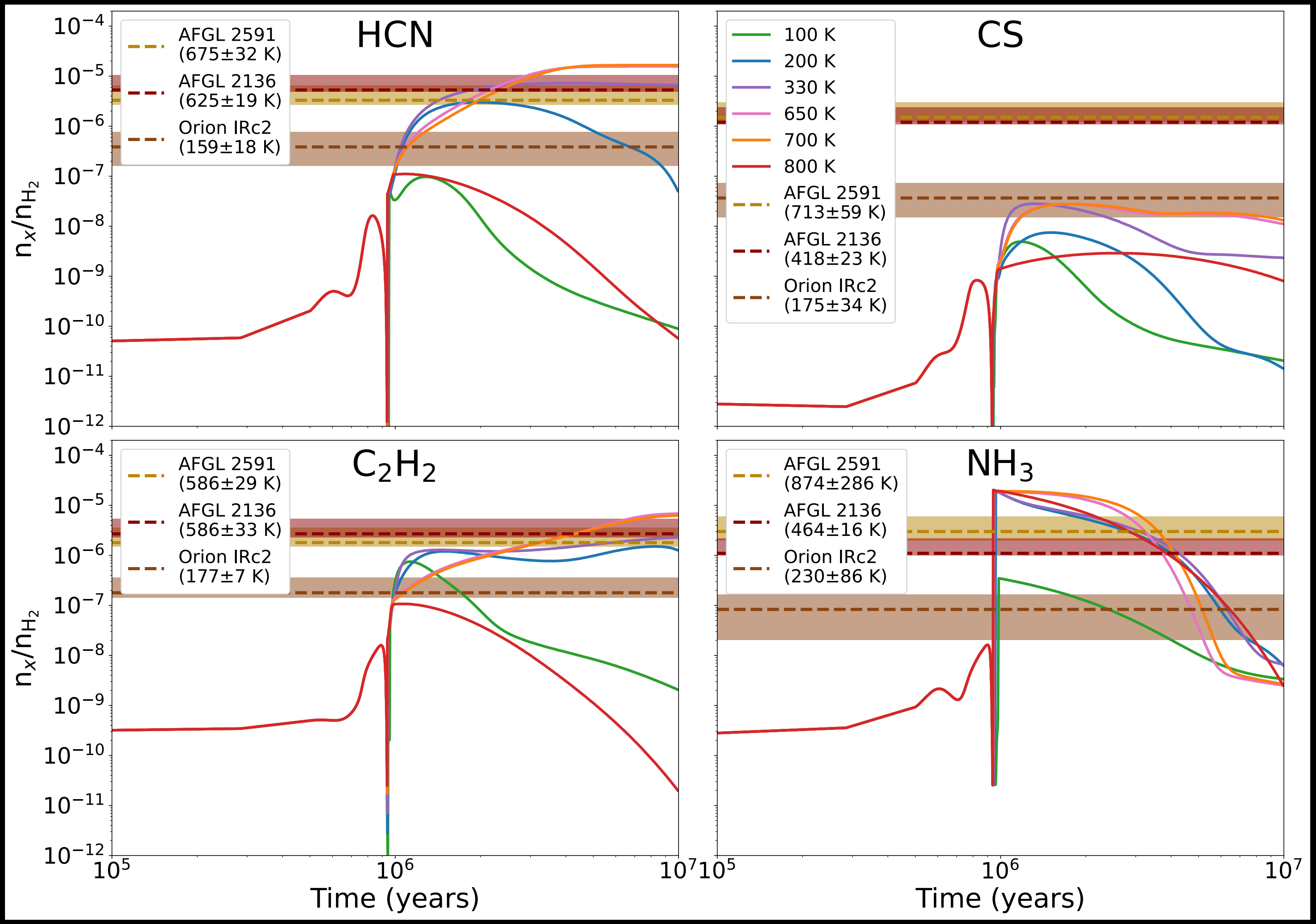
Preliminary: Comparing Species Abundance Ratios Across Hot Cores



- AFGL 2136 and 2591 are conventional hot cores surrounding massive protostars; Orion IRc2 atypical, externally heated
- C_2H_2/HCN similar across hot cores, other species inconsistent
- NH_3 lower in AFGL 2591
- CS lower towards Orion IRc2
- What causes these differences in molecular abundances? Orion IRc2 is expected to be different, but not AFGL 2136 and 2591
- In future will tabulate more species and hot cores

AFGL 2136 and 2591: Barr+ 2020; Orion IRc2: Nickerson+ 2022 arXiv:2211.15707

Preliminary: Comparing Species Abundance Ratios Between Observation and Simulations



- Compare to gas-grain chemical network (Acharyya & Herbst 2018) that traces hot core evolution in three phases: free fall collapse, warmup (9.35 to 9.85 × 10^5 years), and post-warmup
- For HCN, C_2H_2, NH_3 the model matches the observed abundances at some point during its evolution for most temperature models
- CS is much lower in the model compared to the hot cores. Unexpectedly Orion IRc2 is the closest despite it being an atypical situation

- This suggests that there is an unknown mechanism that produces extra CS in massive star forming regions, not accounted for in theoretical models.
- In future, we will add more hot cores and species to this analysis

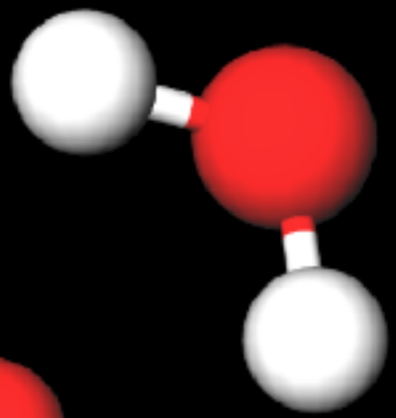
MIR Python Analysis Toolkit

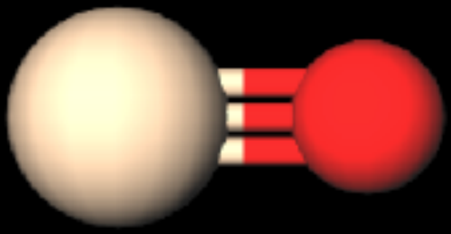
- Publicly available analysis tools for spectroscopy are focussed on longer wavelengths, FIR to sub-mm
- Nothing for the MIR
- Developed Python Toolkit to analyze EXES and TEXES high resolution spectra; includes:
  - Visualization
  - Molecule identification using MIR line lists from databases (HITRAN, GEISA, and ExoMol), and custom line lists
  - Peak finder and noise finder
  - Fitting atmospheric models to data for subtraction
  - Rotation diagram analysis of both absorption and emission lines
  - Production and fitting of simulated spectra
- Presently not ready for public availability but happy to share and collaborate on request
- Considering public release in future

Student Projects

Jose Monzon, Yale University PhD student:

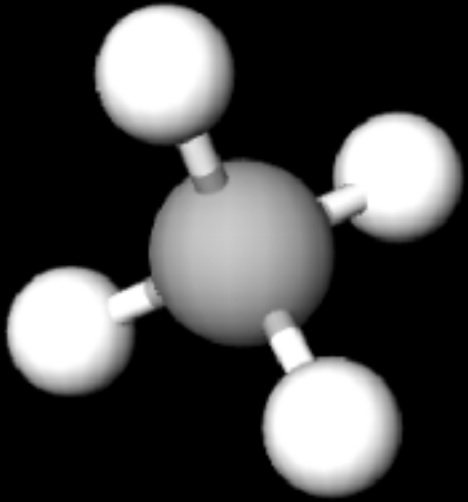
- Working on a paper that focusses on the H_2O and SiO emission lines towards Orion IRc2 with SOFIA/EXES and IRTF/TEXES
- Associated with outflow, not the molecular absorption lines
- (Monzon+ 2023 in prep)





Ciera Knabe, University of Texas at Austin undergraduate student:

- Measuring CH_4 towards the hot core NGC 7538 IRS 1 with SOFIA/EXES
- Comparing methane across hot cores
- An important molecule to life only seen at these wavelengths
- (Knabe+ 2023 in prep)



Ultimately, What Do We Learn From Hot Cores?

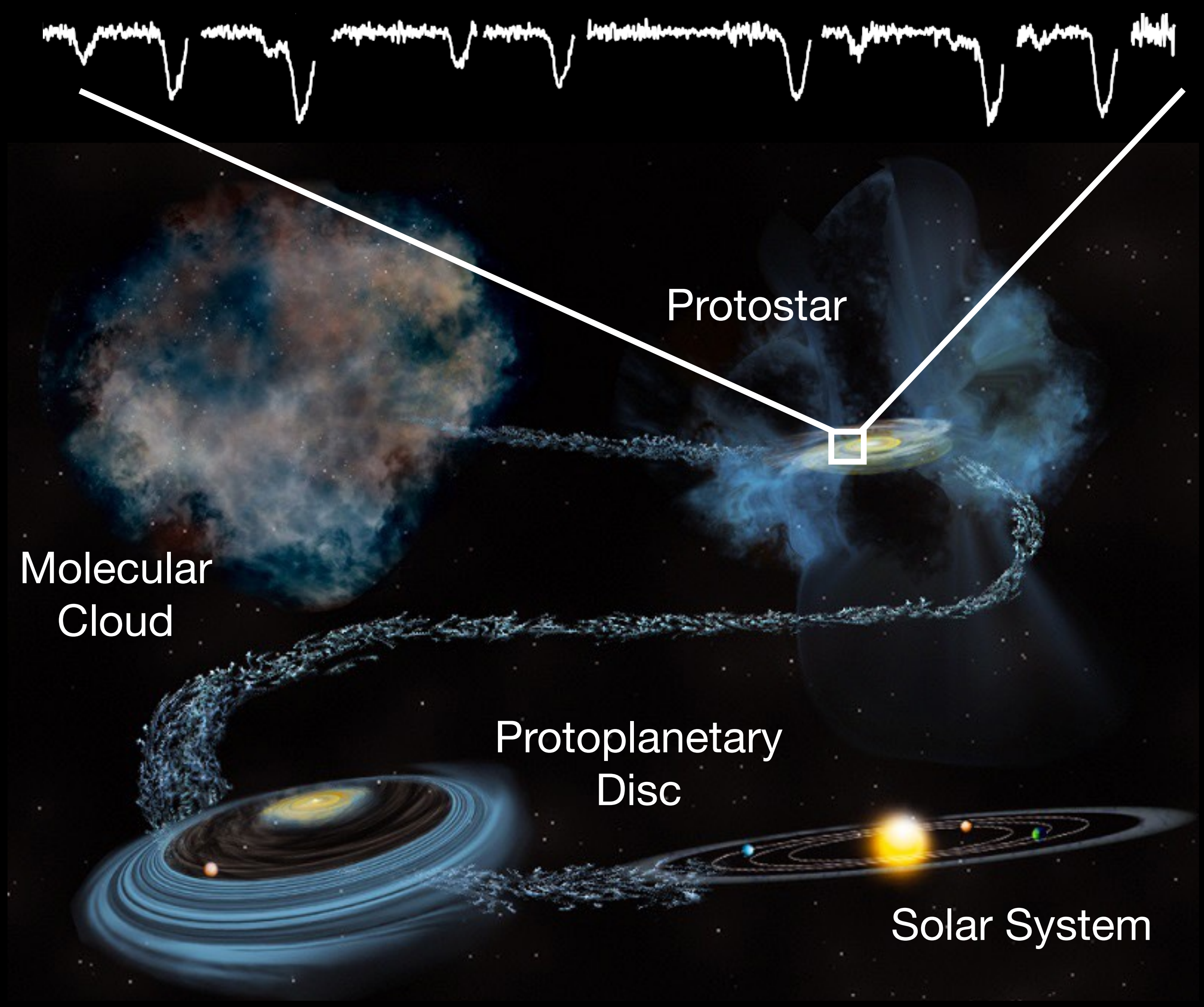


Illustration: Bill Saxton, NSF/AUI/NRAO; Spectra: H_2O towards AFGL 2136 (Indriolo+ 2020)

- Massive protostars probe the state of the interstellar medium at the earliest stages of star formation
- Our own sun may have formed in a massive star-forming region
- This gas contains the precursors to probiotics that will form planetary systems such as our own
- Studying hot cores will elucidate the origins of prebiotic molecules and inform chemical modelling
- We are constructing the first MIR inventory across multiple hot cores
- The MIR accesses unique molecules and transitions
- Will inform low resolution JWST/ MIRI spectra of fainter hot cores and hot corinos around solar mass protostars, as well as protoplanetary discs

Conclusions

- With SOFIA/EXES, we have surveyed the molecular inventory towards Orion IRc2 in MIR from 7.2 to 28 μm (Nickerson+ 2022 arXiv:2211.15707, accepted to ApJ)

- Species reveal new kinematic components in the MIR that are undetectable at longer wavelengths, and clues on the history and structure of these components
- First MIR observations of HNC and $H^{13}CN$ in the ISM, along with numerous HCN transitions (Nickerson+ 2021)
- In preparation:
  - H_2O and SiO emission lines with EXES and TEXES towards IRc2 (Monzon+ 2023 in prep)
  - CH_4 absorption towards hot core tne NGC 7538 IRS 1 (Knabe+ 2023 in prep)

- Analyzing now SOFIA/EXES observations of molecular lines towards other hot cores
- Will unlock what these species reveal about the hot core's histories and physical conditions
- This high resolution work in the MIR will provide a reference to compare lower resolution JWST observations

Only SOFIA/EXES, complemented from the ground by TEXES, could do this science!

Lynette Cook