Building the Mid-Infrared Inventory for the Orion Hot Core

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Bay Area Environmental Research Institute

Stratospheric Observatory for Infrared Astronomy

SOFIA Community Tele-Talk
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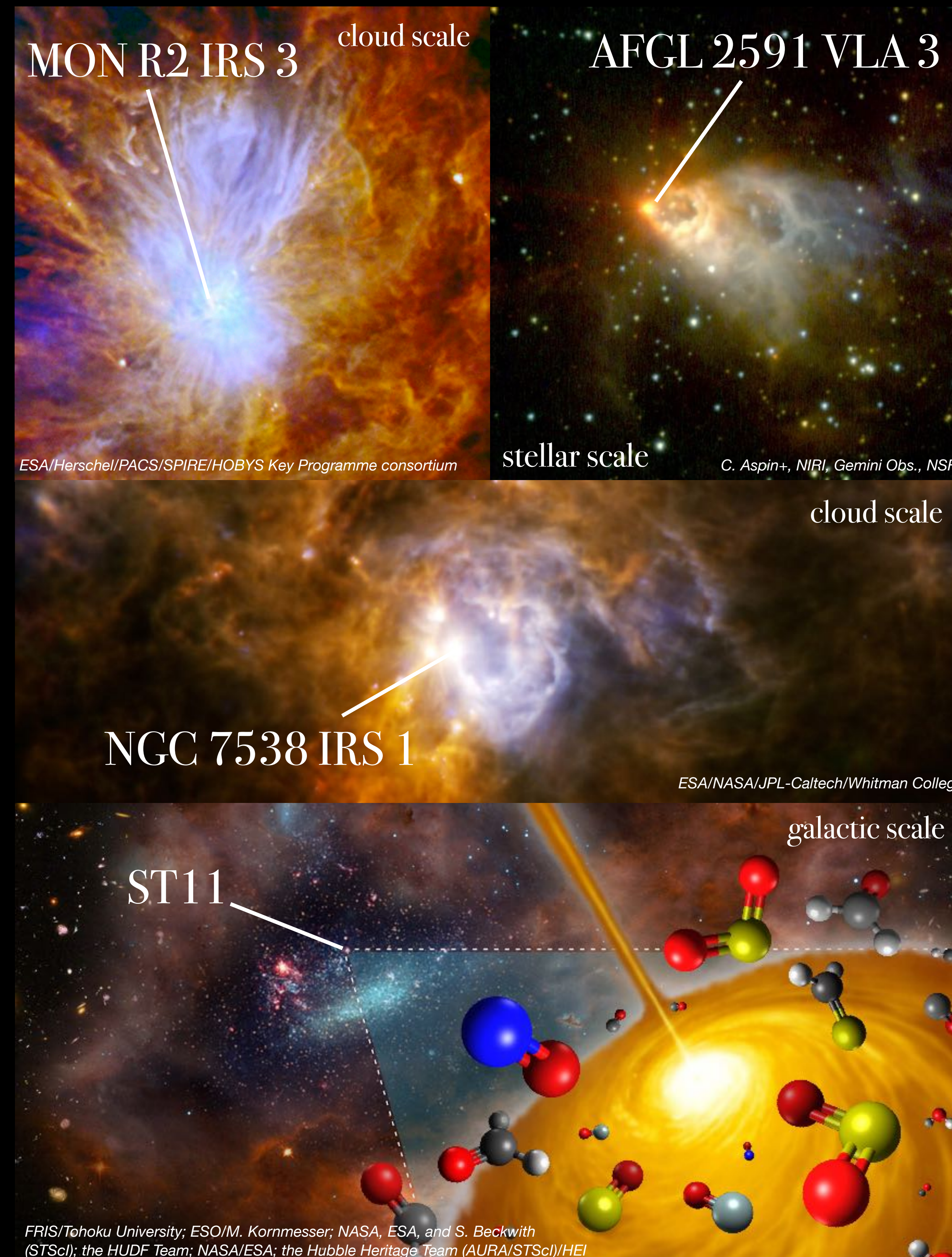
Hot Molecular Cores

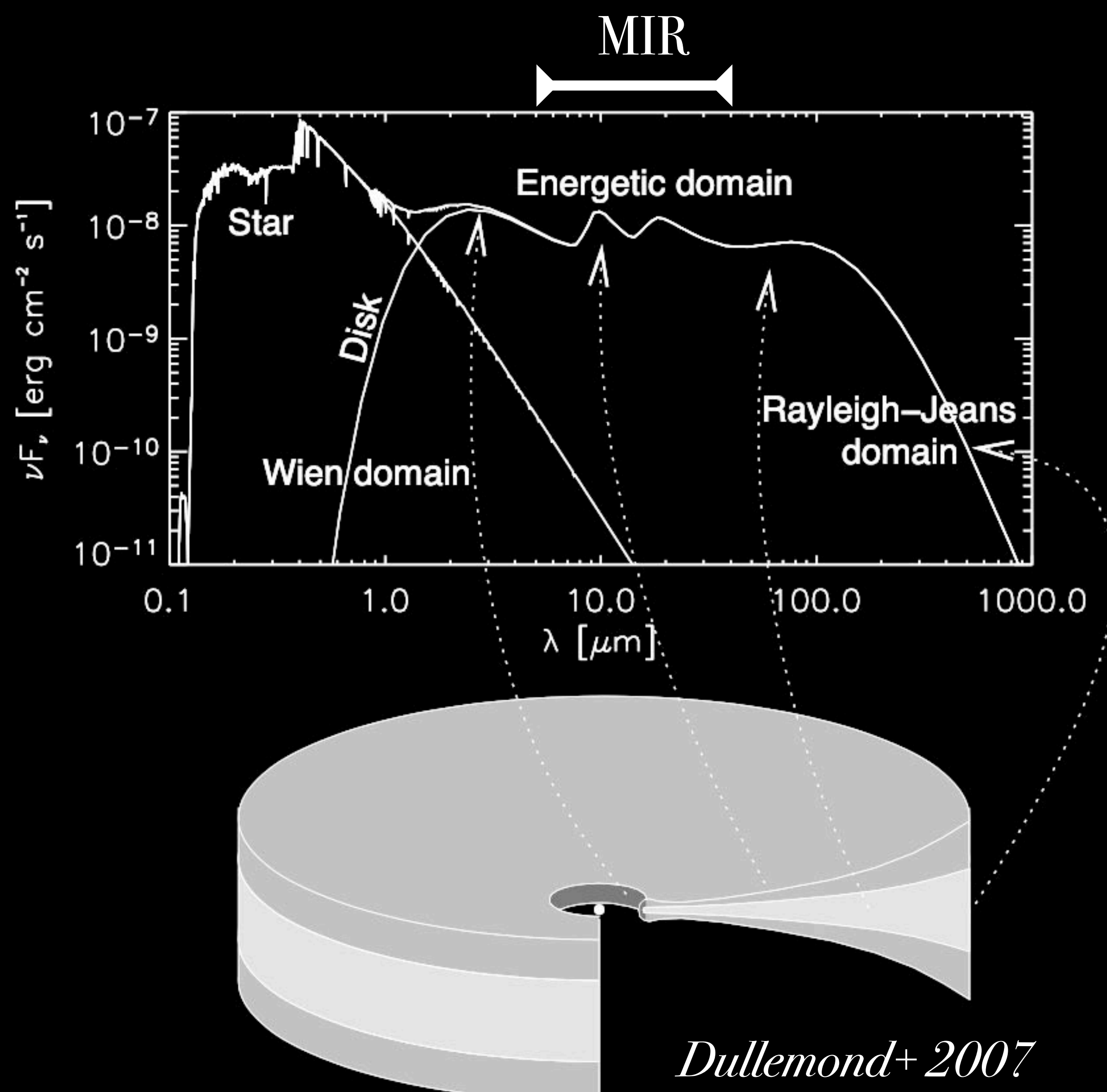
- Warm (≥ 100 K), small (≤0.1 pc) and dense (10^5 to 10^8 cm^{-3}) gas near young, high mass protostars (Ohisi 1997)
- Stellar radiation evaporates ice on dust grains in molecular clouds
- Unlocks chemically rich reservoirs of complex and prebiotic molecules
- Abundant in rare molecular species (Kurtz+ 2000)
- Become the building blocks of planetary systems, such as our own Solar System
- At least 35 discovered in the Milky Way, 4 total in the LMC



Hot Core Molecular Line Surveys

- 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

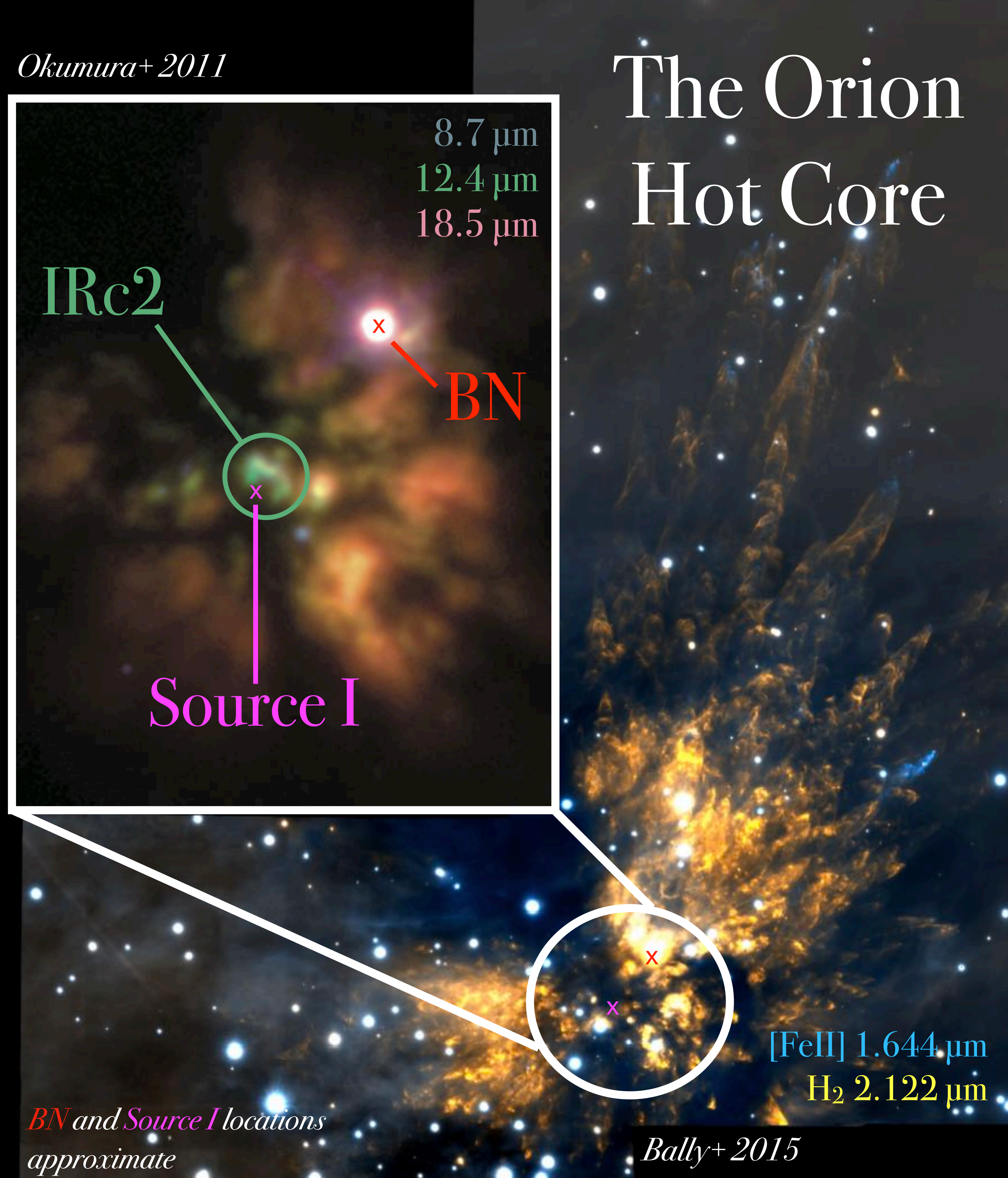
- Only the mid-infrared (MIR) can observe rovibrational transitions and molecules with no permanent dipole moment
- Radio to FIR captures molecules in cooler, outer regions of discs while the MIR to NIR covers the inner regions (Dullemond+ 2007, Barr+ 2020, Nickerson+ 2021)
- MIR difficult to access because of atmospheric interference
- Past space telescopes *ISO* and *Spitzer*, and future *JWST* cannot resolve individual lines of hots cores in the MIR



Dullemond+ 2007

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

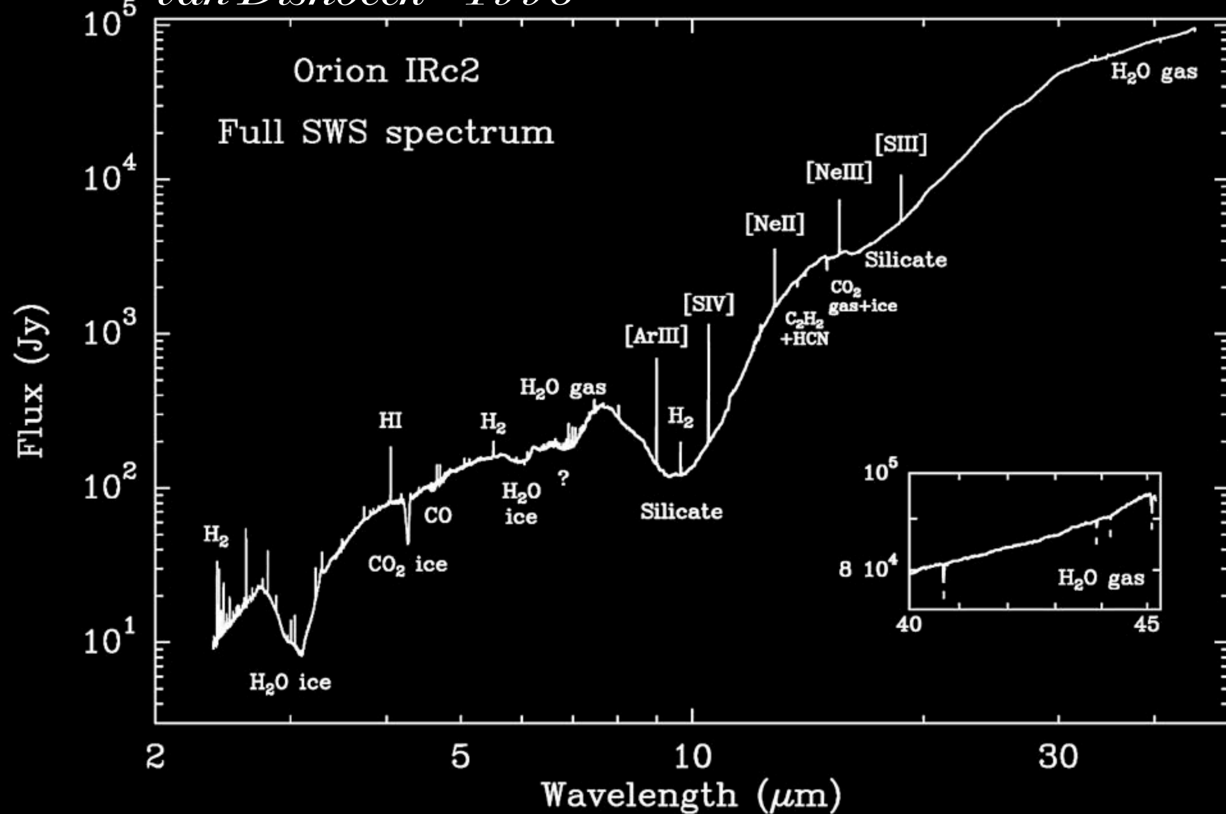
The Orion Hot Core



- Orion BN/KL closest and most studied massive star formation region
- Site of explosion ~500 years ago from multi-body encounter; pushed sources BN and I apart (Bally+ 2015)
- Orion hot core was first hot molecular core discovered, via NH_3 emission (Ho+ 1979)
- Atypical for a hot core; externally heated
- Illuminated in MIR by IRc2, scattered radiation from radio source I (Okumura+ 2011)
- Hot core may be cavity or pre-existing clump (Shuping+ 2004, Zapata+ 2011)
- Possibly heated externally by embedded radio source I which has no IR component

IRc2 in MIR

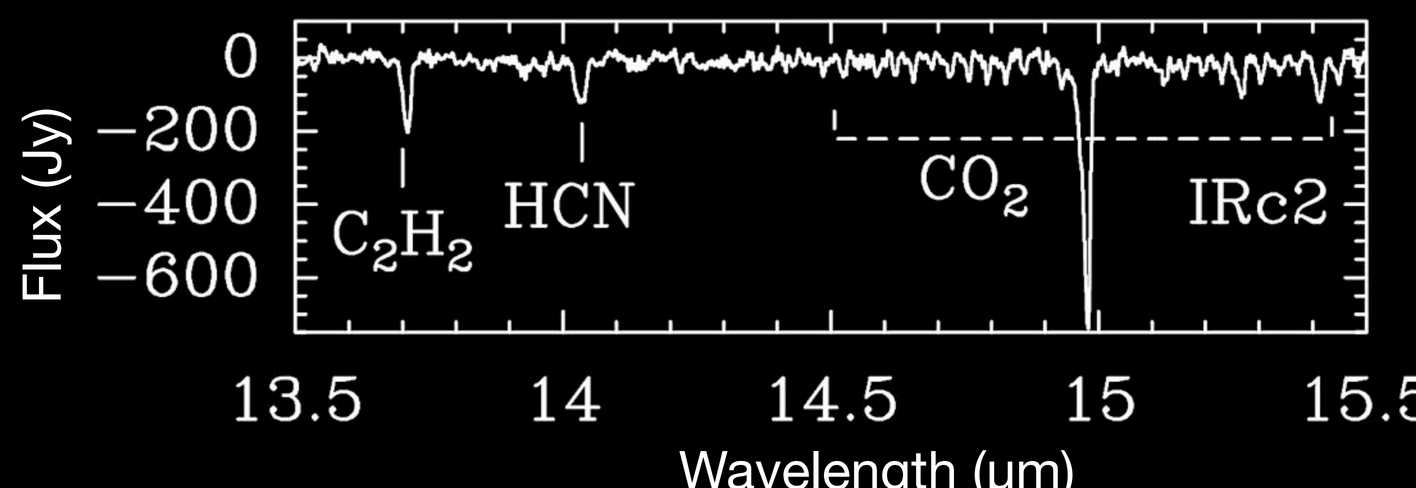
van Dishoeck+ 1998



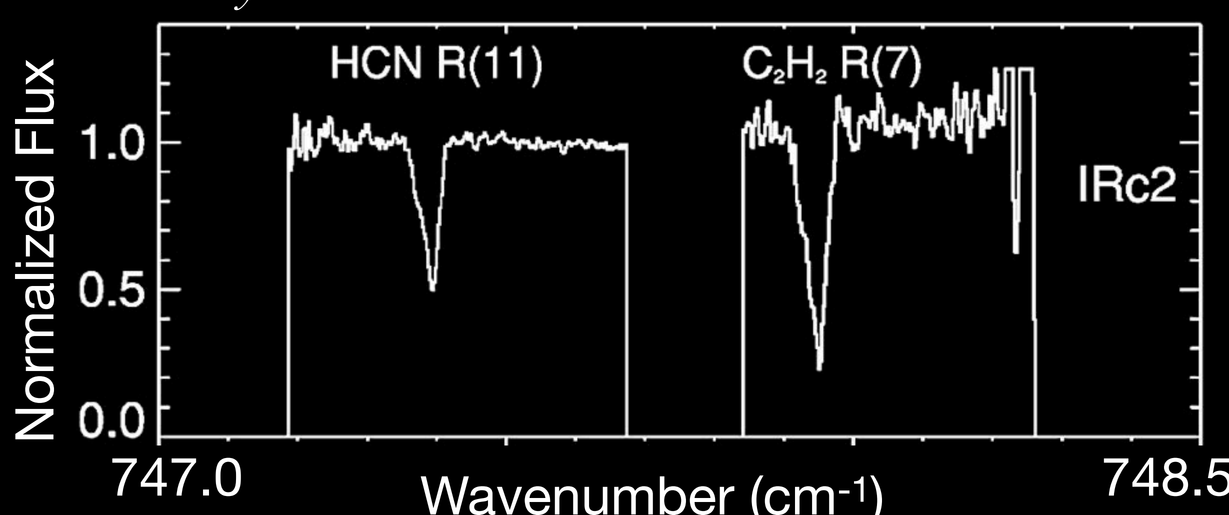
Previous survey in MIR with space-based telescope *ISO* 2.4 to 45.2 μm reveals rich molecular gas chemistry, species CO, H_2, C_2H_2, HCN, SO_2, and CO_2 (van Dishoeck+ 1998)

From 13.5 to 15.5 μm *ISO* only detects strongest absorption features; excitation temperatures of ~175-275 K (Boonman+ 2003)

Boonman+ 2003



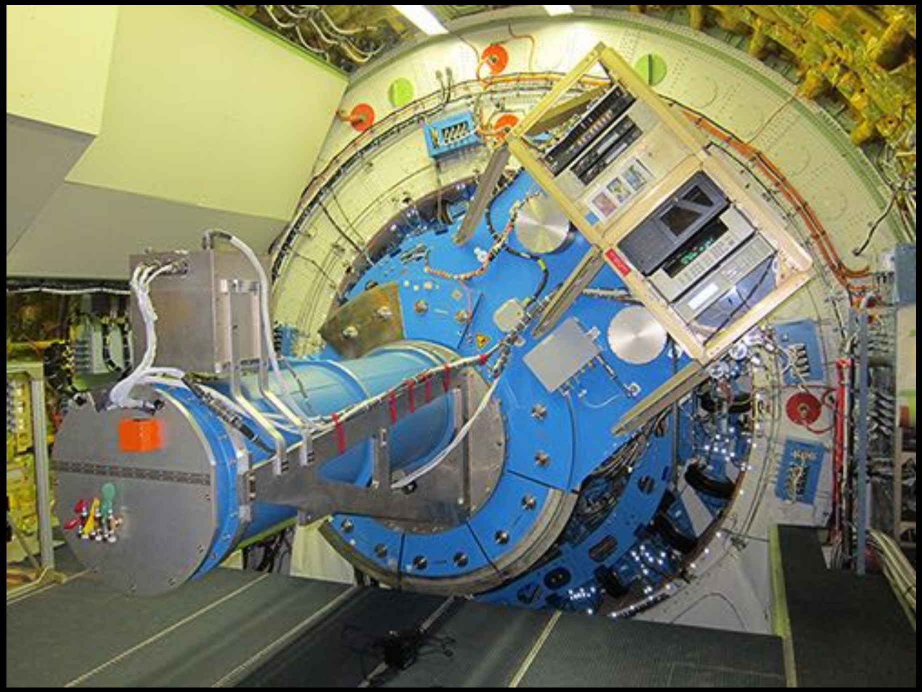
Lacy+ 2002

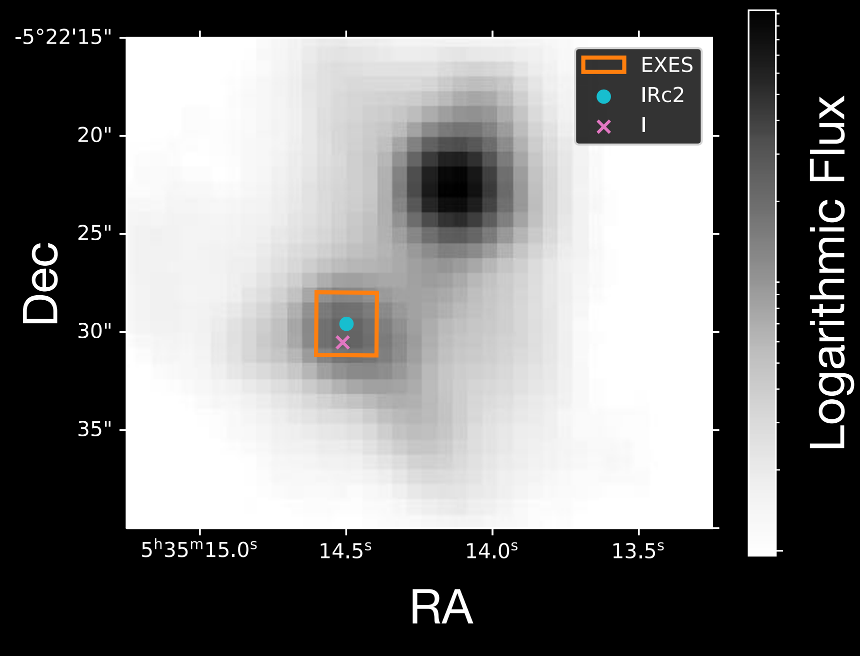


Ground-based TEXES can resolve individual lines of HCN and C_2H_2 in absorption, and SiO in emission but much of MIR is obscured by atmosphere; for absorption lines v_{LSR}~-10 km/s (Lacy+ 2002, 2005)

Note: ambient cloud velocity v_{LSR}~9 km/s (Genzel & Stutzki 1989)

SOFIA/EXES



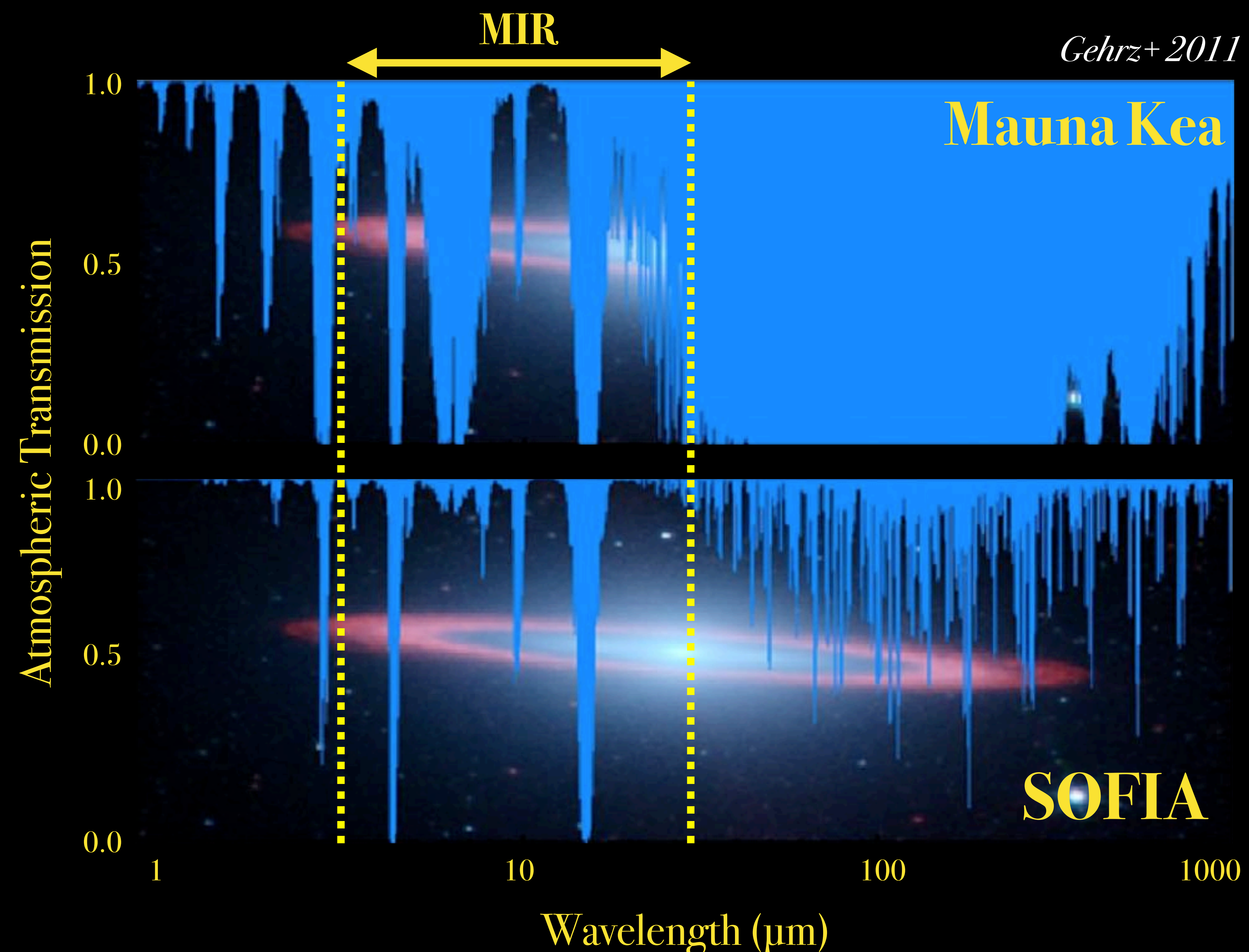


EXES slit at 7.6 μm setting projected onto FORCAST image at 7 μm

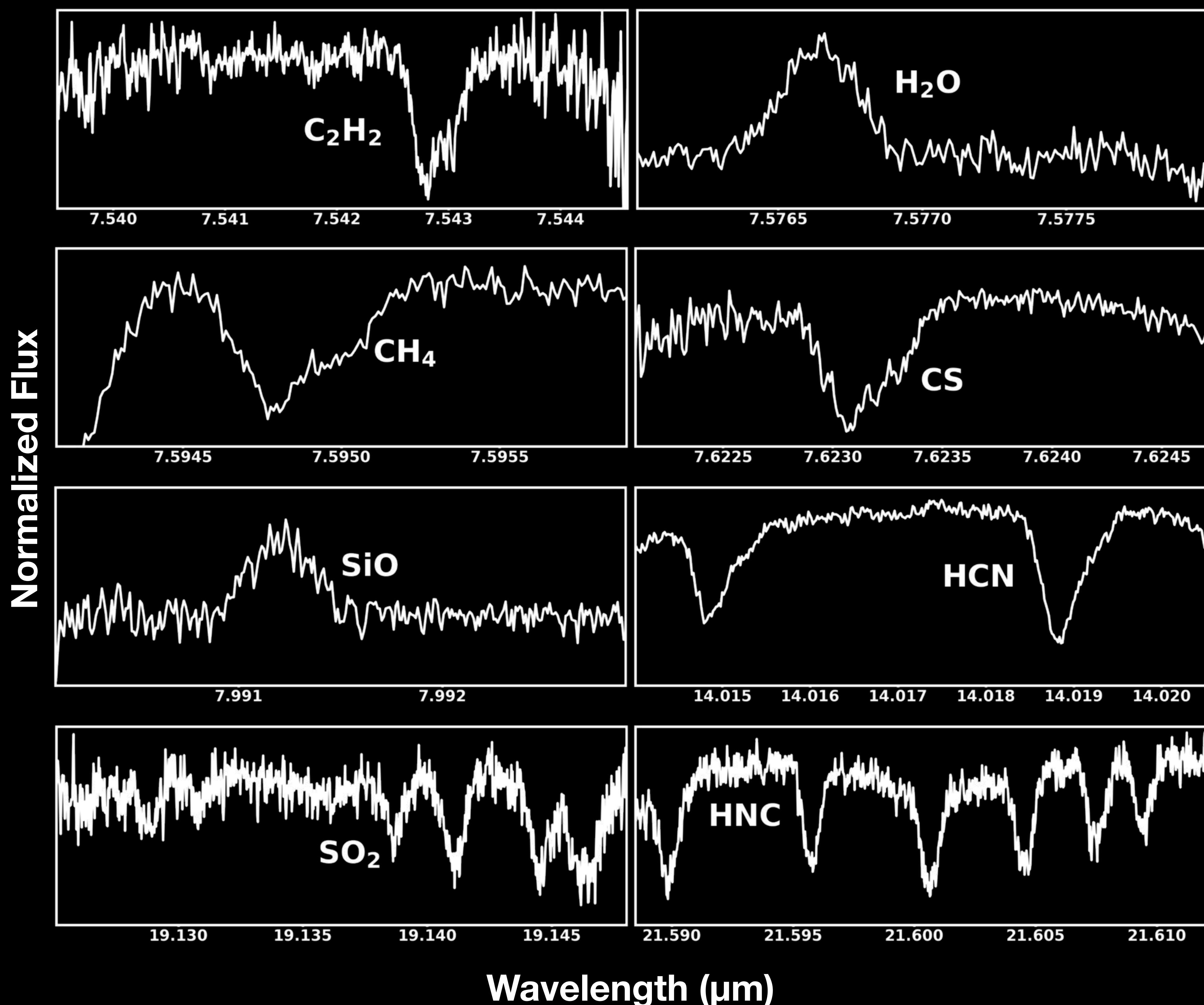
FORCAST: De Buizer et al 2012
Source I: Rodríguez+ 2005

- Stratospheric Observatory for Infrared Astronomy (SOFIA) has high spectral capability in IR
- Flies 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 configuration dependent
- Sister spectrograph to TEXES
- Currently only spectrograph with high enough resolution to identify individual molecules over the whole MIR
- We conduct an unbiased, MIR line survey at high resolution (R ~ 60,000) from 7.2 to 28 μm of Orion IRc2 with SOFIA/EXES

SOFIA versus Ground in MIR

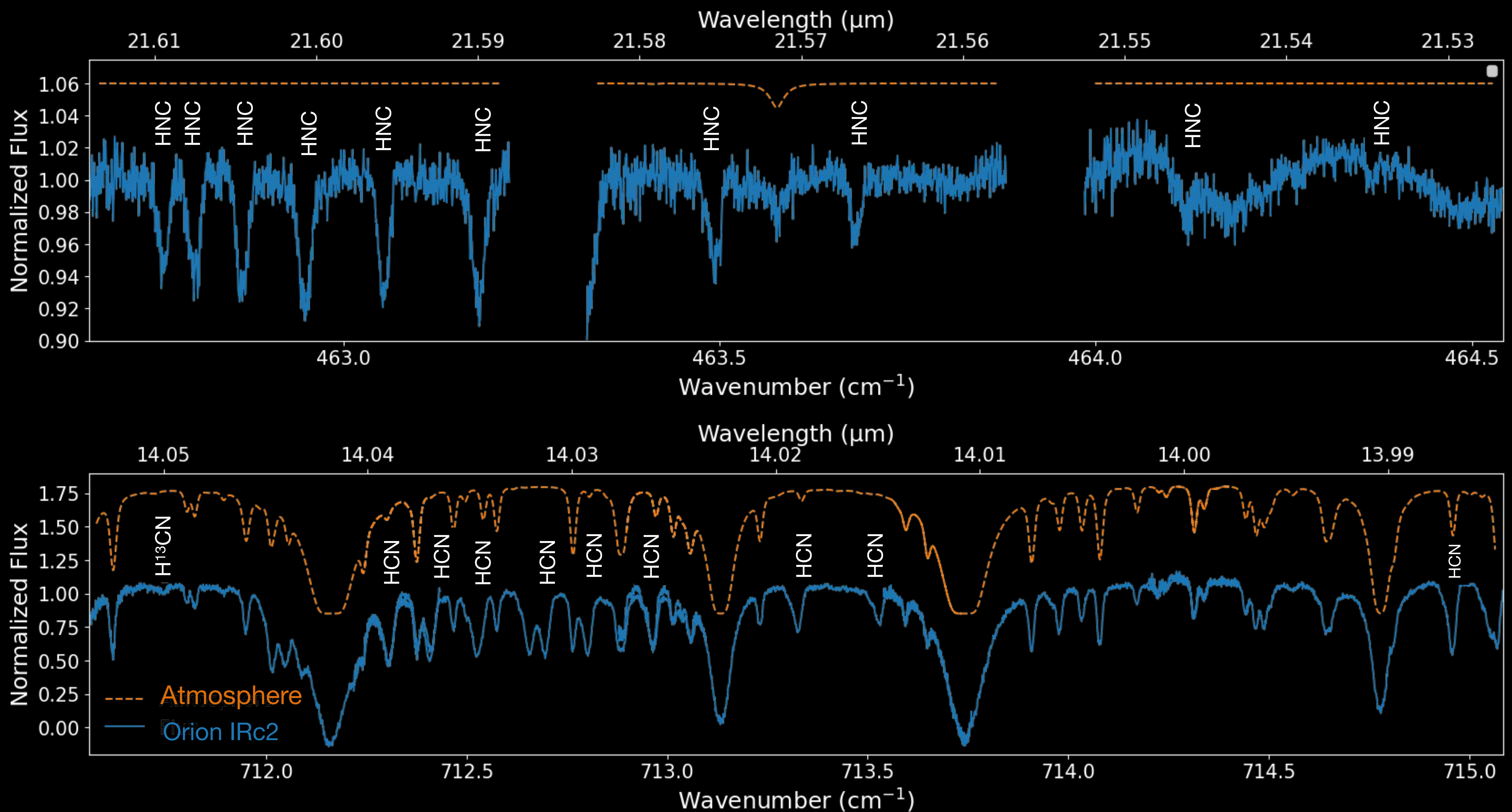


EXES Spectra Towards IRc2



- Over 400 unique lines
- Molecular species identified with certainty: HCN, HNC, H_2, C_2H_2, H_2O, CH_4, SO_2, SiO, and CS; isotopes $H^{13}CN$ and $^{13}CCH_2$
- Tentative: One OH line
- Some species exhibit double Gaussians pointing to two velocity components: C_2H_2, HCN, CH_4, and CS
- Main absorption velocity component ~-7 km/s
- Secondary absorption component ~1 km/s
- Atomic/Ion Lines: FeII, SI, SIII, and NeII

Focus on: HCN, HNC, and $H^{13}CN$



Nickerson+ 2021

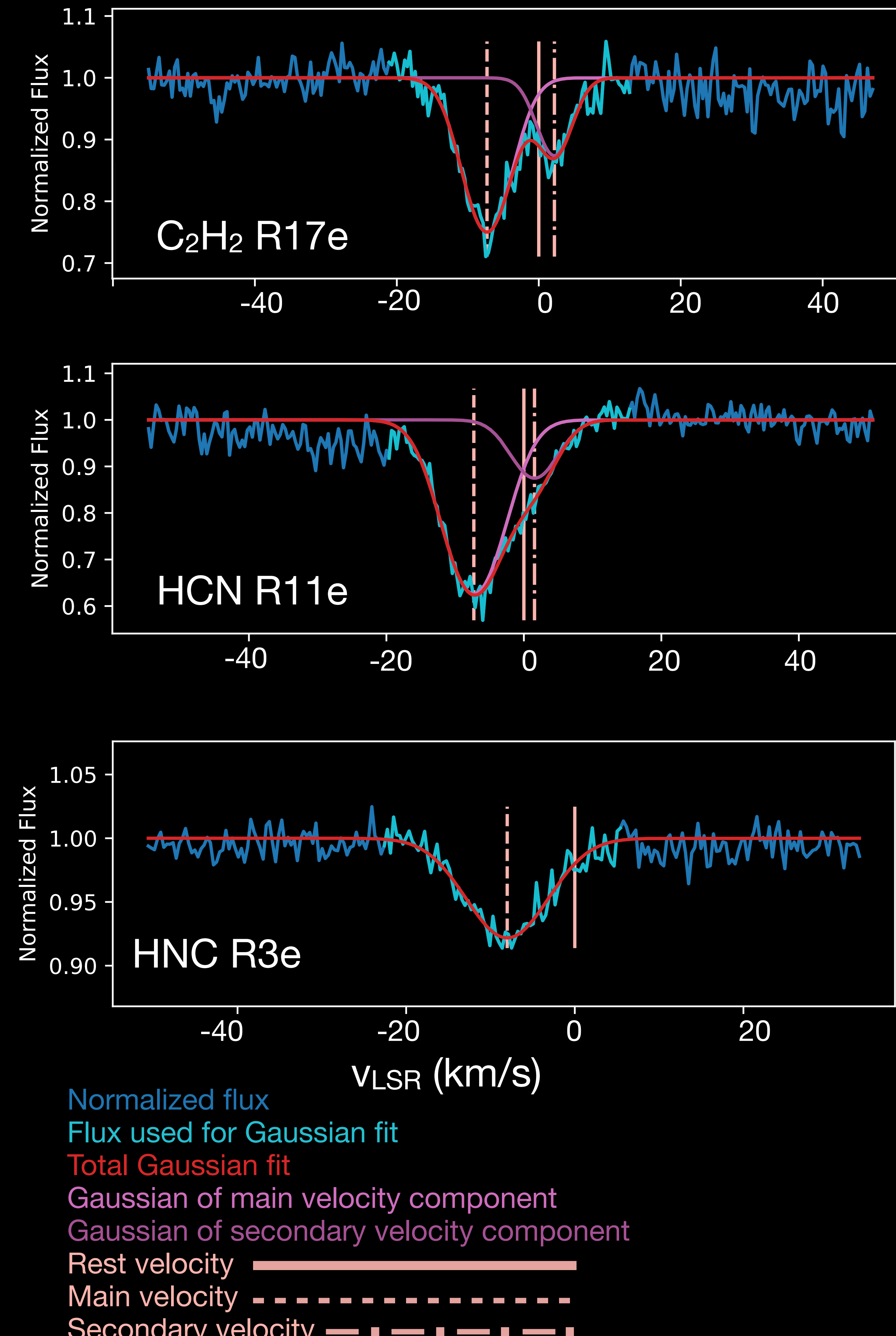
Analysis Recipe

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

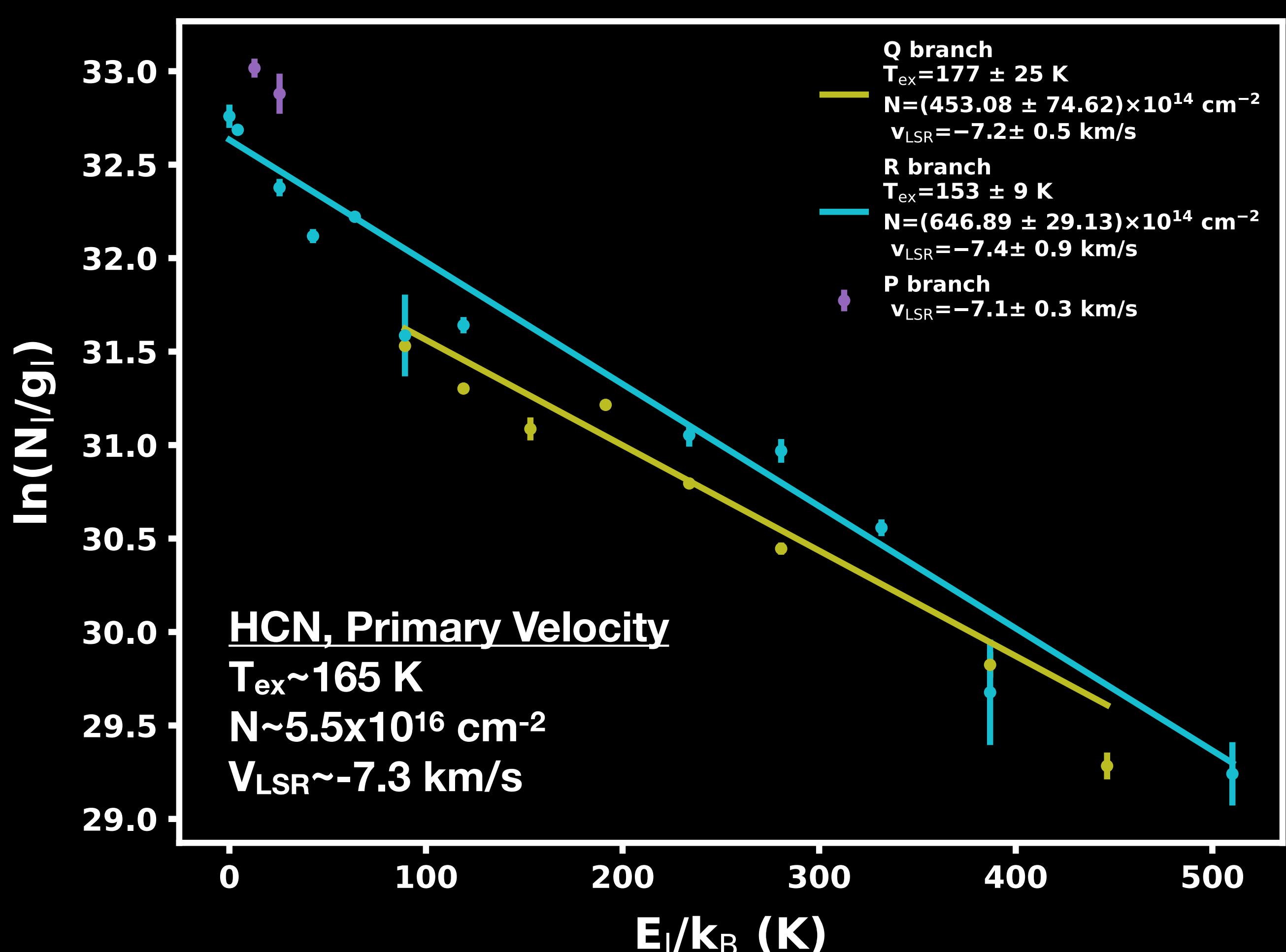


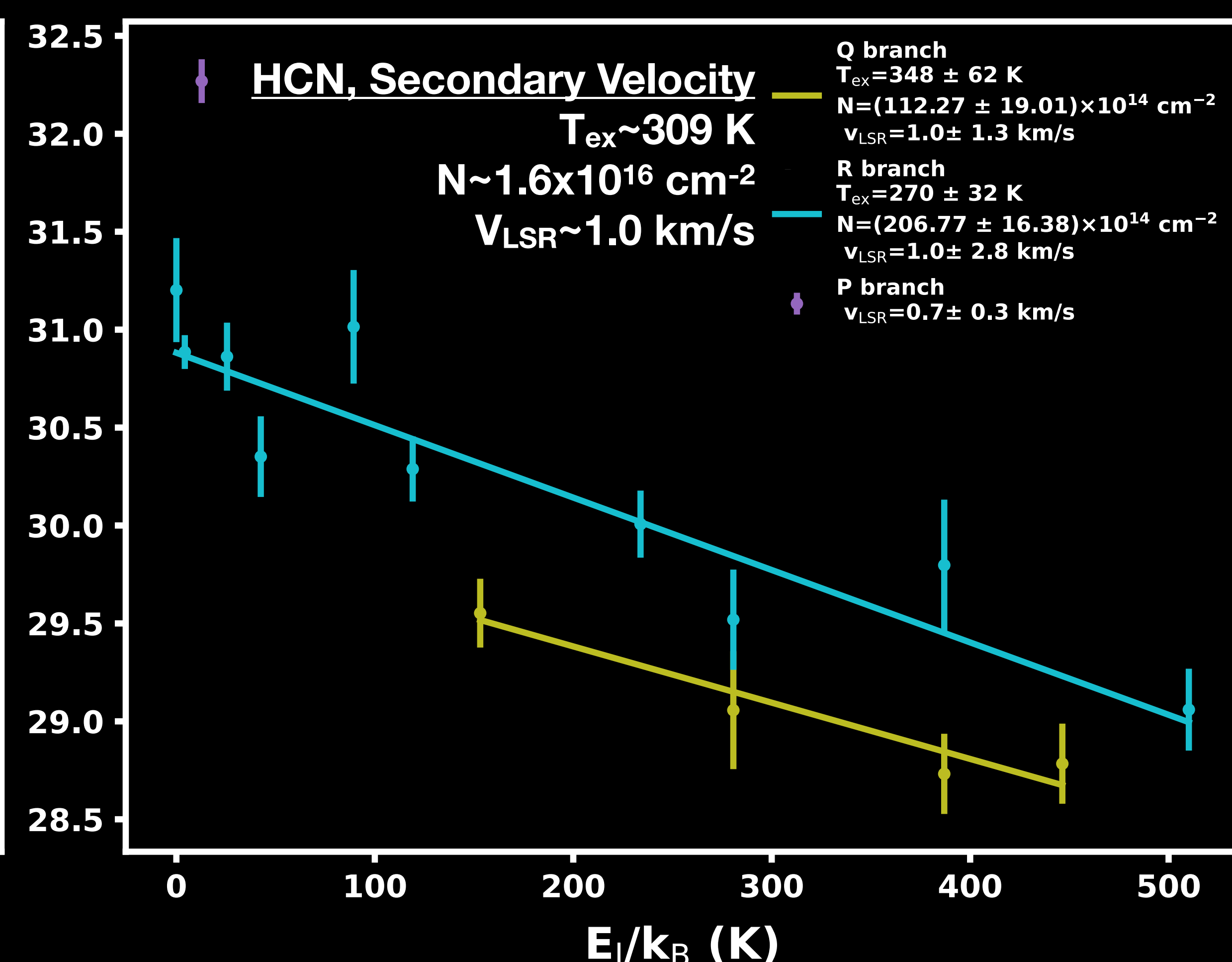
HCN

- Ubiquitous in the Solar System, ISM, and extra-Galactic sources
- Important prebiotic molecule, leads to DNA formation

- Observe two velocity components: primary -7 km/s at 165 K, secondary 1 km/s at 309 K and less abundant

- Primary component velocity similar to outflow from radio source I, likely associated with it, second deeper into hot core





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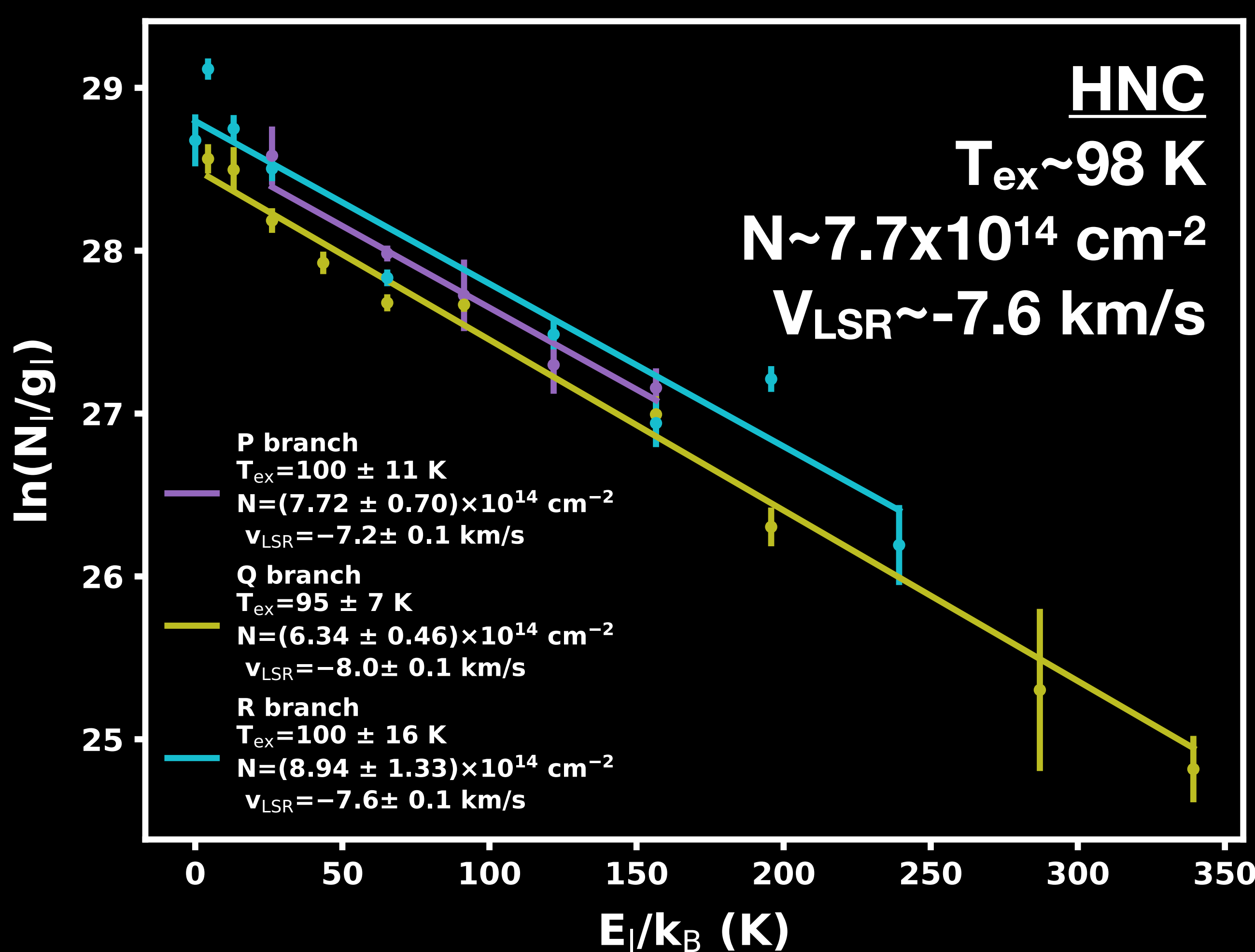
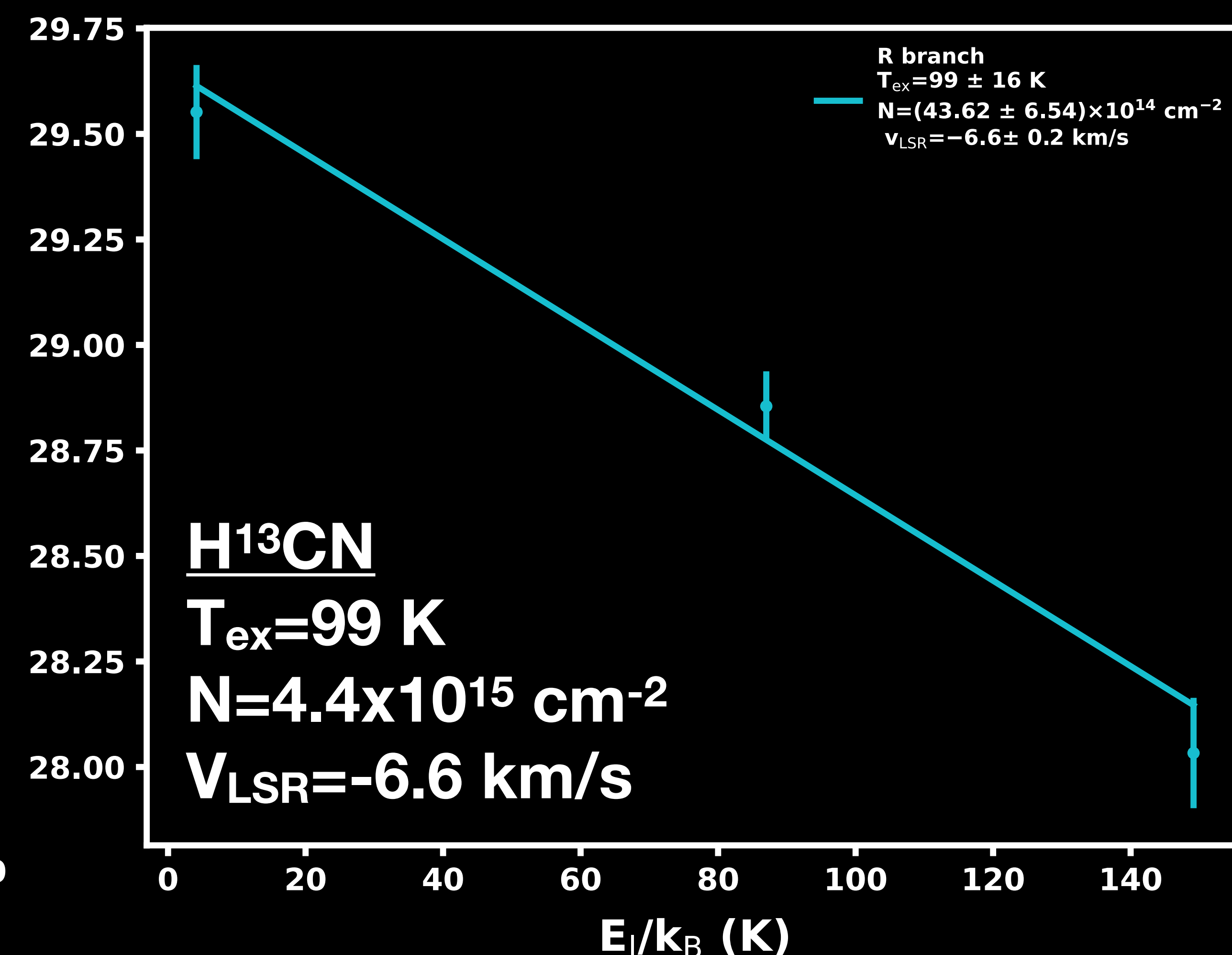
New to the MIR: HNC and $H^{13}CN$

- Isomers HNC and HCN both trace the densest, coldest gas
- HCN/HNC nearly equal at low temperatures (Schilke+ 1992) but HNC depletion increases with temperature (Hirota+ 1998)

- First MIR detections of HNC and $H^{13}CN$ in the ISM; complement the story of HCN
- Both HNC and $H^{13}CN$ exhibit one velocity component, -7 km/s and 100 K
- HNC has wider FWHM than HCN and $H^{13}CN$ lines, hinting at unresolved secondary component





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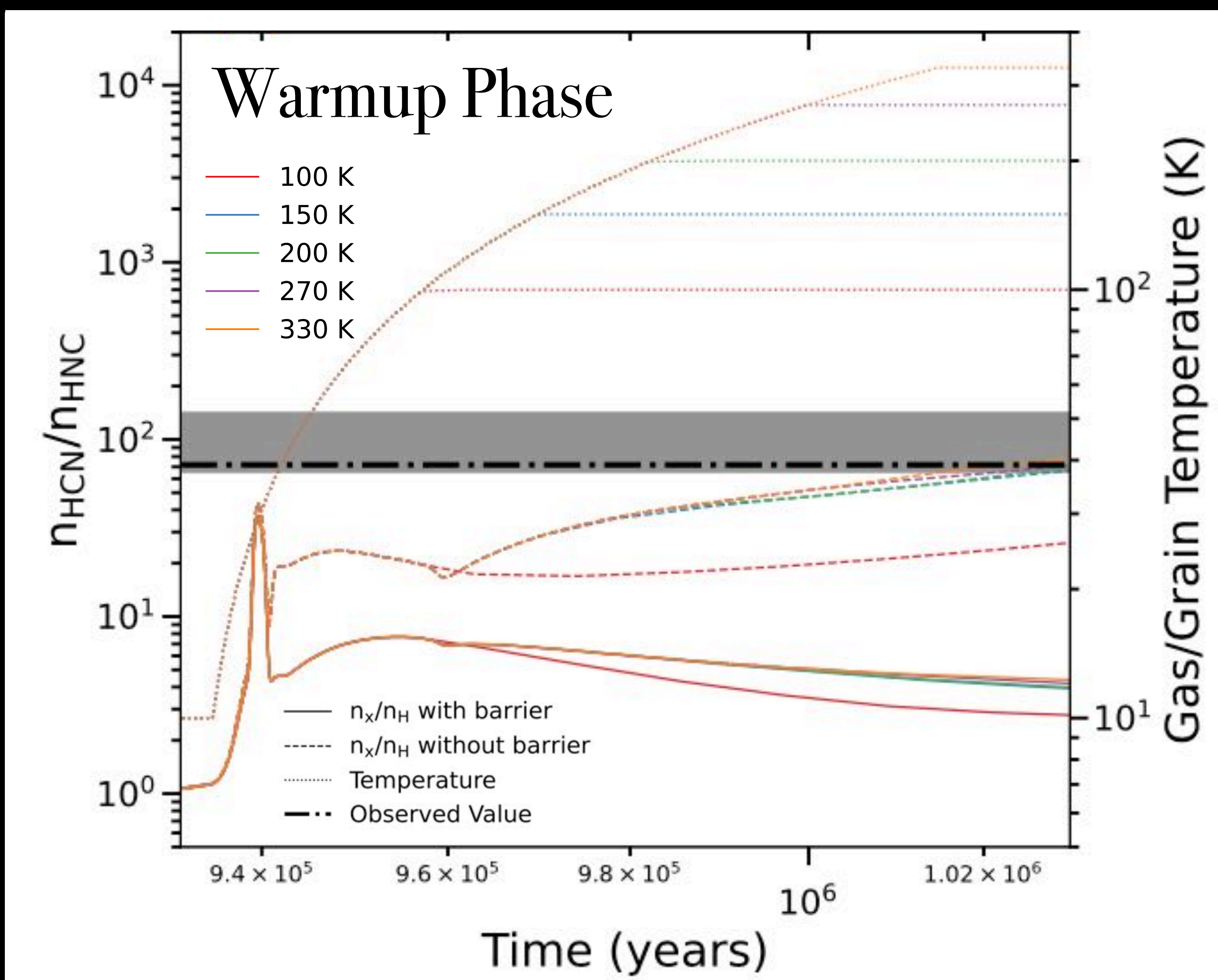
The Ratios

- $^{12}C/^{13}C=13$ much lower than expected for Galactocentric distance; similar result as Rangwala+ 2018, measured with C_2H_2 also with SOFIA/EXES
- Comparable to other star forming regions, wider problem requires followup



- HCN/HNC=72 expected for this extreme environment, previous work showed ratio ~5 in surrounding regions and increases towards IRc2 (Schilke+ 1992)
- Compare to chemical model (Acharyya & Herbst 2018) that traces hot core evolution in three phases: free fall collapse, warmup, and post-warmup
- Test using five different final temperatures, and with or without activation barrier for HNC + H → HCN + H as it is uncertain
- Pinpoint hot core's chemical age ~10^6 years
- Predates region's explosive event, which occurred ~500 years ago
- Hot core irradiated prior to explosion, likely a hot core around radio source I and was separated
- In future, need to incorporate shock physics into model

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MIR versus Sub-mm/mm

Comparison of HNC, HCN, and $H^{13}CN$ observations towards Orion IRc2 between this and previously published works.

Reference	Region	Beam Size	τ	Type	v_{LSR} (km s^{-1})	T (K)	N ($\times 10^{14} cm^{-2}$)
				HNC			
This work	MIR	5.″5–6.″9×3.″2	thin	abs	−7.6±0.1	98±7	7.67±0.52
Persson et al. (2007)	sub-mm	2.′1	thin	emi	9	—	4.4
Comito et al. (2005)	sub-mm	11″	thin	emi	8	150[a]	5
				HCN			
This work	MIR	1.″9–2.″1×3.″2	thin	abs	−7.3±0.5	165±13	549.99±40.05
					1.0±1.5	309±35	159.52±12.55
Rangwala et al. (2018)	MIR	3.″2×3.″2	thin	abs	−5.2 ± 2.8	140 ± 10[b]	840 ± 60
Comito et al. (2005)	sub-mm	11″	thin	emi	5	150[a]	700
Lacy et al. (2005)	MIR	1.″5×8″[c]	—[c]	abs	−10[d]	150[d]	—
Boonman et al. (2003)	MIR	14″×27″	thick	abs	—	275[e]	450
Schilke et al. (2001)	sub-mm	12″	thin	emi	—	100[f]	260
Stutzki et al. (1988)	sub-mm	32″	thick	emi	6	—	—
Blake et al. (1987)	mm	30″	thick	emi	5.8	—	250
				$H^{13}CN$			
This work	MIR	2.″1×3.″2	thin	abs	−6.6±0.2	97±13	42.08±5.67
Schilke et al. (1992)	mm	26″	thin	emi	9.2[g]	70[g]	0.57

- The MIR finds the molecules in absorption and at hotter temperatures and a different velocity component compared to longer wavelengths
- Secondary component of HCN the hottest measured towards IRc2: closest gas to the hot core's centre

The MIR is critical to accessing material nearest to the centres of hot cores and tracing unique components of the gas

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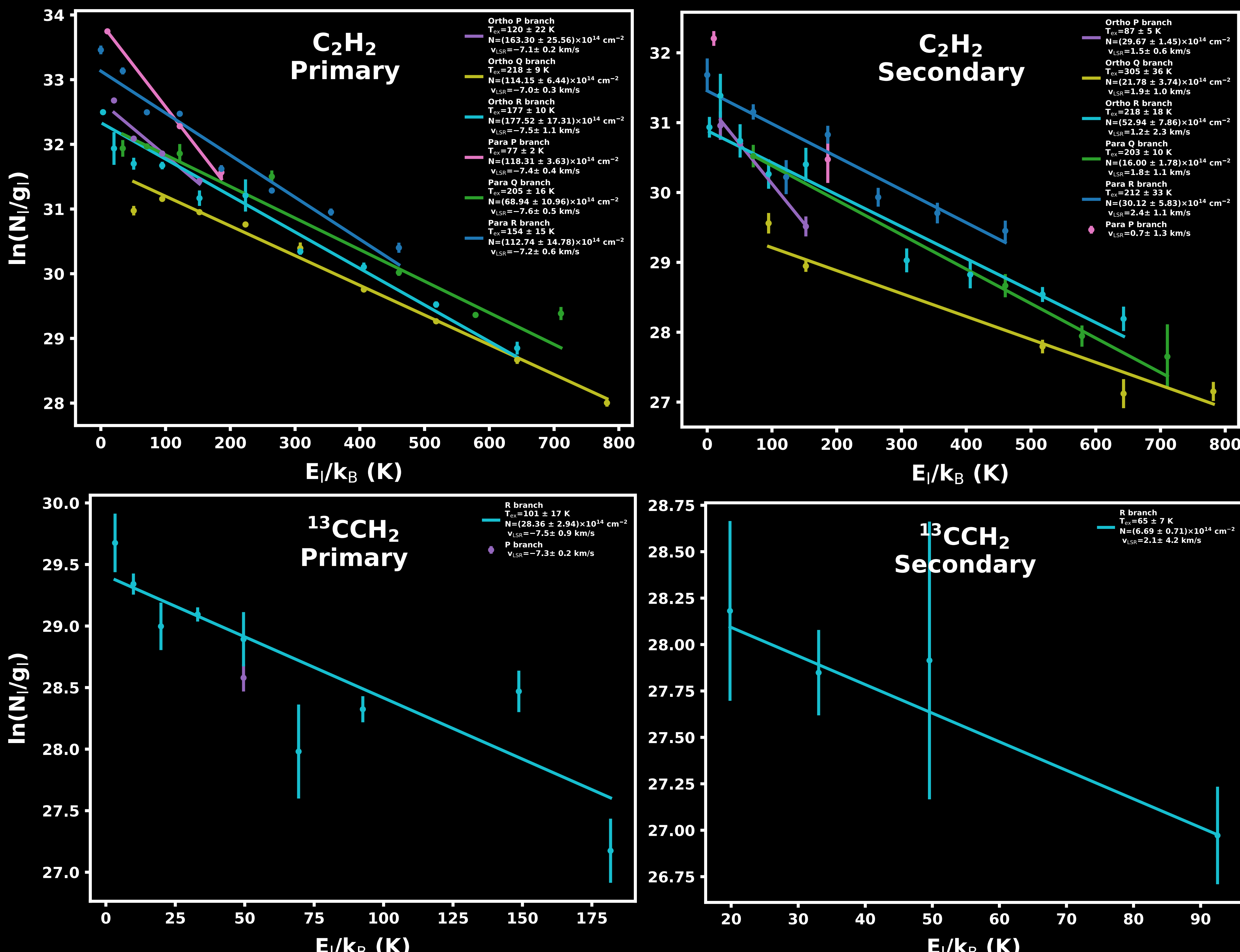
Future: Building the MIR Chemical Inventory of the Orion Hot Core



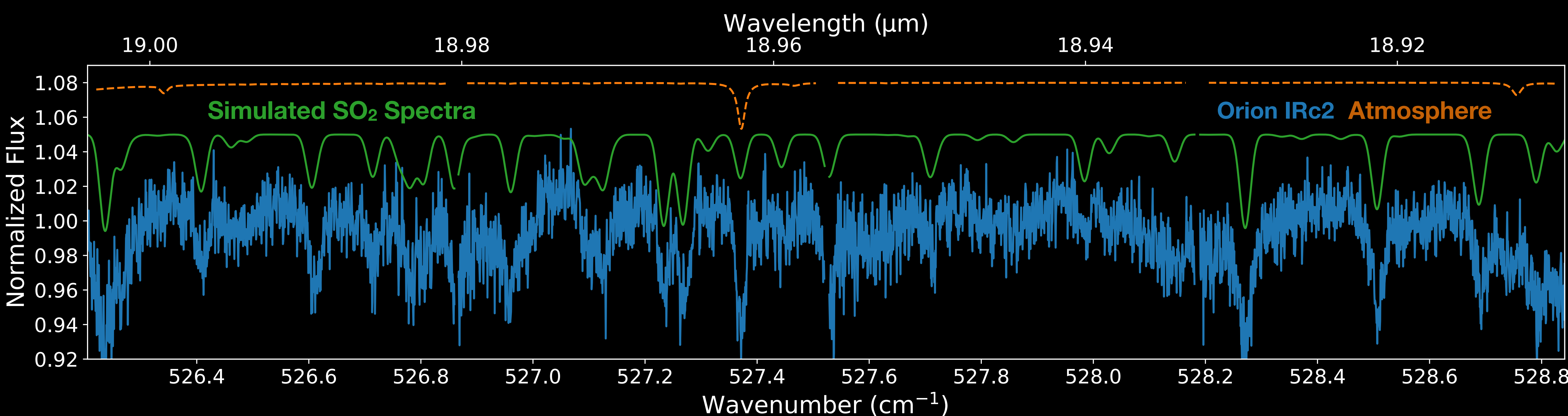
- Two components: -7 km/s and 1 km/s
- Ortho and para ladders not in LTE, separate properties
- Secondary C_2H_2 component hotter for both ortho and para ladders on average (ignoring P branch which as few lines, para Q about the same)
- For each component, ortho hotter than para
- Primary $^{13}CCH2$ 101K (like HNC, $H^{13}CN$), secondary 65 K cooler
- $^{12}C/^{13}C$ ~ 9 for both velocity components

Nickerson+ in prep

Future: Building the MIR Chemical Inventory of the Orion Hot Core

- 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 primary velocity component
- Future: fit two components?

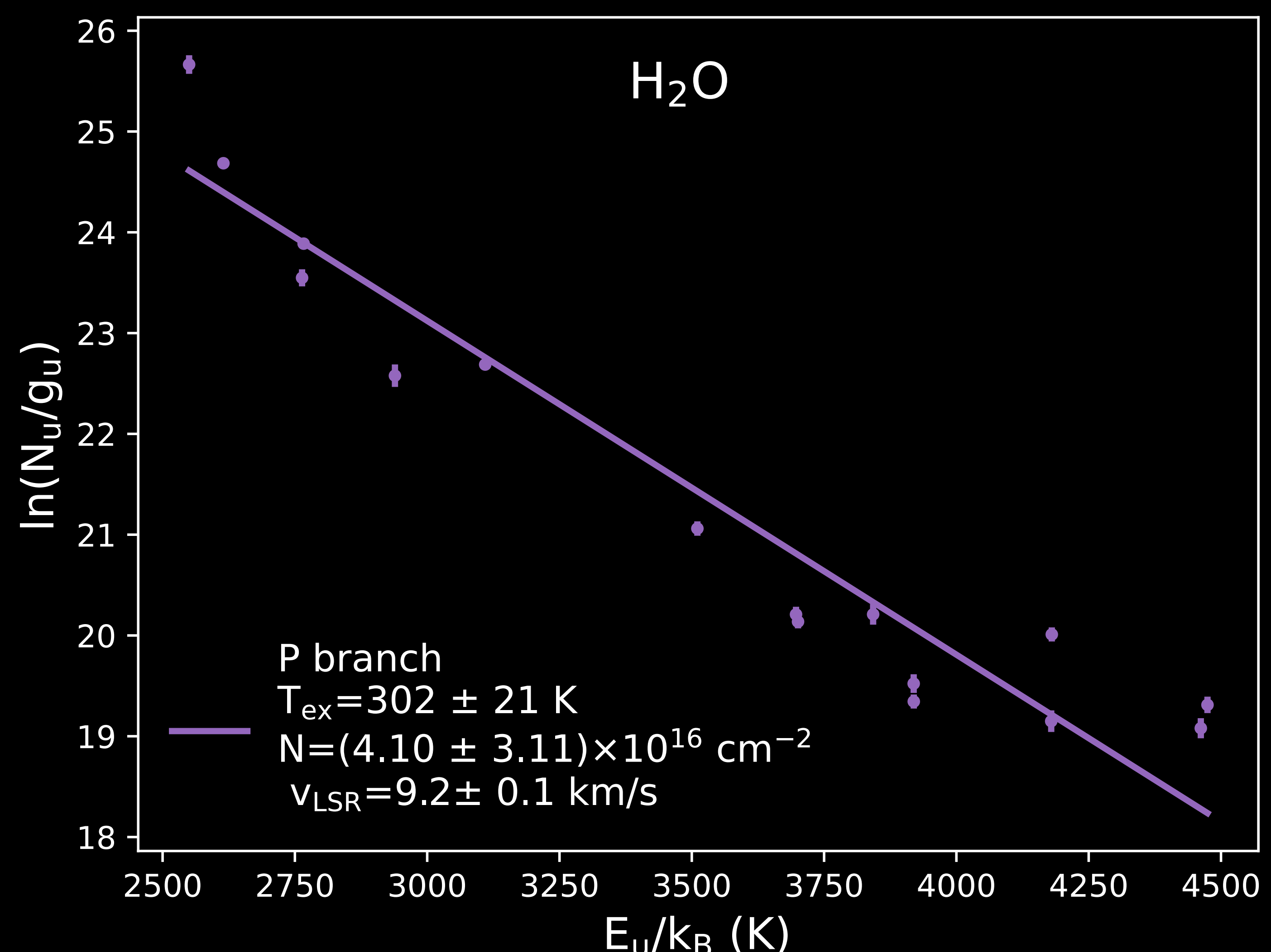
<u>SO_2</u>
T_{ex}=93.8 K
N=6.2×10^{16} cm^{-2}
V_{LSR}=-6.0 km/s

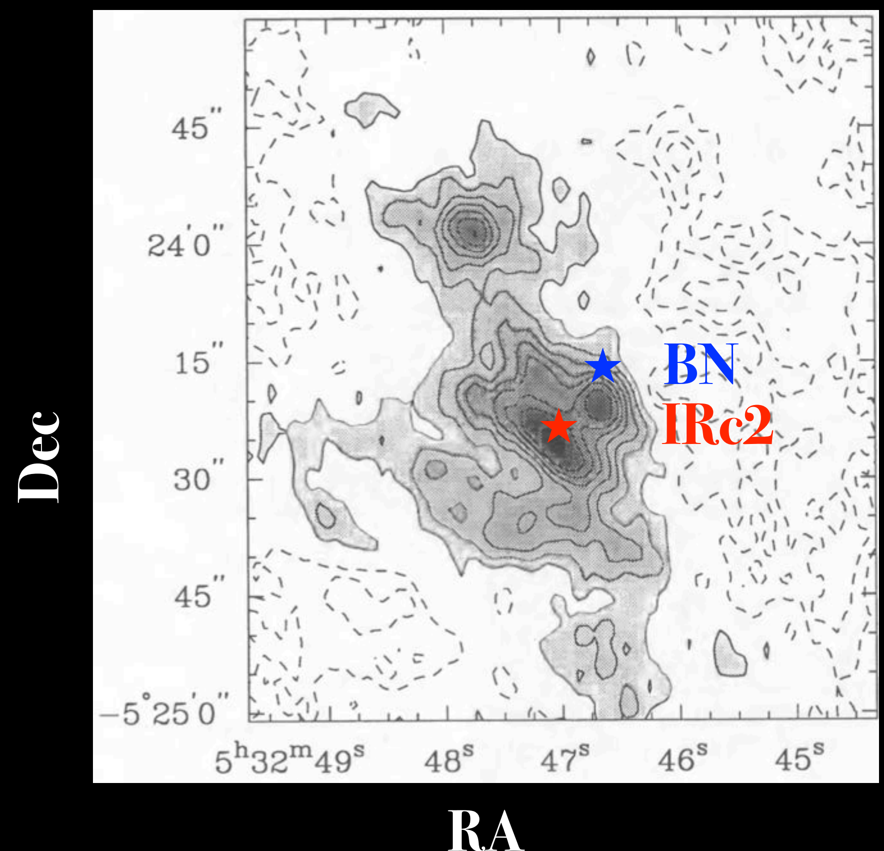


Nickerson+ in prep

Water Emission Towards IRc2

- H_2O and SiO appear in emission
- With Jose Monzon, analyzing the H_2O emission lines; paper in preparation
- v_{LSR} ~ 9 km/s different than absorption lines of other species (but similar to SiO emission)
- Similar velocity to the extended ridge feature (Blake+ 1987); emission lines towards IRc2 likely not associated with the hot core itself



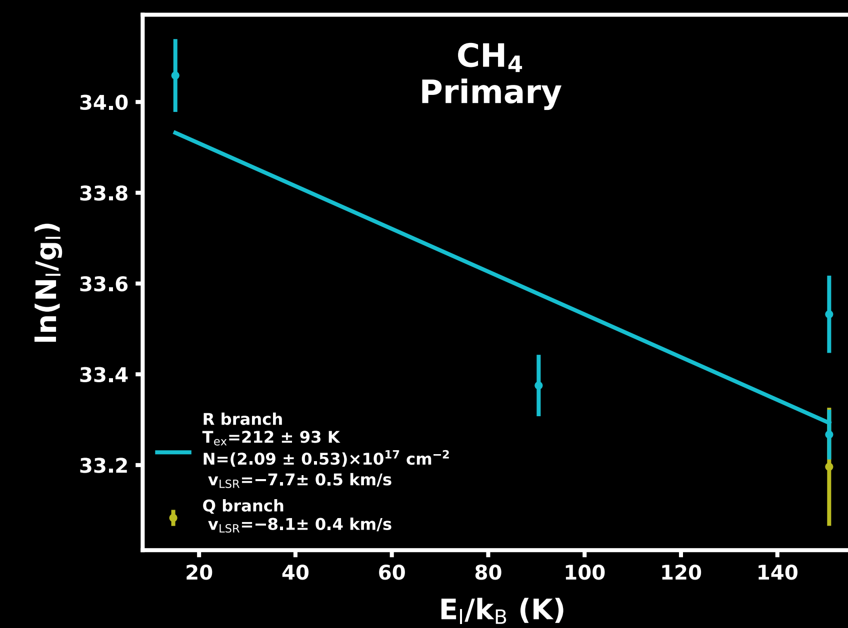


- Left: map of dust emission of Orion BN/KL region at 82 to 95 GHz (Wright+ 1992); peaks where IRc2 heats the dust
- Hot core is suggested to be a dense region within the larger extended ridge (Zapata+ 2011)

Monzon+ 2021 in prep

Undergraduate Projects

Jose Monzon: measured the CH_4 lines in Orion IRc2 and currently measuring the H_2O emission lines; Monzon+ 2021 in prep



Ciera Knabe:

Constructing a database for all EXES hot core observations in the SOFIA archive at IRSA; measuring CH_4 towards the hot core NGC 7538 IRS 1

Jorge Vazquez:

Manipulating the SOFIA/EXES spectra to JWST/MIRI's lower resolution for future observation predictions; measuring H_2O towards the hot core W3 IRS 5

MIR Python Analysis Toolkit

- Publicly available analysis tools for spectroscopy are focussed on longer wavelengths, FIR to sub-mm
- Nothing for the MIR… until now!
- Will publicly release to the community a Python Toolkit to analyze EXES/TEXES spectra; could expand to other instruments and NIR if demand exists (and suggestions welcome)
- Will include:
    - 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
- Catchy acronym forthcoming

Conclusions

- With SOFIA/EXES, we are building a molecular inventory for the Orion Hot Core in MIR (7.2 to 28 μm)
- Have identified over 400 features, at least 9 molecular species, and 2 isotopes; also 4 atomic/ion lines
- First MIR observations of HNC and $H^{13}CN$ in the ISM, along with numerous HCN transitions
- HCN/HNC=72, used to chemically age gas to 10^6 years; predates 500 year old explosion, which likely tore hot core from its natal star
- $^{12}C/^{13}C=13$ below expectations; similar results from C_2H_2; requires follow-up
- HNC/HCN/$H^{13}CN$: Nickerson+ 2021, published in ApJ
- H_2O emission: Monzon+ 2021 in prep
- Data release of MIR chemical inventory of Orion Irc2: Nickerson+ in prep

- Our MIR results trace unique components of the ISM that are separate from those measured longer wavelengths
- MIR detects hottest material closest to hot core's centre
- Completing a python package of MIR analysis tools for public release

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

Lynette Cook