

Molecular line survey of “The Rotten Egg”



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Goals

- Characterize the chemistry in CSEs around O-rich AGB stars (most chemistry studies on C-rich CSEs: IRC+10216 & CRL 618)
- Study non-equilibrium, shock-induced chemistry.

Methods

- **Molecular line survey:** IRAM 30m/EMIR (80-350GHz) & HSO/HIFI (480-1245 GHz)
- Two targets:

IK Tau ('normal' Mira-type, O-rich AGB)

➔ OH231.8+4.2 (a.k.a "The Rotten Egg") = shock-accelerated, fast+bipolar flow & unusually rich chemistry



The 'bipolar' disorder of OH231.8+4.2

- Mira-type variable ($P=700\text{d}$)
- M6-9III
- $L \sim 10^4 L_{\odot}$, $T_{\text{eff}} \sim 2200\text{K}$
- $\dot{M} \approx 10^{-4} M_{\odot}/\text{yr}$
- SiO maser emission (+OH, H_2O)
- $d \sim 1500\text{ pc}$



I'm an AGB star

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I'm an AGB star



I'm a post-AGB nebula

- Fast, Bipolar outflow

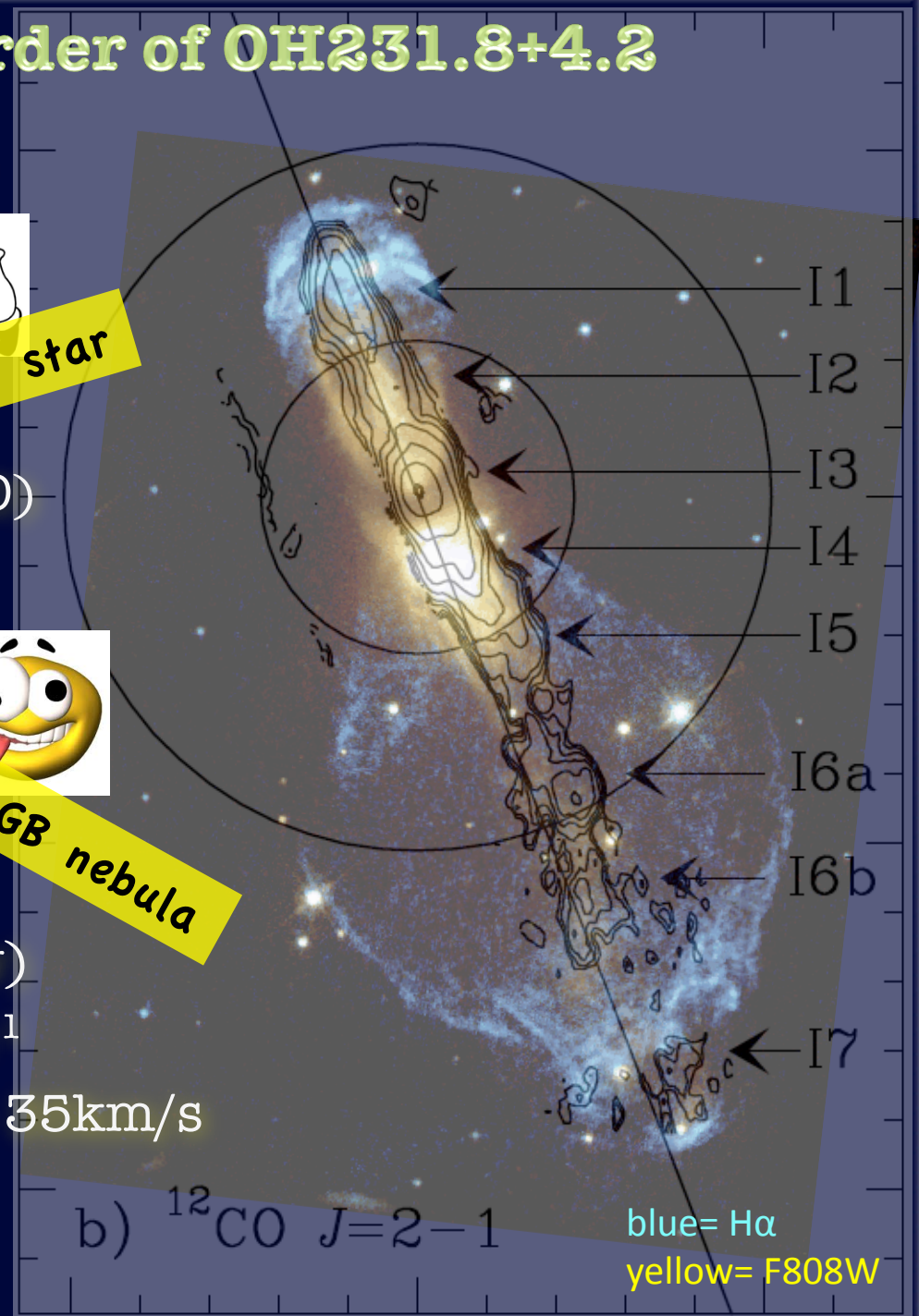
$v_{\text{exp}} \sim 7\text{-}30\text{ km/s}$ (core)

$v_{\text{exp}} \sim 30\text{-}400\text{ km/s}$ (axial flow)

$\nabla v \sim 6.5\text{ km/s arcsec}^{-1}$

- Central core (torus), $v_{\text{exp}} \sim 7\text{-}35\text{ km/s}$

$M_{\text{mol}} \sim 1 M_{\odot}$, $\text{cool} \sim 10\text{-}35\text{ K}$



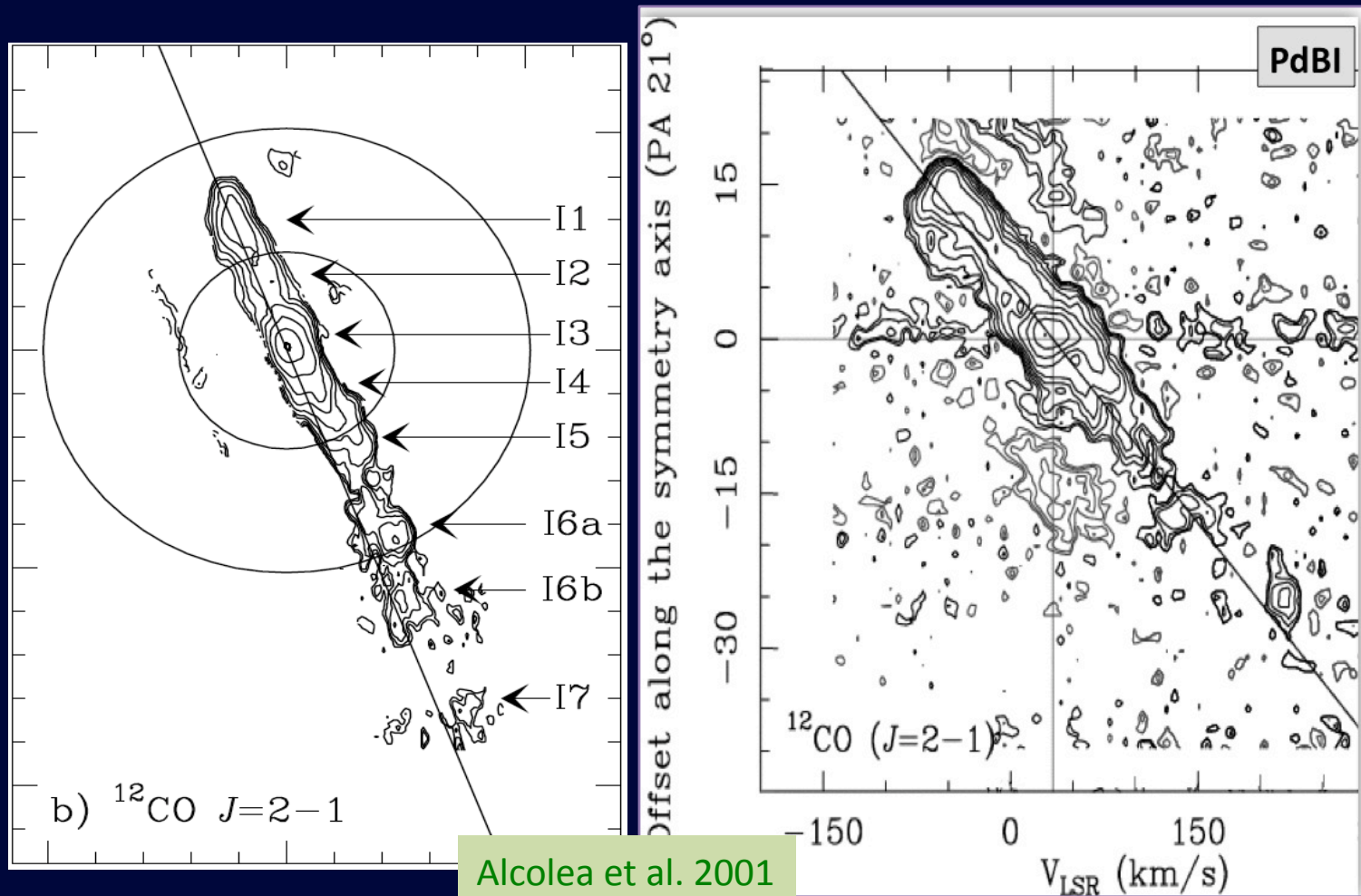
The 'bipolar' disorder of OH231.8+4.2

"Hubble-law" kinematics, $V \propto r$ (common in pPNs)

Sudden interaction between

jet+'AGB CSE'

1000yr ago, in $\lesssim 150$ yr



The 'bipolar' disorder of OH231.8+4.2

Atypical CHEMISTRY:

- CO, H₂O, OH, SiO, SO, SO₂,...



I'm Oxygen-rich

The 'bipolar' disorder of OH231.8+4.2

Atypical CHEMISTRY:

- CO, H₂O, OH, SiO, SO, SO₂,...

.... BUT ALSO

- C-, S-, and N-bearing species unexpected to be abundant in O-rich CSEs:

H₂S (Rotten Egg), HCO⁺, HNC,
HNC, CS, NS, OCS, H₂CO, NH₃
(isotopologs ¹³CO & H¹³CN)

Morris et al. 1987

Lindqvist et al. 1990

Sánchez Contreras et al. 1997, 2000



I'm Oxygen-rich



I'm a "Rotten Egg"

shocks → endothermic reactions, molecule desorption from dust, grain destruction, **dissociating molecules**

IRAM 30m mm-line survey: OH231.8+4.2 & IKTau



- Single-pointed observations (HPBW $\approx$ 29''–8'')
- EMIR receivers [79-350GHz]
- WILMA (2MHz $\approx$ 1.7–7.5km/s), FTS (195kHz $\approx$ 0.2–0.7km/s)
- Several runs: 2009, 2010, 2011 & 2013
- sensitive survey $\rightarrow$ rms[2MHz]=0.8–20 mK

Velilla et al., in prep.

Table 1. Iram-30 m efficiencies and parameters of the EMIR receivers at representative frequencies.

Frequency (GHz)	Beam eff. (%)	Forward eff. (%)	HPBW ('')	S/T _a [*] (Jy/K)
86	81	95	29	5.9
145	74	93	16	6.4
210	63	94	11	7.5
260	53	88	9	8.4
340	35	81	7.5	10.9

Notes. (#1) Frequency in GHz; (#2) Beam efficiency percentage; (#3) Forward efficiency percentage; (#4) Half Power Beam Width in arc-sec; (#5) Flux to antenna temperature conversion factor in Jansky per Kelvin.

Table 2. Relevant observational information.

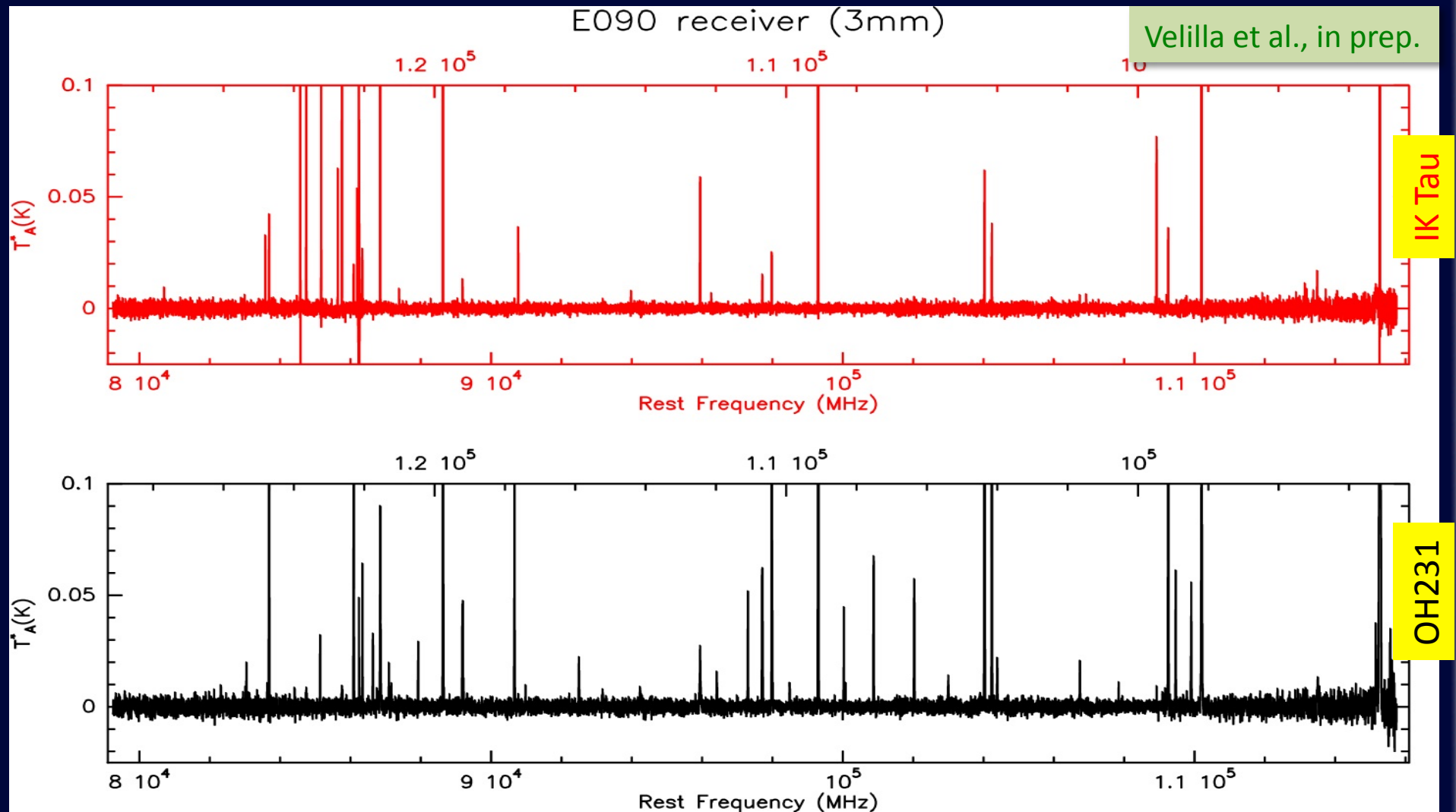
Band	Mode & IBW (GHz)	ν_{obs} (GHz)	RMS (mK)	Opacity
E090 (3mm)	DSB - 8	79.2 - 115.7	1 - 2	0.07 - 0.3
E150 (2mm)	SSB - 4	128.3 - 167.6	1 - 4	0.09 - 0.4
E230 (1mm)	DSB - 16	202.0 - 270.8	5 - 9	0.12 - 0.3
E330 (0.9mm)	DSB- 16	258.3 - 348.9	9 - 20	0.17 - 0.8

Notes. (#1) EMIR receiver band; (#2) Observing mode Single side-band or Dual sideband (SSB/DSB) and Instantaneous bandwidth (IBW) in GHz; (#3) Observed frequency windows; (#4) Root Mean Square (rms) noise for a spectral resolution of $\Delta\nu=2$ MHz; (#5) Zenith atmospheric opacities at the observed frequency.

IRAM 30m mm-line survey: OH231.8+4.2 & IKTau

0.8mm-3mm: ~ 200 lines detected, few mK

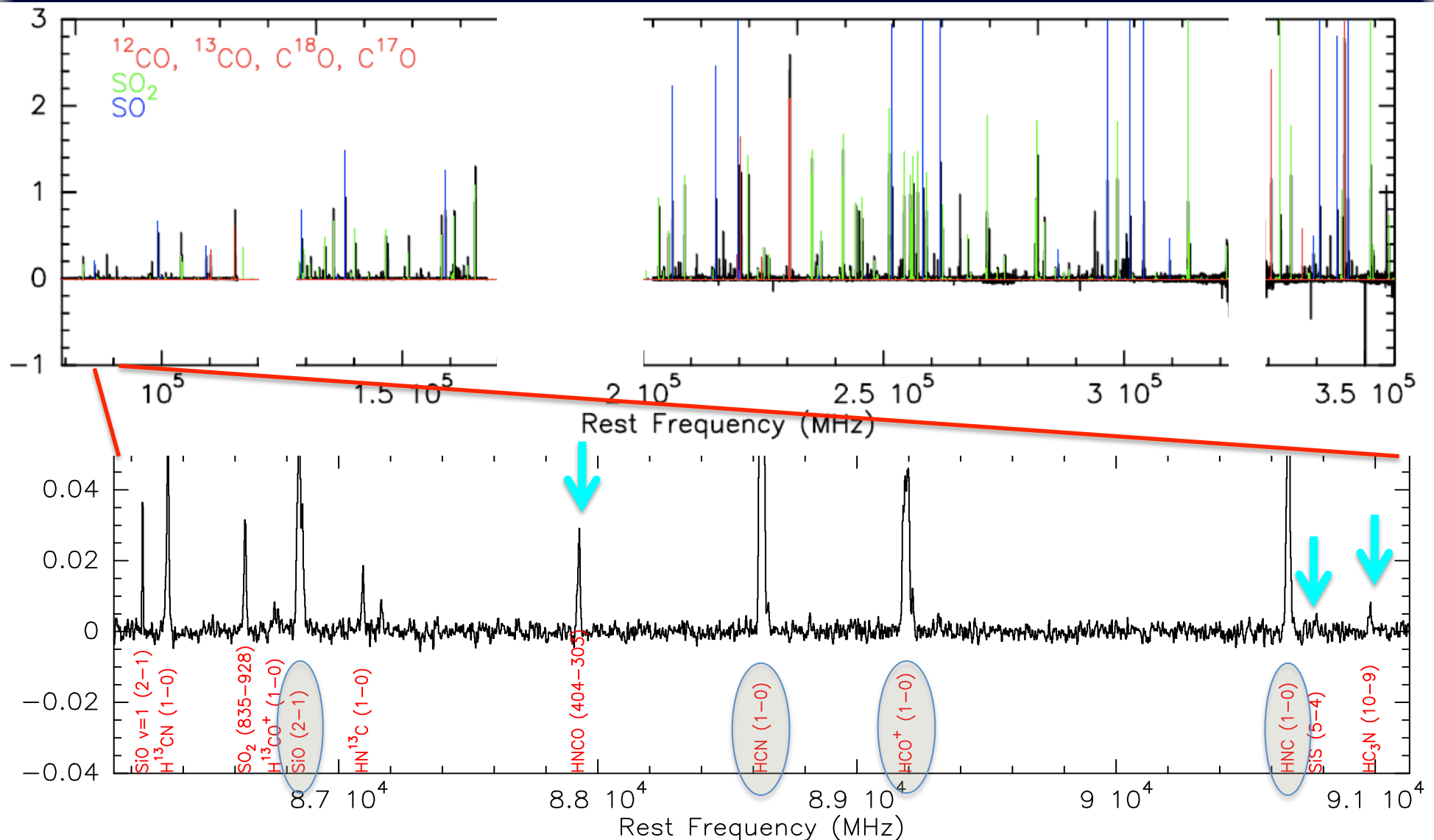
OH231 has a richer spectrum: CO, SO₂, SO, (+isotopologues) ...



IRAM 30m mm-line survey: OH231.8+4.2 & IKTau

OH231 spectrum dominated: CO, SO₂, SO, (+isotopologues) ...

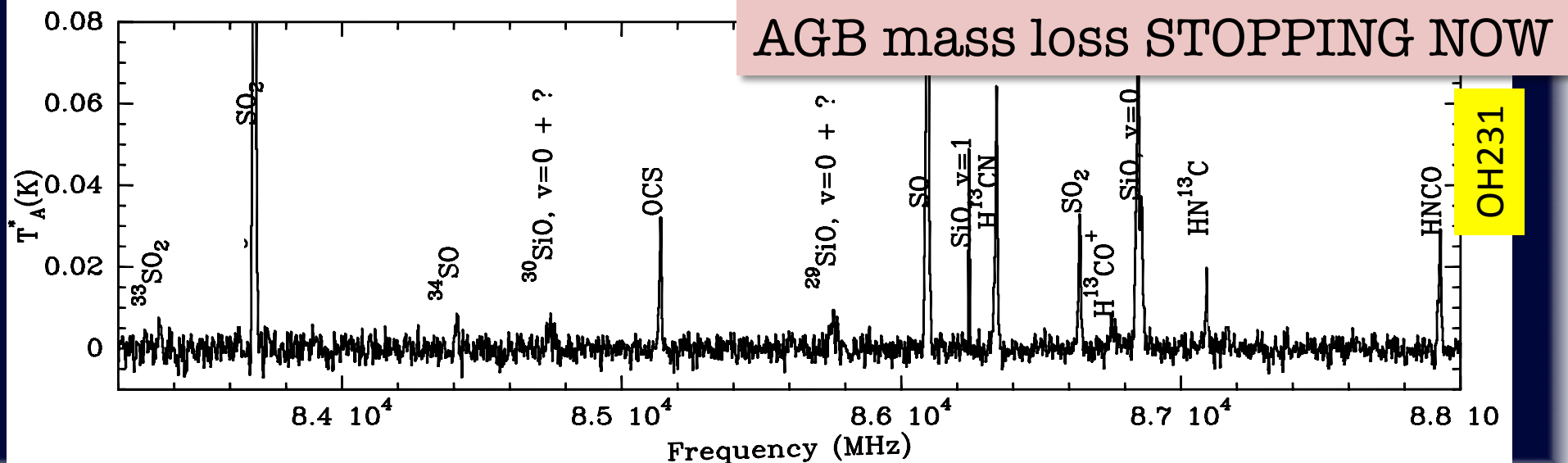
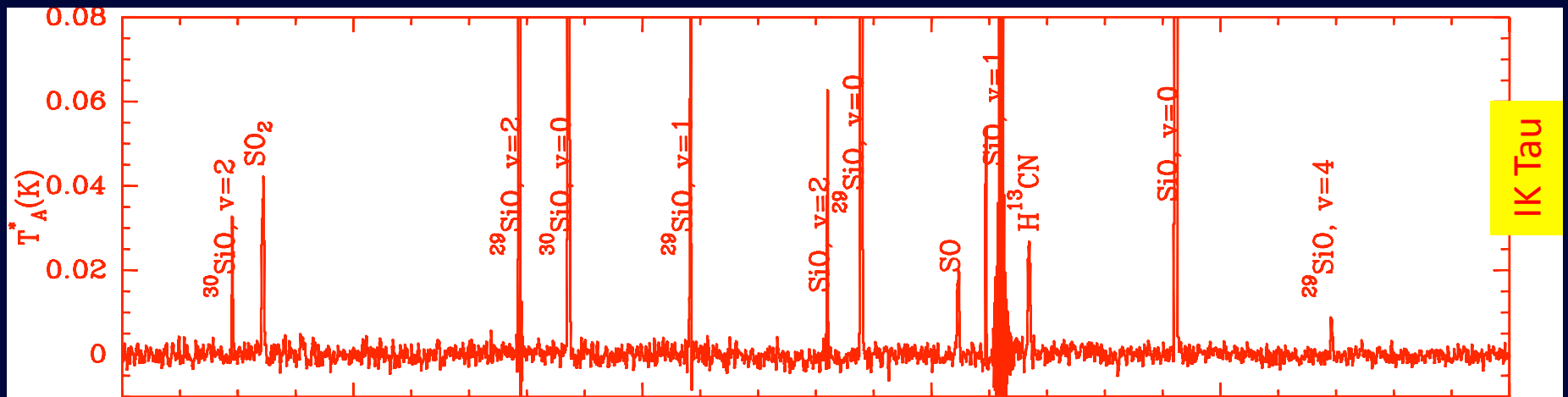
³³S, ³⁴S, ¹⁸O, ¹⁷O, ¹³C, ²⁹Si, ³⁰Si



IRAM 30m mm-line survey: OH231.8+4.2 & IKTau

Lines present in IK Tau but NOT/weak in OH231.8: SiO, SiS, NaCl, PN, PO.. → inner envelope → growing inner hole

Progressive weakening of SiO masers in OH231.8 (in prep.) →



IRAM 30m mm-line survey: OH231.8+4.2 & IKTau

Lines present in OH231.8 but NOT/weak in IK Tau: SO, SO₂, OCS, HCO⁺, H₂CO, HNCO, HNCS, HC₃N, CN, NO, SO⁺, N₂H⁺, H₃O⁺...

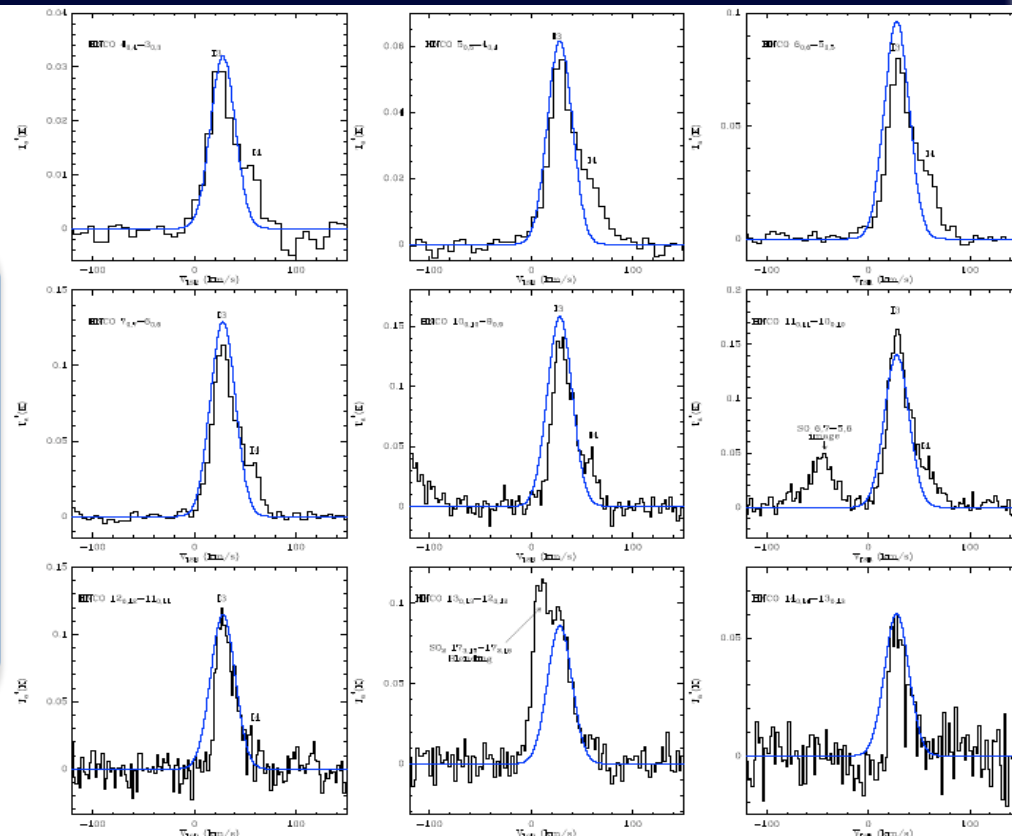
discovered in this survey



IRAM 30m mm-line survey: OH231.8+4.2

HNCO, HNCS, HC₃N (Velilla et al., in prep.)

Molecule	$J_u - J_l$ $J_{K_u - k_u}^u - J_{K_l - k_l}^l$	ν_{rest} (MHz)	E_u (K)	A_{ul} s^{-1}
¹³ CO	1 - 0	110201.35399	5.3	6.336×10^{-8}
	2 - 1	220398.68356	15.9	6.082×10^{-7}
	3 - 2	330587.96441	31.7	2.199×10^{-6}
HNCO	4 _{0,4} - 3 _{0,3}	87925.237	10.5	9.025×10^{-6}
	5 _{0,5} - 4 _{0,4}	109905.749	15.8	1.802×10^{-5}
	6 _{1,6} - 5 _{1,5}	131394.230	65.3	3.006×10^{-5}
	6 _{0,6} - 5 _{0,5}	131885.734	22.2	3.163×10^{-5}
	7 _{1,7} - 6 _{1,6}	153291.935	72.7	4.863×10^{-5}
	7 _{0,7} - 6 _{0,6}	153865.086	29.5	5.078×10^{-5}
	7 _{1,6} - 6 _{1,5}	154414.765	72.9	4.971×10^{-5}
	10 _{0,10} - 9 _{0,9}	219798.274	58.0	1.510×10^{-4}
HNCO ⁺	11 _{1,11} - 10 _{1,10}	240875.727	112.6	1.957×10^{-4}
	11 _{0,11} - 10 _{0,10}	241774.032	69.6	2.019×10^{-4}
	12 _{0,12} - 11 _{0,11}	263748.625	82.3	2.630×10^{-4}
	13 _{0,13} - 12 _{0,12}	285721.951	96.0	3.355×10^{-4}
	14 _{0,14} - 13 _{0,13}	307693.905	110.8	4.200×10^{-4}
HNCS	8 _{0,8} - 7 _{0,7}	93830.07049	20.3	1.217×10^{-5}
	9 _{0,9} - 8 _{0,8}	105558.07582	25.3	1.744×10^{-5}
	11 _{0,11} - 10 _{0,10}	129013.25917	37.2	3.215×10^{-5}
	12 _{0,12} - 11 _{0,11}	140740.37808	43.9	4.189×10^{-5}
	13 _{0,13} - 12 _{0,12}	152467.14243	51.2	5.342×10^{-5}
	14 _{0,14} - 13 _{0,13}	164193.52268	59.1	6.690×10^{-5}
HC ₃ N	9 - 8	81881.46210	19.6	4.215×10^{-5}
	10 - 9	90978.98877	24.0	5.812×10^{-5}
	11 - 10	100076.38486	28.8	7.770×10^{-5}
	12 - 11	109173.63729	34.1	1.012×10^{-4}
	15 - 14	136464.40210	52.4	1.993×10^{-4}
	16 - 15	145560.94935	59.4	2.424×10^{-4}
	17 - 16	154657.28766	66.8	2.912×10^{-4}



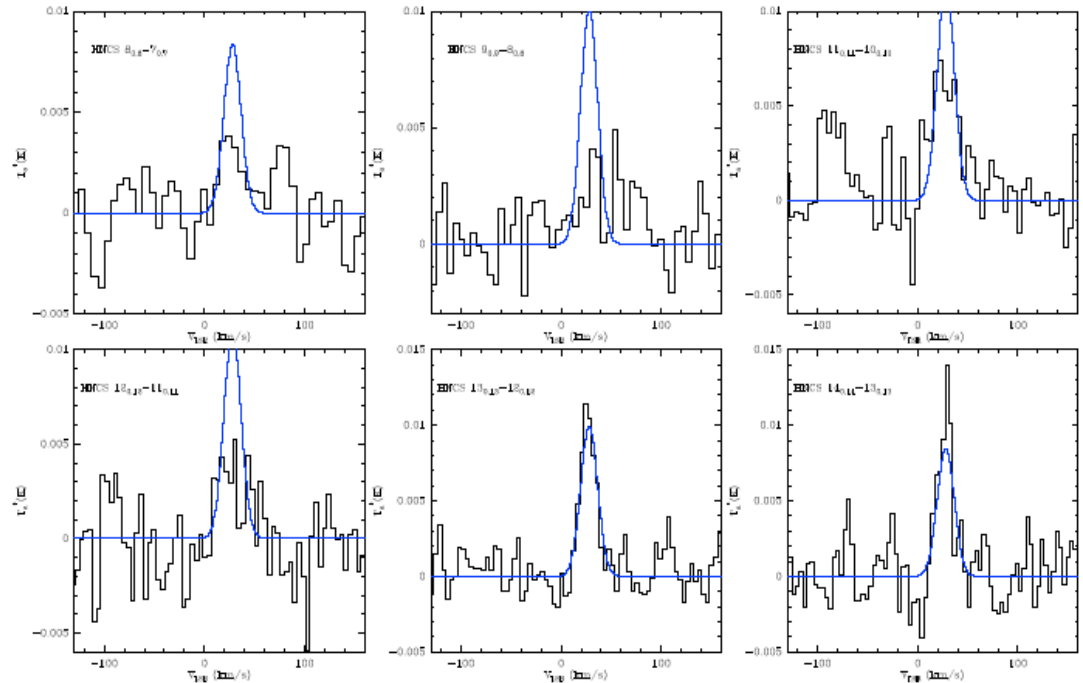
FWHM ~ 20 km/s → central core (I3)
wing, $v_{\text{lsr}} = 60 \text{ km/s}$ → base of the SOUTH lobe (I4)



IRAM 30m mm-line survey: OH231.8+4.2

HNCO, **HNCS**, HC₃N= Velilla et al., in prep.

Molecule	$J_u - J_l$ $J_{K_u - k_u}^u - J_{K_l - k_l}^l$	ν_{rest} (MHz)	E_u (K)	A_{ul} s^{-1}
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HNCO	4 _{0,4} - 3 _{0,3}	87925.237	10.5	9.025×
	5 _{0,5} - 4 _{0,4}	109905.749	15.8	1.802×
	6 _{1,6} - 5 _{1,5}	131394.230	65.3	3.006×
	6 _{0,6} - 5 _{0,5}	131885.734	22.2	3.163×
	7 _{1,7} - 6 _{1,6}	153291.935	72.7	4.863×
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	11 _{1,11} - 10 _{1,10}	240875.727	112.6	1.957×
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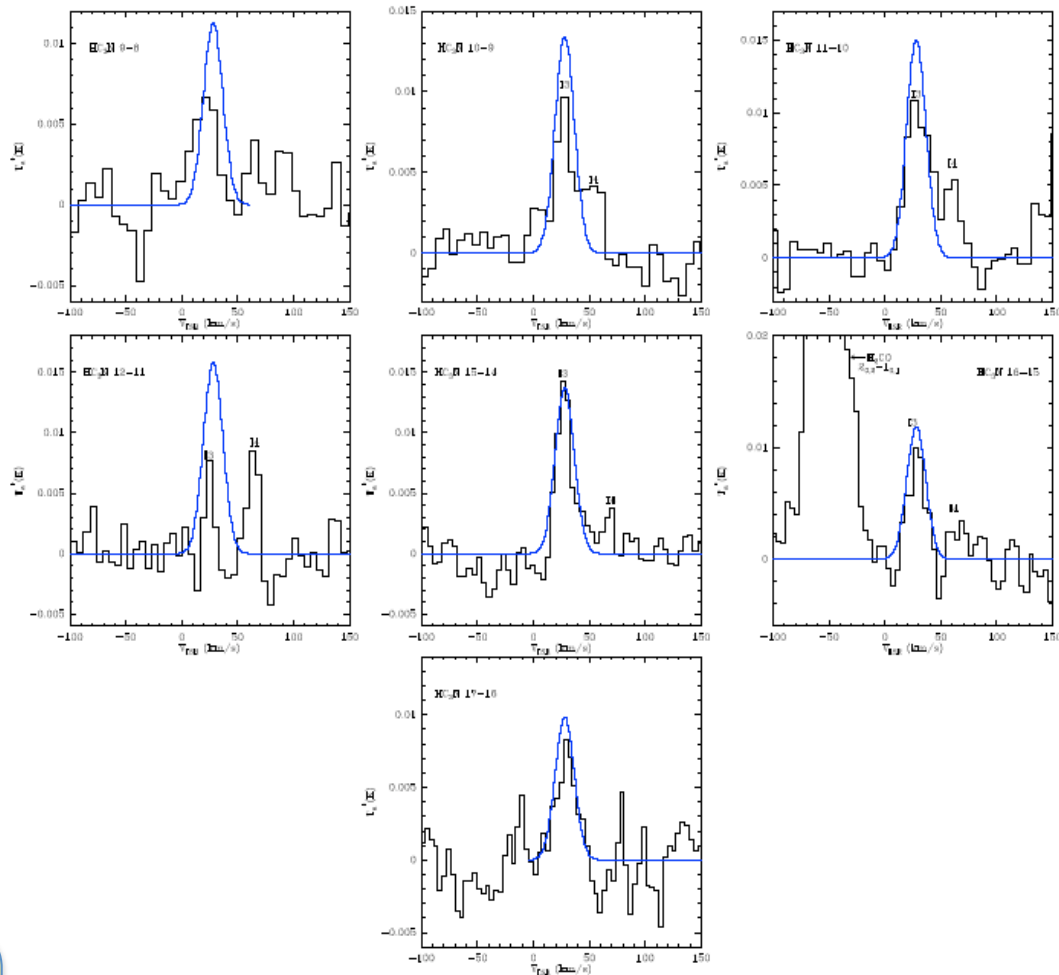
FWHM~20km/s → central core (I3)
weak wings? (low S/N)



IRAM 30m mm-line survey: OH231.8+4.2

HNCO, HNCS, **HC₃N** = Velilla et al., in prep.

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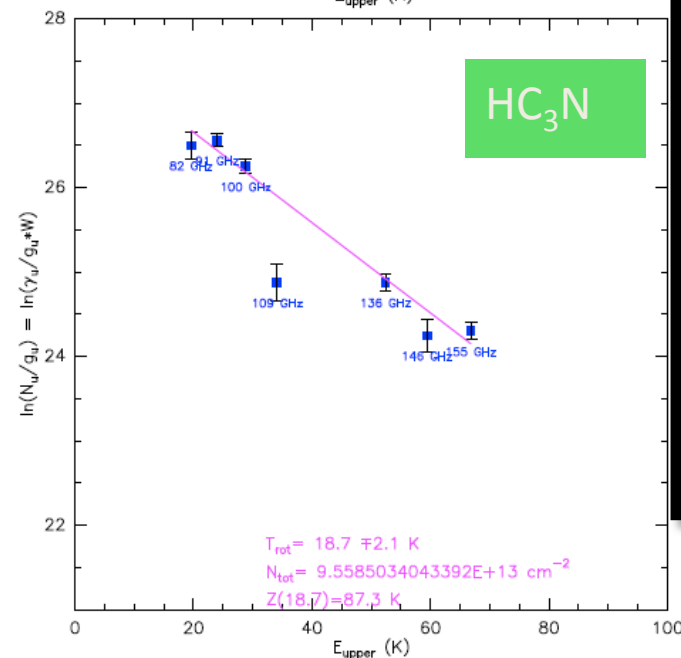
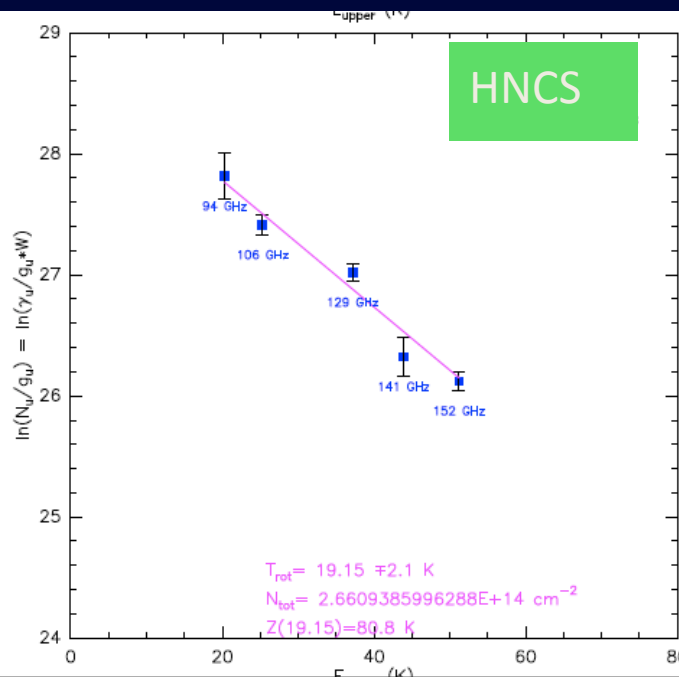
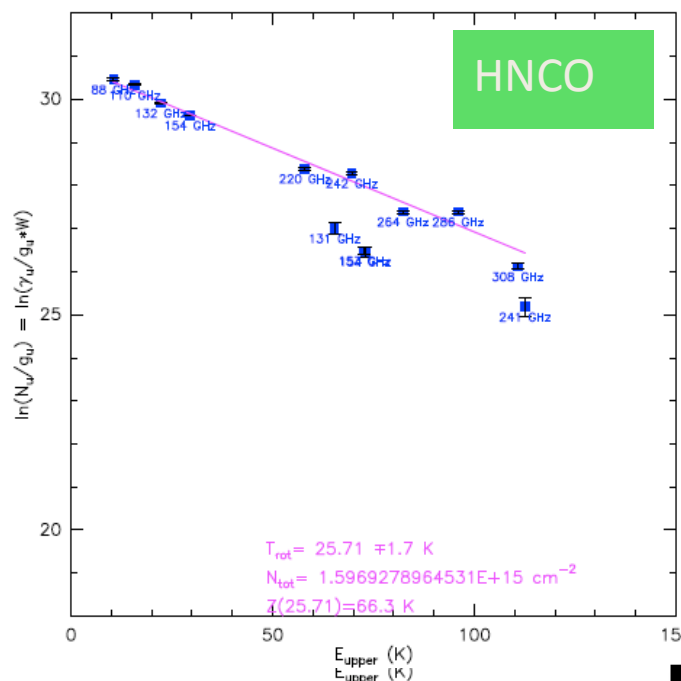


FWHM ~ 20 km/s → core (I3)

$v_{\text{lsr}} = 60 \text{ km/s}$ base of the SOUTH lobe (I4)



IRAM 30m mm-line survey: OH231.8+4.2

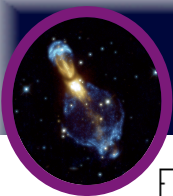


RDA (LTE, $\tau < 1$):
 beam-averaged
 $N, T_{\text{rot}} \rightarrow X$
 (MOL) w.r.t.
 $^{13}\text{CO} \approx 5 \times 10^{-5}$

$n(\text{H}_2) \sim > 10^6 - 10^{4-5} \text{ cm}^{-3}$

Molecule	ds (arcsec)	N (cm^{-2})	T_{rot} (K)	X
(i) LTE RESULTS				
^{13}CO	4 × 8	6.7 (1.9) × 10 ¹⁷	10 (1)	5 × 10 ⁻⁵
HNC	3 × 5	1.6 (0.2) × 10 ¹⁵	26 (2)	1 × 10 ⁻⁷
HNCS	3 × 5	2.6 (0.7) × 10 ¹⁴	18 (2)	2 × 10 ⁻⁸
HC ₃ N	3 × 5	1.1 (0.3) × 10 ¹⁴	17 (2)	8 × 10 ⁻⁹

$X(\text{HCN}) \approx X(\text{HNC}) \approx 10^{-8}$



IRAM 30m mm-line survey: OH231.8+4.2

Chemical kinetics model (Agúndez et al 2007): gas-phase + UV-chemistry

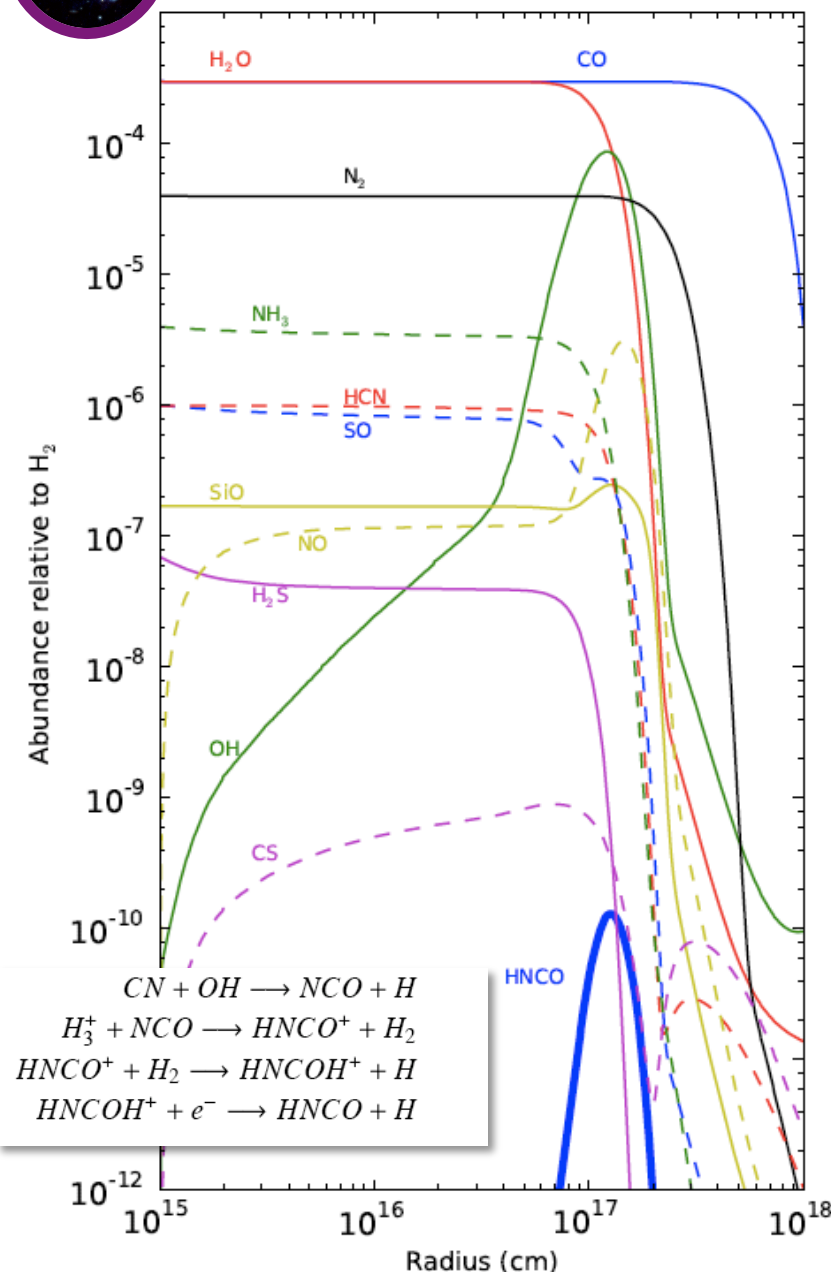
HNCO, HNCS, and HC₃N abundances by factor >100

Other astronomical environments:

- **HNCO**: SgrB2, Taurus, shocked outflow L1157 ($X_{\text{HNCO}} \approx 9.6 \times 10^{-8}$)
- **HNCS**: SgrB2, TMC-1 ($X_{\text{HNCS}} \approx 10^{-11}$)
- **HC₃N**: SgrB2, Ori ($X_{\text{HC3N}} \approx 10^{-6}$)

what is different?
shocks

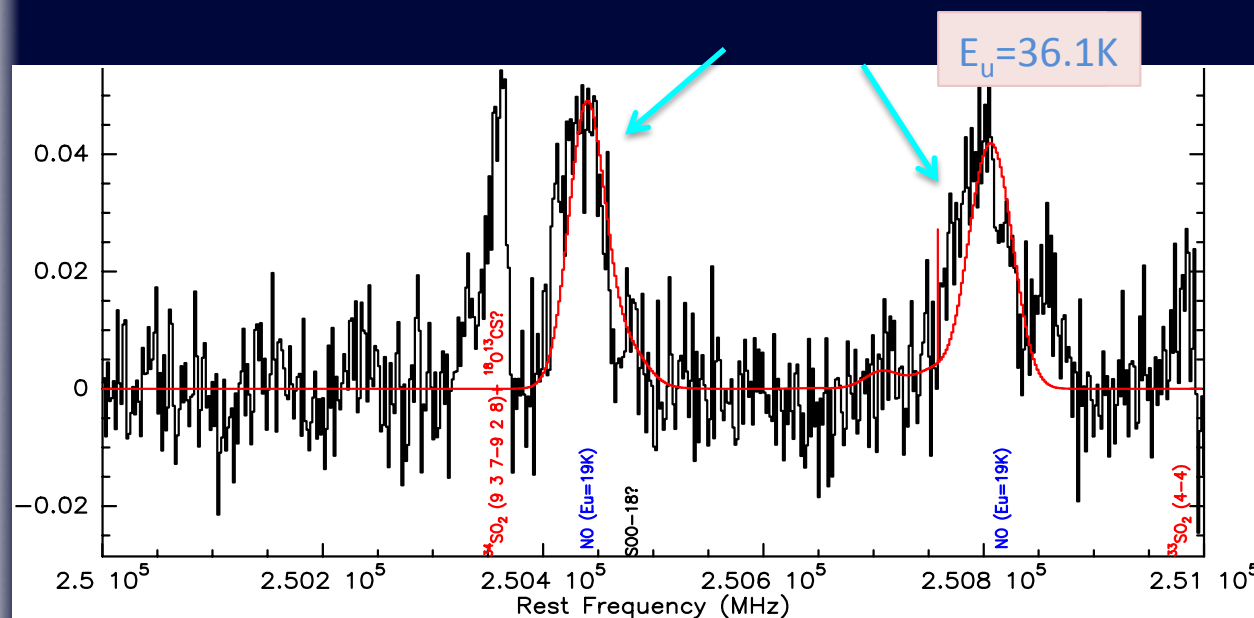
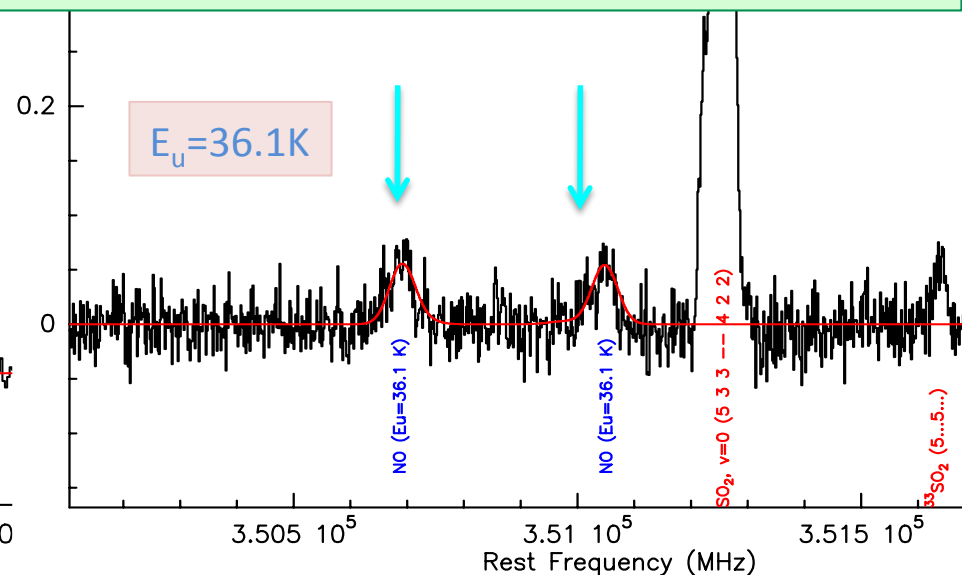
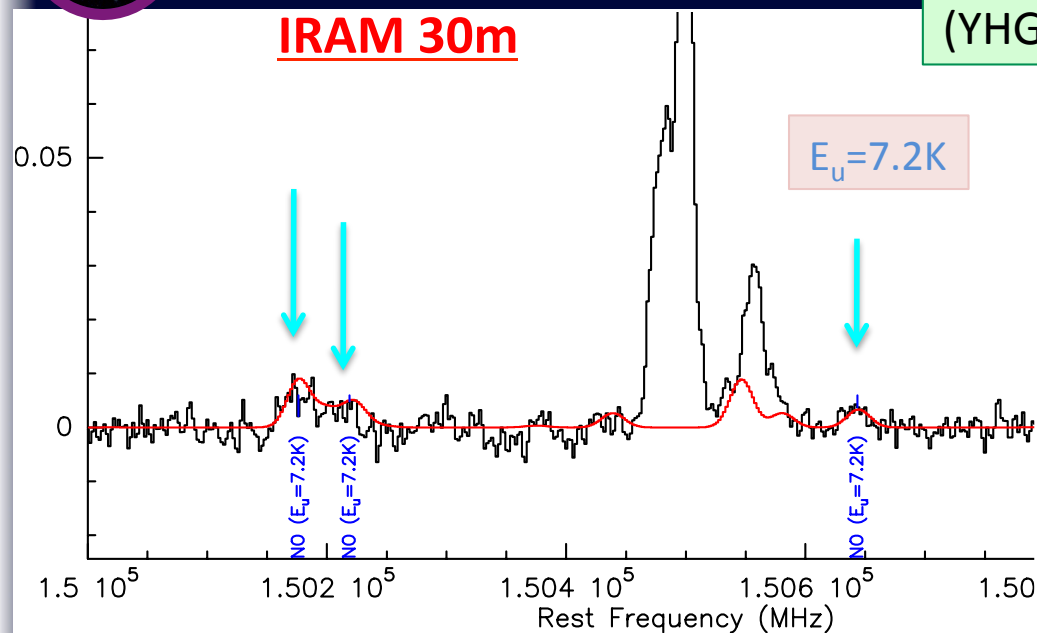
Non detected (O-rich CSE):
IK Tau $< 10^{-9} - 10^{-10}$
(VY CMa, IRC+10420)





New detections in OH231.8+4.2: **NO**

first detection in an **AGB CSE** (Velilla et al., in prep)
(YHG IRC+10420 G. Quintana-Lacaci 2013)



NO broad → FWHM=55km/s

preliminary ETL:

$N(\text{NO}) \sim 8 \times 10^{15} \text{ cm}^{-2}$

$T_{\text{rot}} \sim 15 \text{ K}$

$X(\text{NO}) \approx 1.3 \times 10^{-6}$

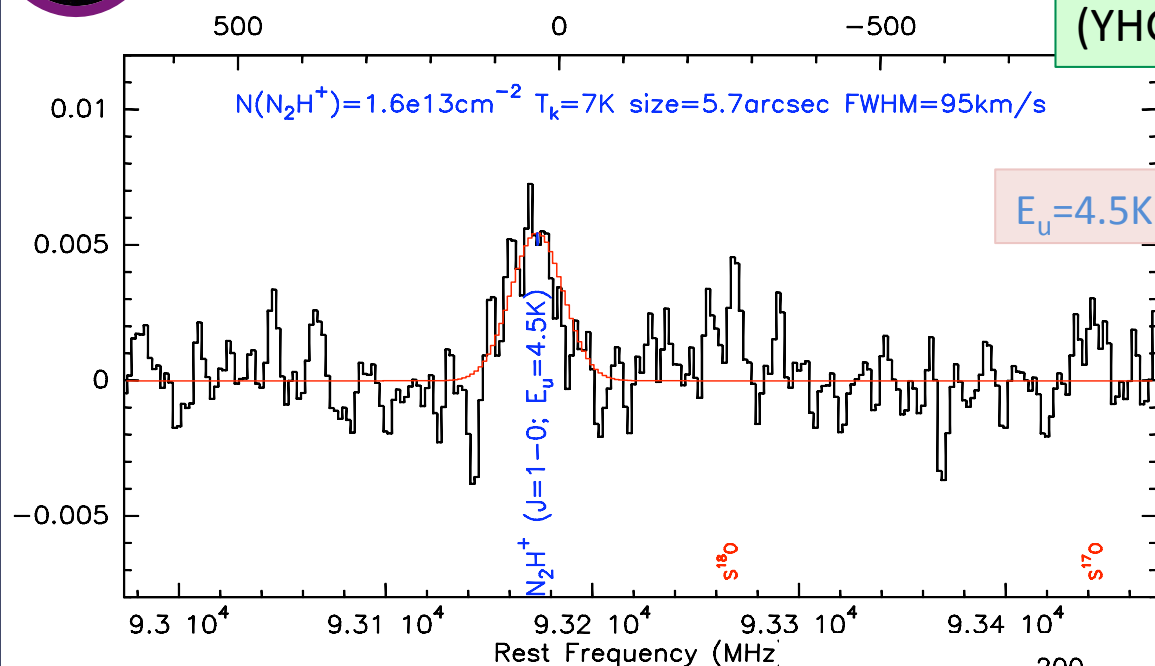
$X(\text{SO}) \approx X(\text{SO}_2) \approx 10^{-6}$



New detections in OH231.8+4.2: N_2H^+

IRAM 30m

first detection in an **AGB CSE**
(YHG IRC+10420, G. Quintana-Lacaci 2013)



N_2H^+ broad $\rightarrow$ FWHM = 90 km/s

preliminary ETL:

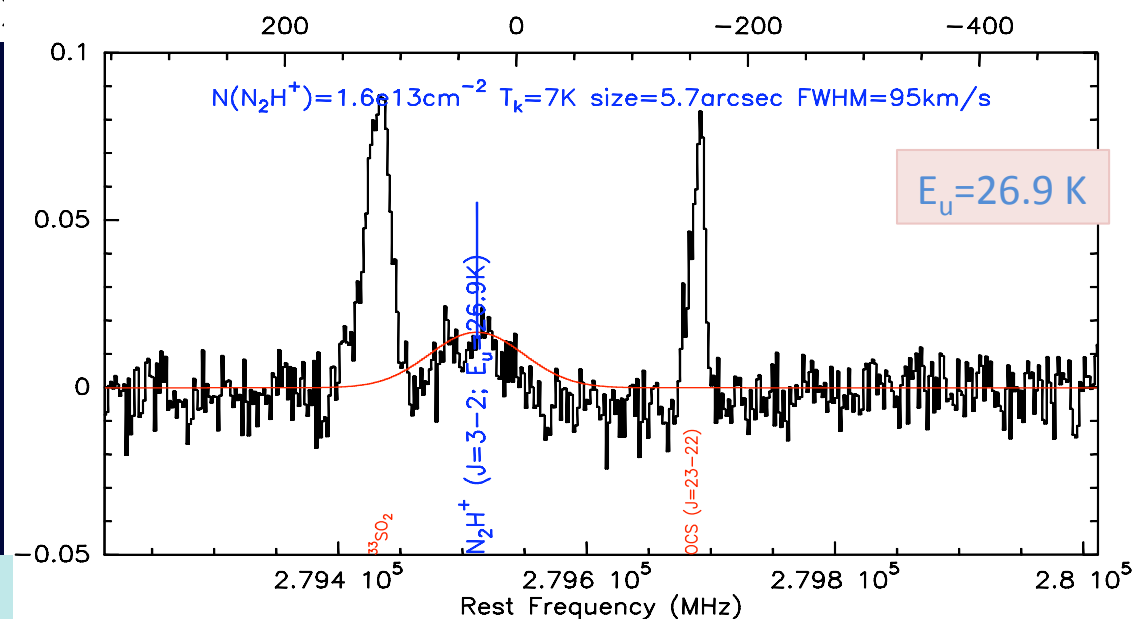
$$N(N_2H^+) \sim 1.6 \times 10^{13} \text{ cm}^{-2}$$

$$T_{\text{rot}} \sim 5-10 \text{ K}$$

$$X(N_2H^+) \approx 3 \times 10^{-9}$$

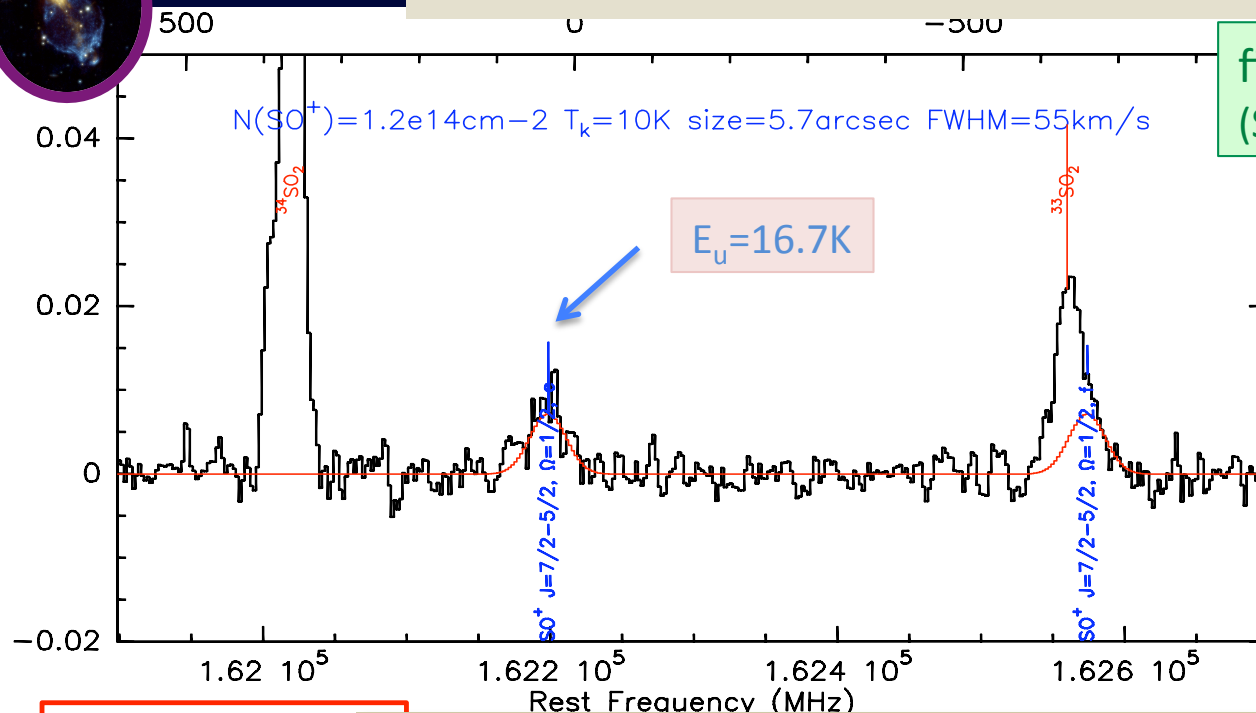
N_2H^+ probably enhanced in the
fast flow (+hyperfine splitting)

(Sánchez Contreras et al., in prep)





New detections in OH231.8+4.2: SO^+



first detection in an **AGB CSE**
(Sánchez Contreras et al., in prep)

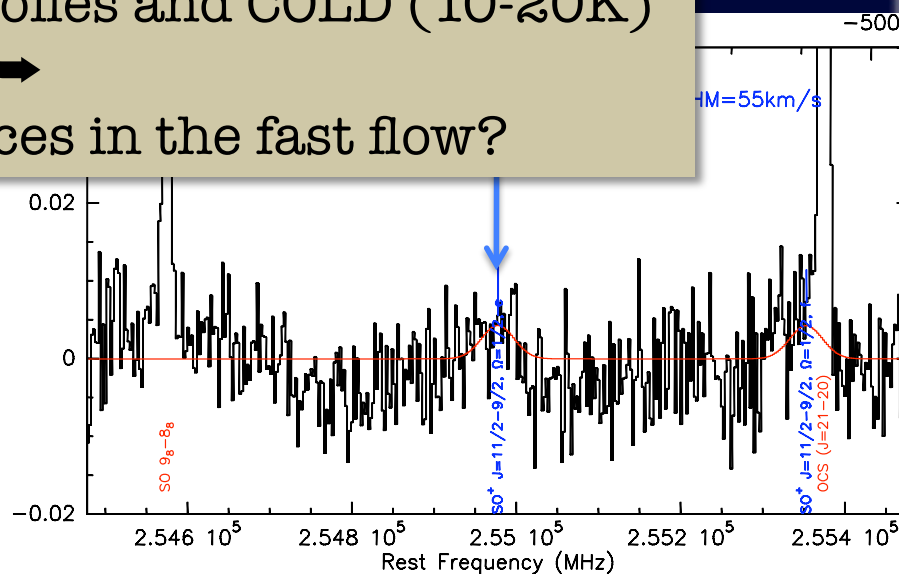
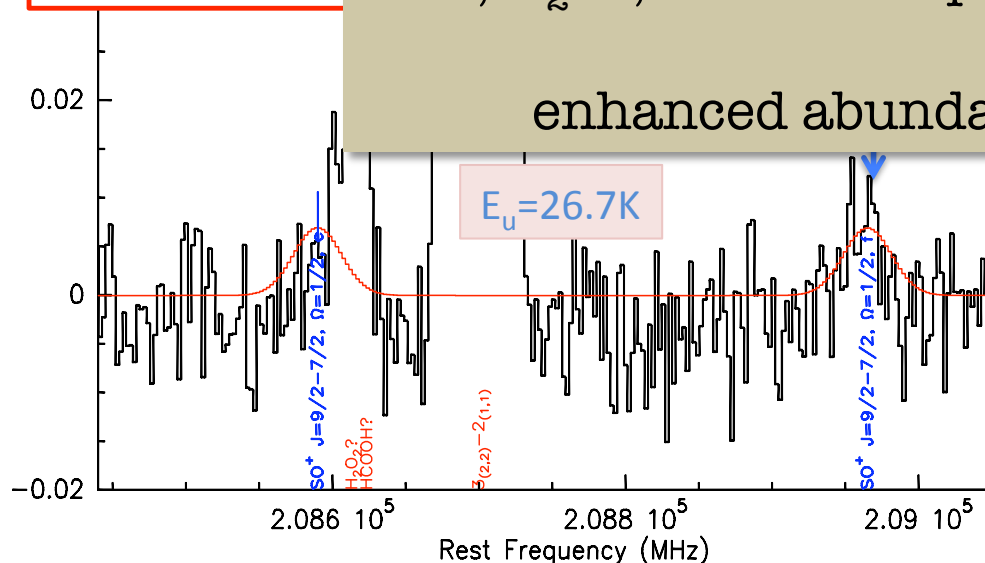
SO^+ broad profile:
FWHM ~ 55 km/s
~ 100 km/s-wide wings
→ **shocked outflow**

preliminary ETL:
 $N(\text{SO}^+) \sim 10^{14} \text{ cm}^{-2}$ and **COOL** ~ 10 K
 $X(\text{SO}^+) \sim 2 \times 10^{-8} \sim X(\text{SO})/100$

IRAM 30m

SO^+ , N_2H^+ , NO : broad profiles and COLD (10-20 K)

enhanced abundances in the fast flow?





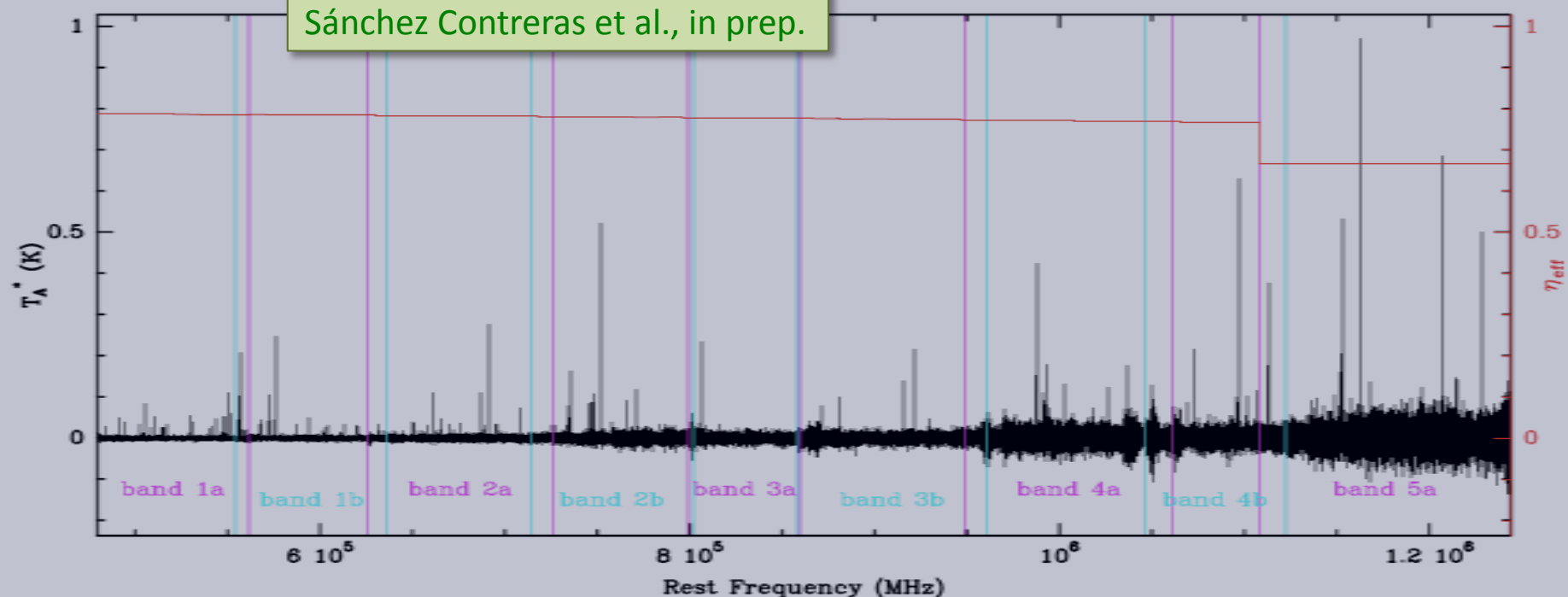
HSO/HIFI line survey: OH231.8+4.2



- 760 GHz, ~600 transitions (80% identified)
- No new species discovered: CO, SO, SO₂, H₂S, H₂O dominate
- Rotational ladders → physical and chemical properties

¹²CO, ¹³CO, C¹⁸O, **H₂O**, **H₂¹⁸O, **H₂¹⁷O (30 transitions, 3 vibrationally excited), SO, SO₂, H₂S, CS, HCN, HNC, HCO⁺, SiO, SiS, NS (+isotopologues)****

- Sensitive to warmer regions + spectral resolution (slow vs. fast)





HSO/HIFI line survey: OH231.8+4.2

Results: Line profiles



^{12}CO

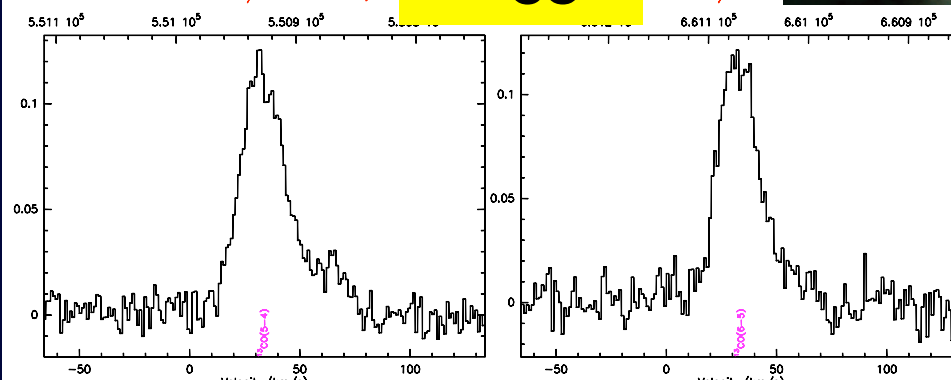
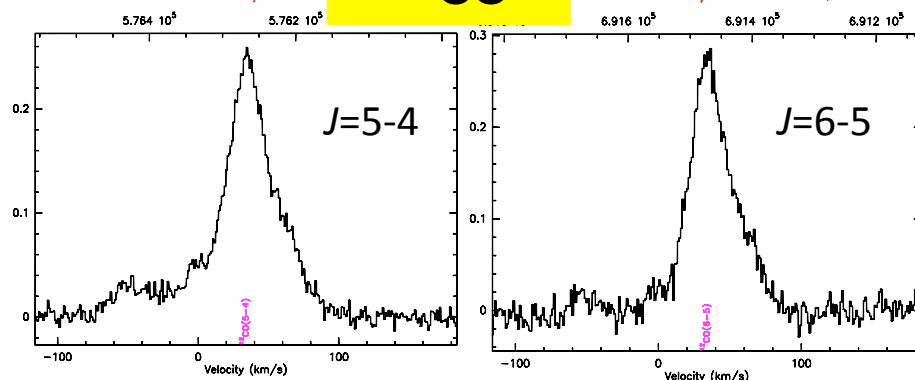
^{13}CO

Area= 12.71K*km/s Eu=8

a= 11.17K*km/s Eu=116.2K; co

Area= 3.26K*km/s Eu=79.3K; 1

.85K*km/s Eu=

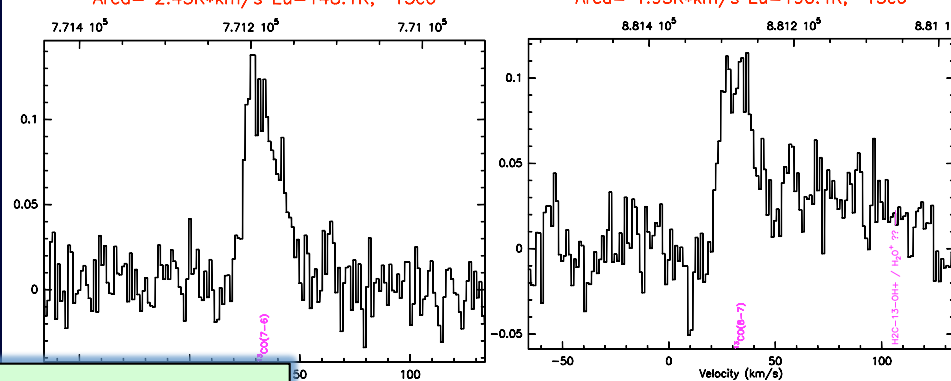
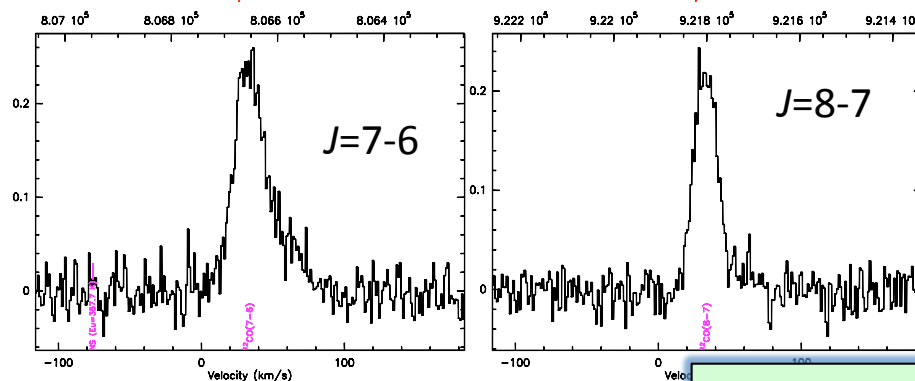


Area= 7.14K*km/s Eu=154.9K; co

Area= 5.16K*km/s Eu=199.1K; co

Area= 2.45K*km/s Eu=148.1K; 13co

Area= 1.95K*km/s Eu=190.4K; 13co

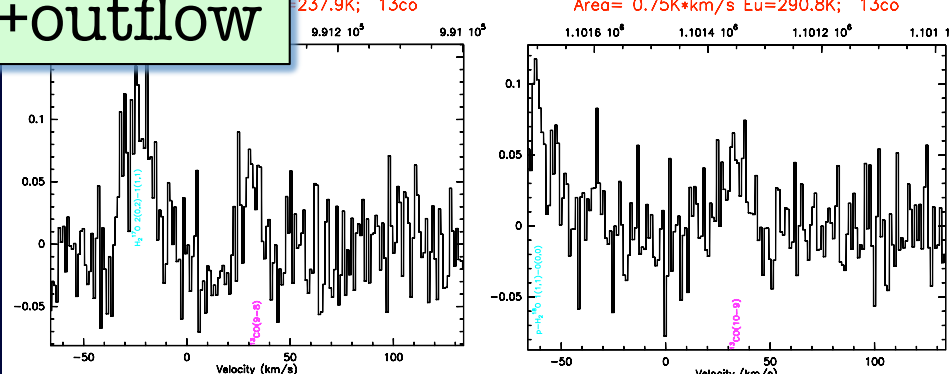
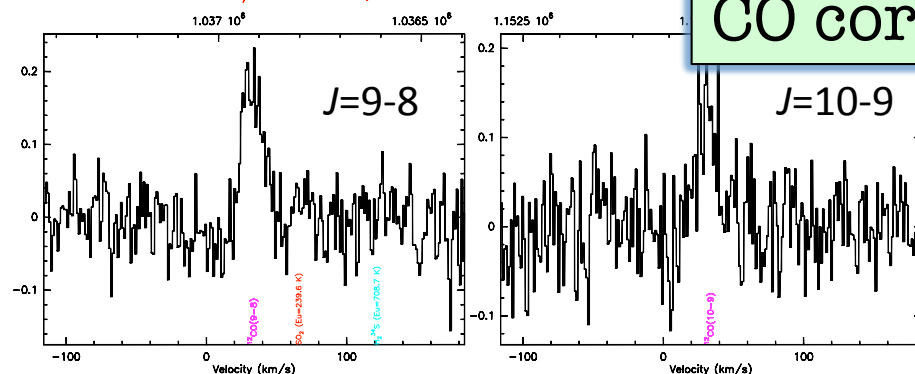


Area= 3.68K*km/s Eu=248.9K; co

Area= 2.11K*km/s Eu=137.9K; co

Area= 0.75K*km/s Eu=290.8K; 13co

Area= 0.75K*km/s Eu=290.8K; 13co



CO core+outflow



HSO/HIFI line survey: OH231.8+4.2



Line profiles

H_2O , H_2^{18}O , H_2^{17}O

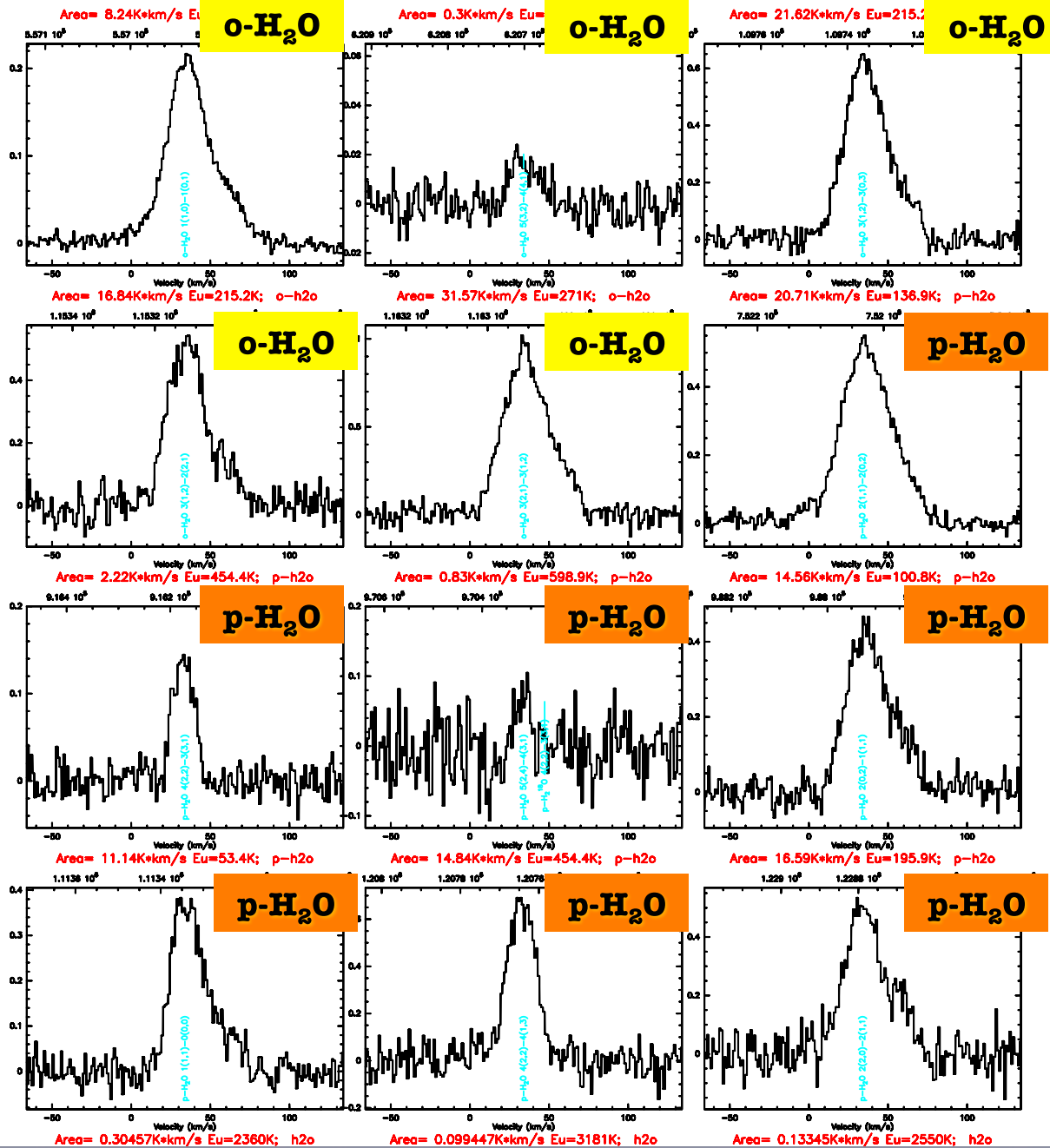
- $E_u = 26-698\text{K}$ ($v=0$)
- $E_u = 2-3 \times 10^3\text{K}$ ($v_2=1$)

$v=0$

core $\sim 10-40\text{ km/s}$

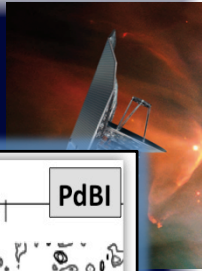
wings $\sim 100\text{ km/s}$

→ similar to CO profile





HSO/HIFI line survey: OH231.8+4.2



H₂O & CO similar spatio-kinematic structure

H₂O traces warm (>200K)

CO traces cool (10-30K)

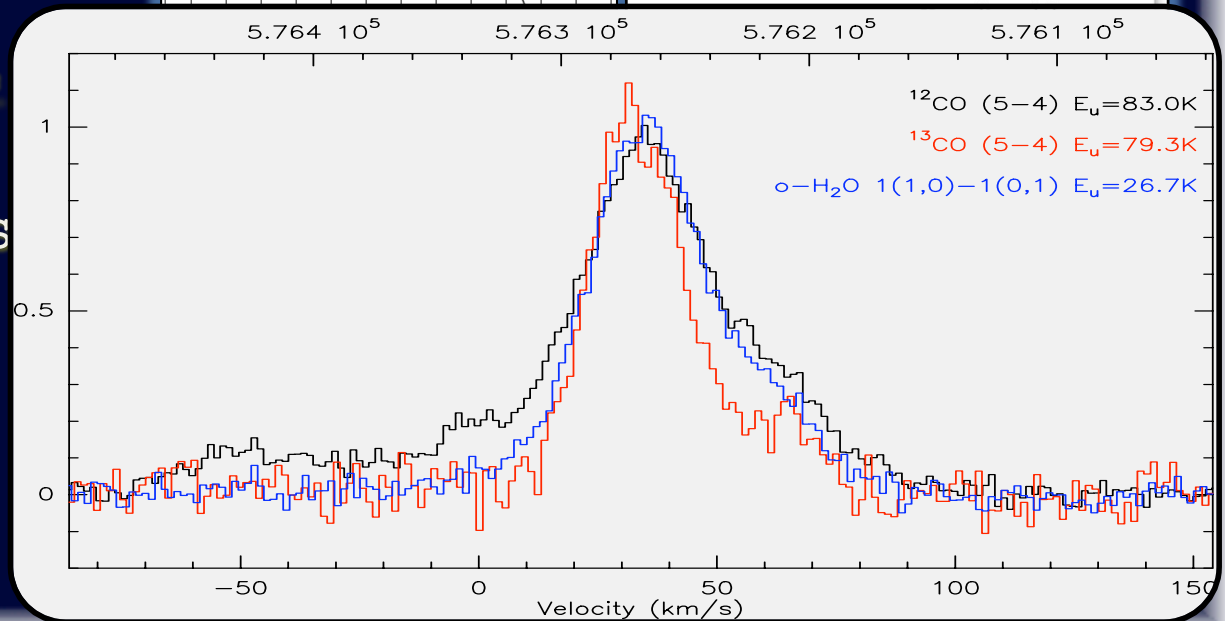
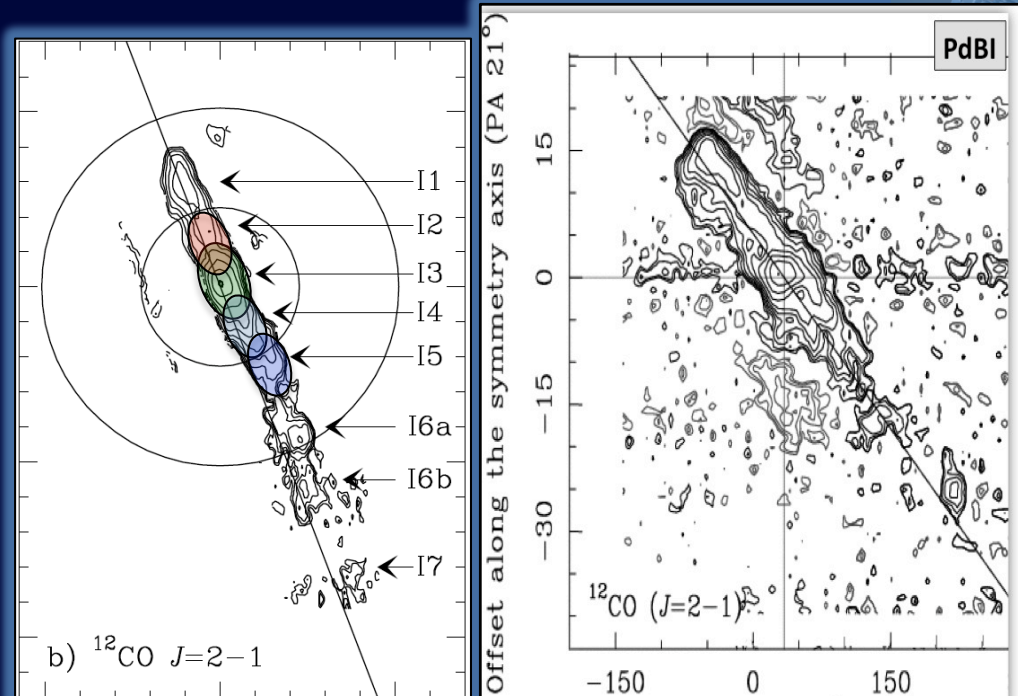
OUTFLOW=WARM+COOL



∇T ACCROSS the lobe walls

CO=outer walls

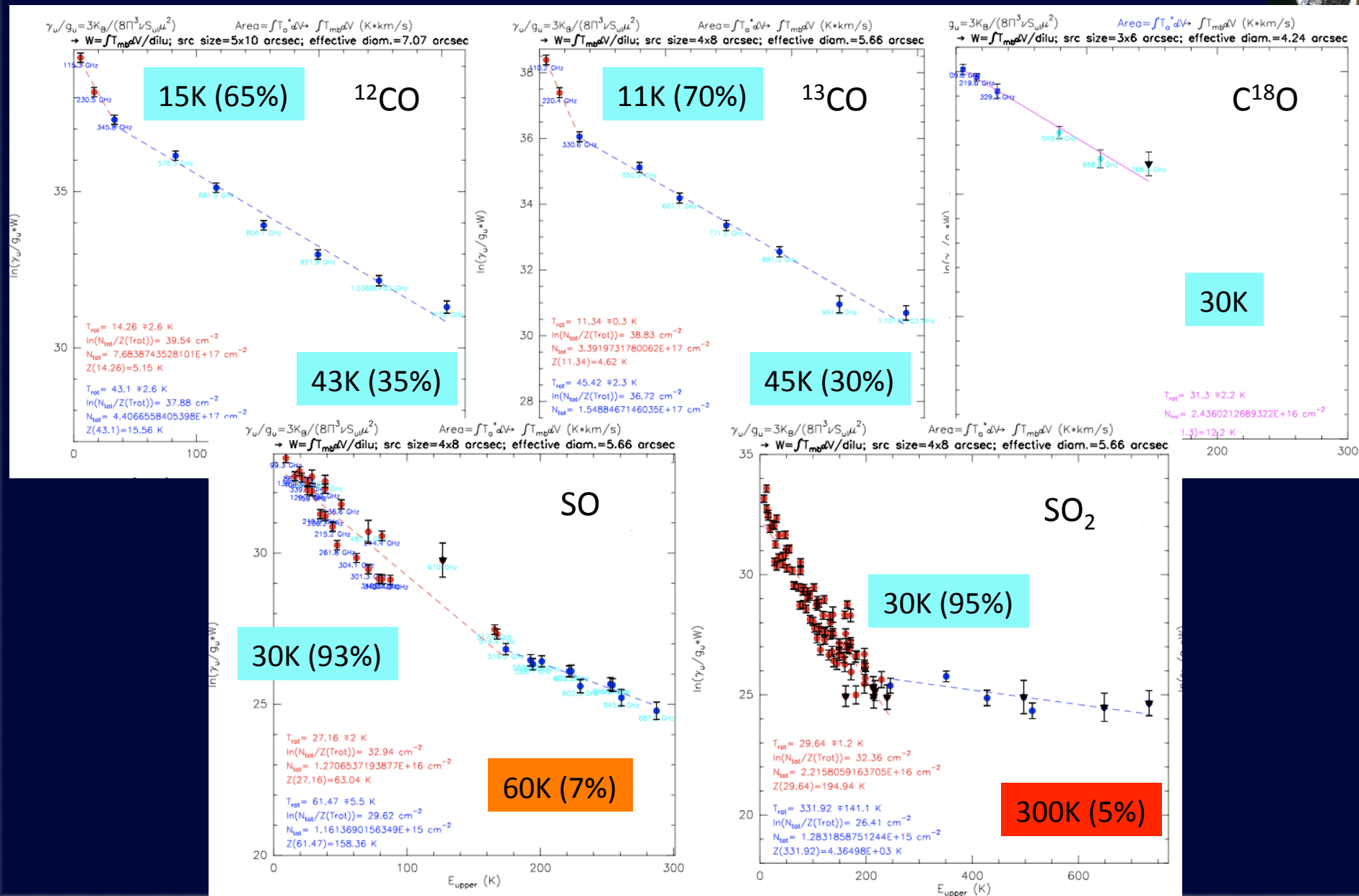
H₂O=inner walls





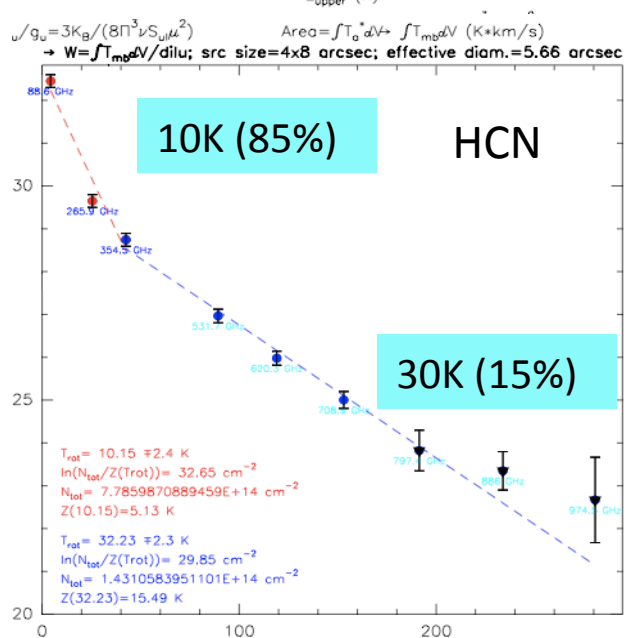
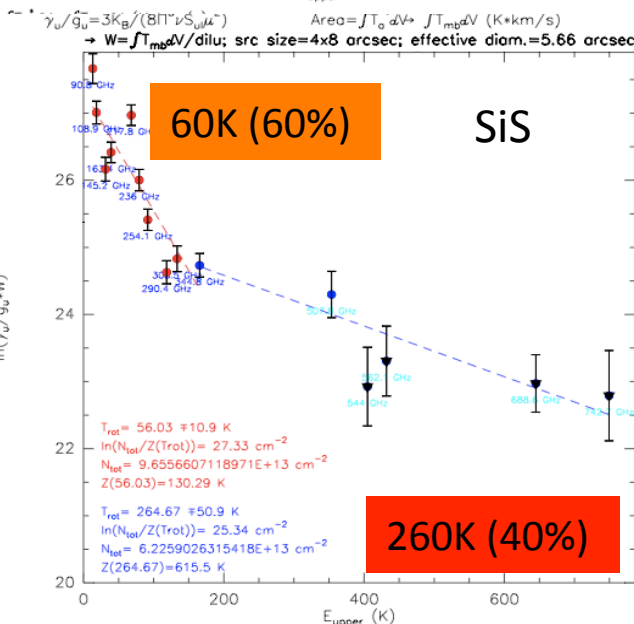
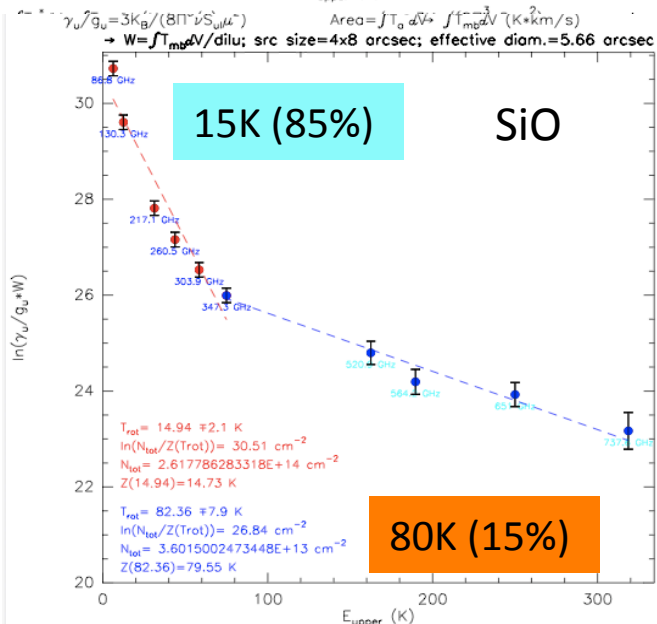
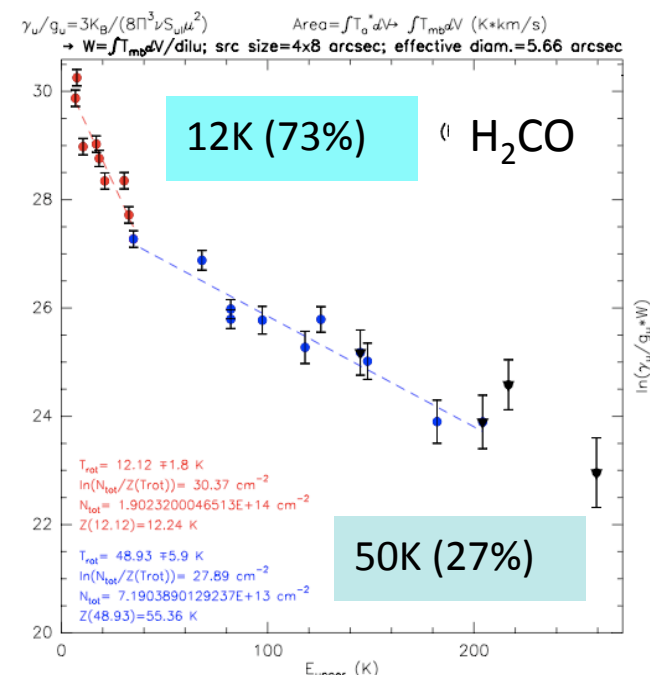
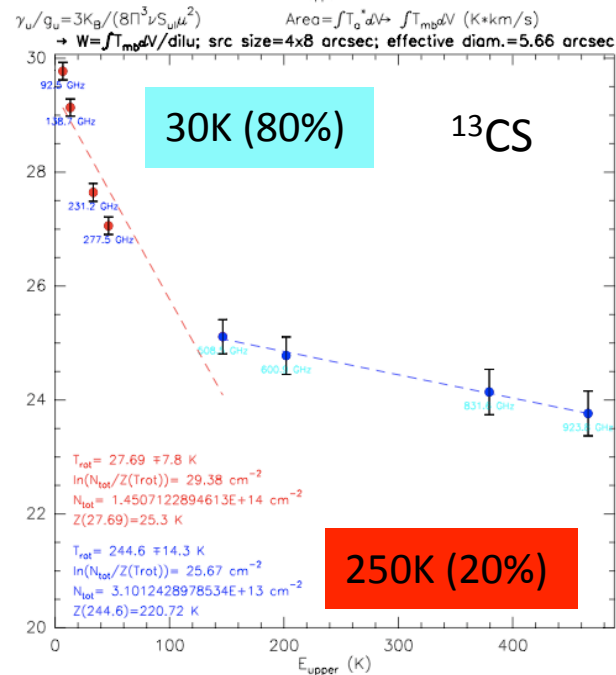
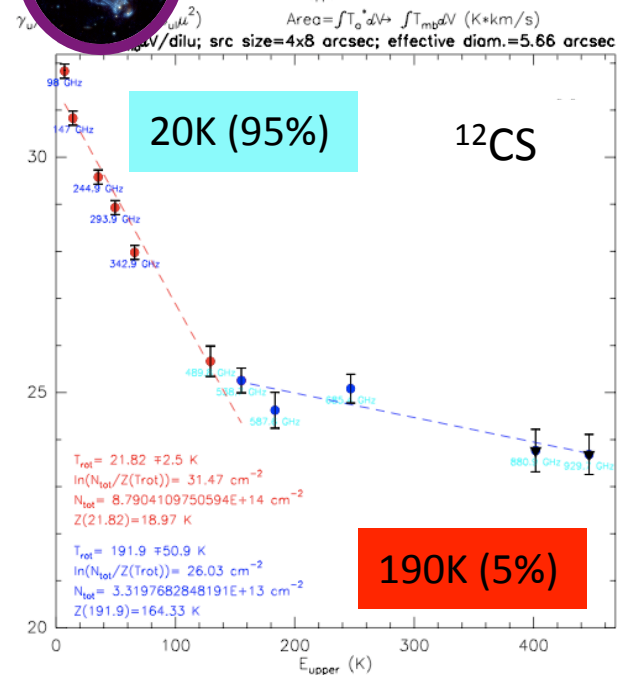
HSO/HIFI line survey: OH231.8+4.2

Results: Rotational diagrams (+ IRAM 30m data)



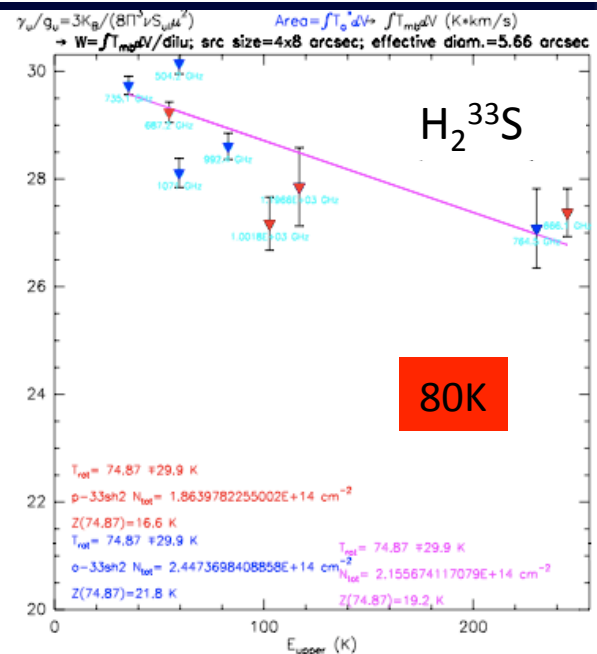
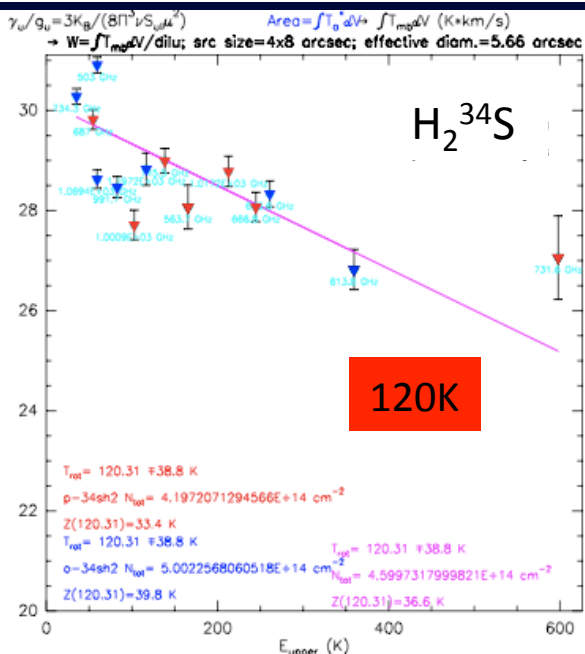
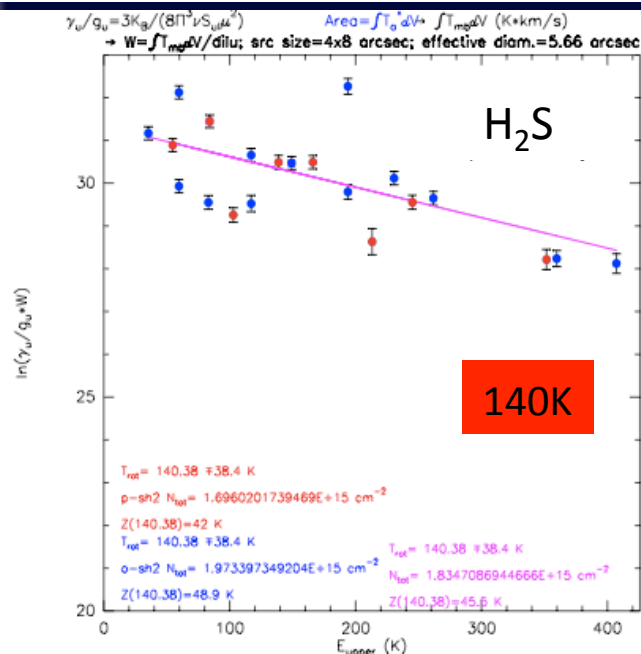
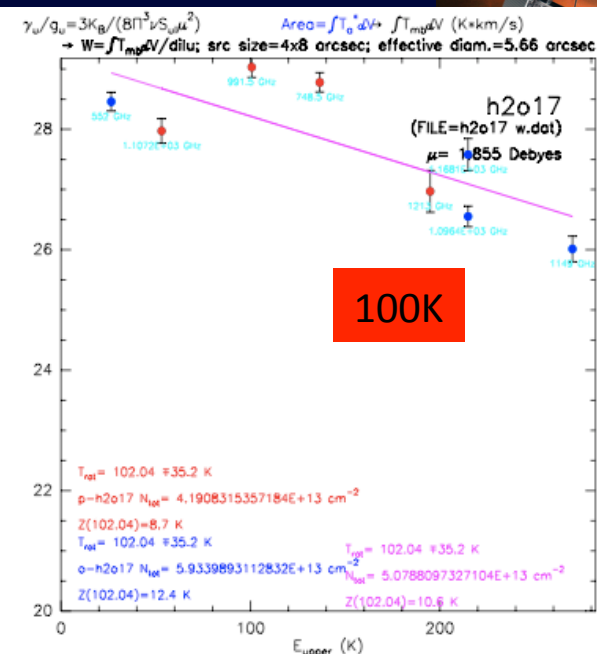
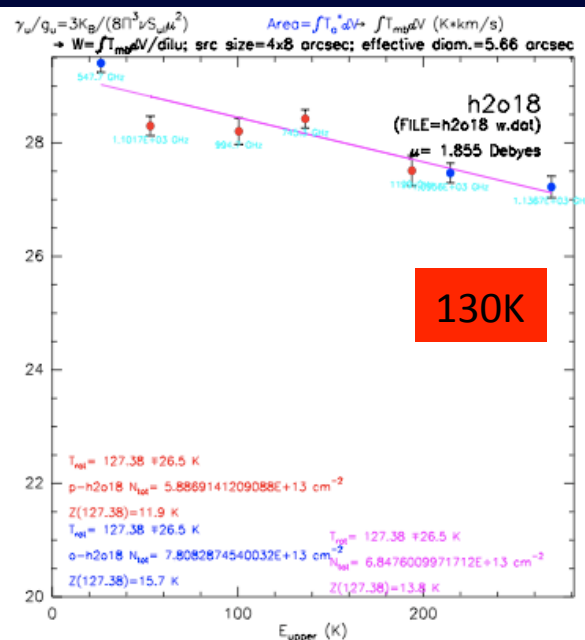
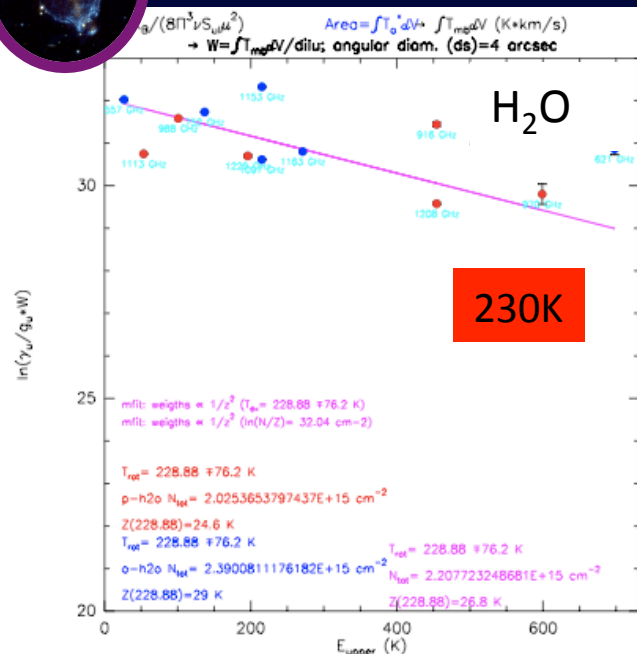
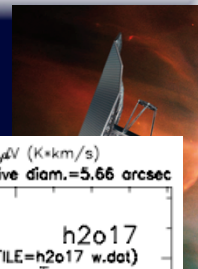


HSO/HIFI line survey: OH231.8+4.2





HSO/HIFI line survey: OH231.8+4.2





HSO/HIFI line survey: OH231.8+4.2

Results: Rotational diagrams

- N_{tot} , X for all molecules
non-LTE, radiative transfs. in progress
o/p ratio ≈ 1 (?) in progress...
isotopic ratios (C, S, O, Si) in progress...

- Temperature stratification

COLD $\sim 10\text{-}50\text{ K}$ CO, CS, SiO, HCN, HNC,
HCO⁺, NH₃, H₂CO, SO⁺,
N₂H⁺, OCS, NS, NO

WARM $>50\text{-}100\text{ K}$ SO, SiO, SiS, H₂CO

HOT $>100\text{-}200\text{ K}$ H₂O, H₂S, H₃O⁺, SO₂, CS,
SiO (maser), SiS, NS

VT not only at the CORE but also
across the LOBE walls!

Species	$\theta \times \theta$ (") $\times$ (")	N_{tot} (cm ⁻²)	T_{rot} (K)	$f(X)$
¹² CO	5 $\times$ 10	$\approx 7.7(2.0) \times 10^{17}$	14 (3)	1.5×10^{-4}
	5 $\times$ 10	$4.4(1.0) \times 10^{17}$	43 (3)	
¹³ CO	4 $\times$ 8	$3.4(0.2) \times 10^{17}$	11 (1)	5×10^{-5}
	4 $\times$ 8	$1.6(0.3) \times 10^{17}$	45 (2)	
C ¹⁸ O	4 $\times$ 8	$1.4(0.2) \times 10^{16}$	31 (2)	2×10^{-6}
SO ₂	4 $\times$ 8	$2.2(0.3) \times 10^{16}$	29 (1)	3×10^{-6}
	4 $\times$ 8	$1.3(0.7) \times 10^{15}$	330 (140)	
SO	4 $\times$ 8	$1.3(0.3) \times 10^{16}$	27 (2)	2×10^{-6}
	4 $\times$ 8	$1.2(0.4) \times 10^{15}$	61 (5)	
NH ₃	4 $\times$ 8	$\approx 7.0(4.0) \times 10^{14}$	21 (4)	$\approx 3 \times 10^{-7}$
CS	4 $\times$ 8	$8.8(0.3) \times 10^{14}$	21 (2)	1.0×10^{-7}
	4 $\times$ 8	$3.3(1.2) \times 10^{13}$	190 (50)	
HCN	4 $\times$ 8	$7.8(0.50) \times 10^{14}$	10 (2)	$\approx 2 \times 10^{-8}$
	4 $\times$ 8	$1.4(0.04) \times 10^{14}$	32 (2)	
HCO ⁺	4 $\times$ 8	$3.0(0.5) \times 10^{14}$	14 (1)	5×10^{-8}
HNC	4 $\times$ 8	$2.6(1.7) \times 10^{14}$	24 (5)	4×10^{-8}
SiO	4 $\times$ 8	$2.6(0.1) \times 10^{14}$	14 (2)	4×10^{-8}
	4 $\times$ 8	$3.6(0.7) \times 10^{13}$	82 (8)	
SiS	4 $\times$ 8	$9.7(3.0) \times 10^{13}$	60 (11)	3×10^{-8}
	4 $\times$ 8	$6.2(1.6) \times 10^{13}$	260 (50)	
H ₂ CO	4 $\times$ 8	$1.9(0.05) \times 10^{14}$	12 (2)	2.5×10^{-8}
	4 $\times$ 8	$7.2(1.70) \times 10^{13}$	48 (6)	
¹³ CS [†]	4 $\times$ 8	$1.5(0.07) \times 10^{14}$	27 (8)	2.5×10^{-8}
	4 $\times$ 8	$3.1(0.2) \times 10^{13}$	244 (14)	
H ₂ O [*]	4 $\times$ 8	$> 1.2(0.3) \times 10^{15}$	230 (70)	$> 2 \times 10^{-7}$
H ₂ ¹⁸ O [*]	4 $\times$ 8	$7.0(1.8) \times 10^{13}$	130 (30)	$> 1.3 \times 10^{-8}$
H ₂ ¹⁷ O [*]	4 $\times$ 8	$5.1(2.1) \times 10^{13}$	100 (35)	$\approx 1.0 \times 10^{-8}$
H ₂ S [*]	4 $\times$ 8	$\approx 1.8(0.7) \times 10^{15}$	140 (40)	$\approx 3 \times 10^{-7}$
H ₂ ³⁴ S [*]	4 $\times$ 8	$4.6(1.7) \times 10^{14}$	120 (40)	8.0×10^{-8}
H ₂ ³³ S [*]	4 $\times$ 8	$2.2(0.9) \times 10^{14}$	75 (30)	4.0×10^{-8}
NS	4 $\times$ 8	$9.8(4.0) \times 10^{13}$	170 (50)	2×10^{-8}

¹²I2 4 $\times$ 8 $\approx 8(4.0) \times 10^{13}$ 130 (20) 5×10^{-8}
H₂³³S₂ 4 $\times$ 8 $5.5(0.8) \times 10^{14}$ 32 (30) 4.0×10^{-8}



Molecular Inventory in OH231.8+4.2

2 atoms	3 atoms	4 atoms	5 atoms
^{12}CO , ^{13}CO , C^{18}O , C^{17}O	SO_2 , $^{33}\text{SO}_2$, $^{34}\text{SO}_2$, SO^{18}O , SO^{17}O	H_2CO , H_2^{13}CO	HC_3N
SO , ^{33}SO , ^{34}SO , S^{18}O , S^{17}O	HCN , H^{13}CN	HNCO	
CS , ^{13}CS , C^{34}S , C^{33}S	HNC , HN^{13}C	HNCS	
NS , N^{33}S , N^{34}S	HCO^+ , H^{13}CO^+	NH_3	
CN , ^{13}CN	H_2S , H_2^{33}S , H_2^{34}S	H_3O^+	17 → 51 species Line identification NOT finished 20% features remaining...
SiO , ^{29}SiO , ^{30}SiO	OCS , O^{13}CS		
SiS	H_2O , H_2^{18}O , H_2^{17}O		
NO	N_2H^+		
SO^+			

Summary

- Molecular Line survey of O-rich CSE OH231.8: IRAM 30m + HSO
- ~1000 GHz explored mm/fIR, ~800 lines detected
- Line identification ~80%: 17 → 51 species
- Lack of/weak em. from the INNER layers → $\dot{M}_{\text{AGB}}$ STOPPING
- OH231's chemistry unparalleled amongst O-rich AGB & post-AGB
→ non-equilibrium molecule reformation in the shocked outflow
- New detections: HNCO, HNCS, HC₃N, NO, N₂H⁺, SO⁺, CN, SiS, H₃O⁺ ...
NOT EXPLAINED chemical kinetics models
- Many transitions of H₂O, CO, SO₂, SO, H₂S, etc → physical and chemical properties, molecular abundances
- Temperature comps.: 10-50, 50-100, >100 K (across lobe walls)

Thank you for your attention