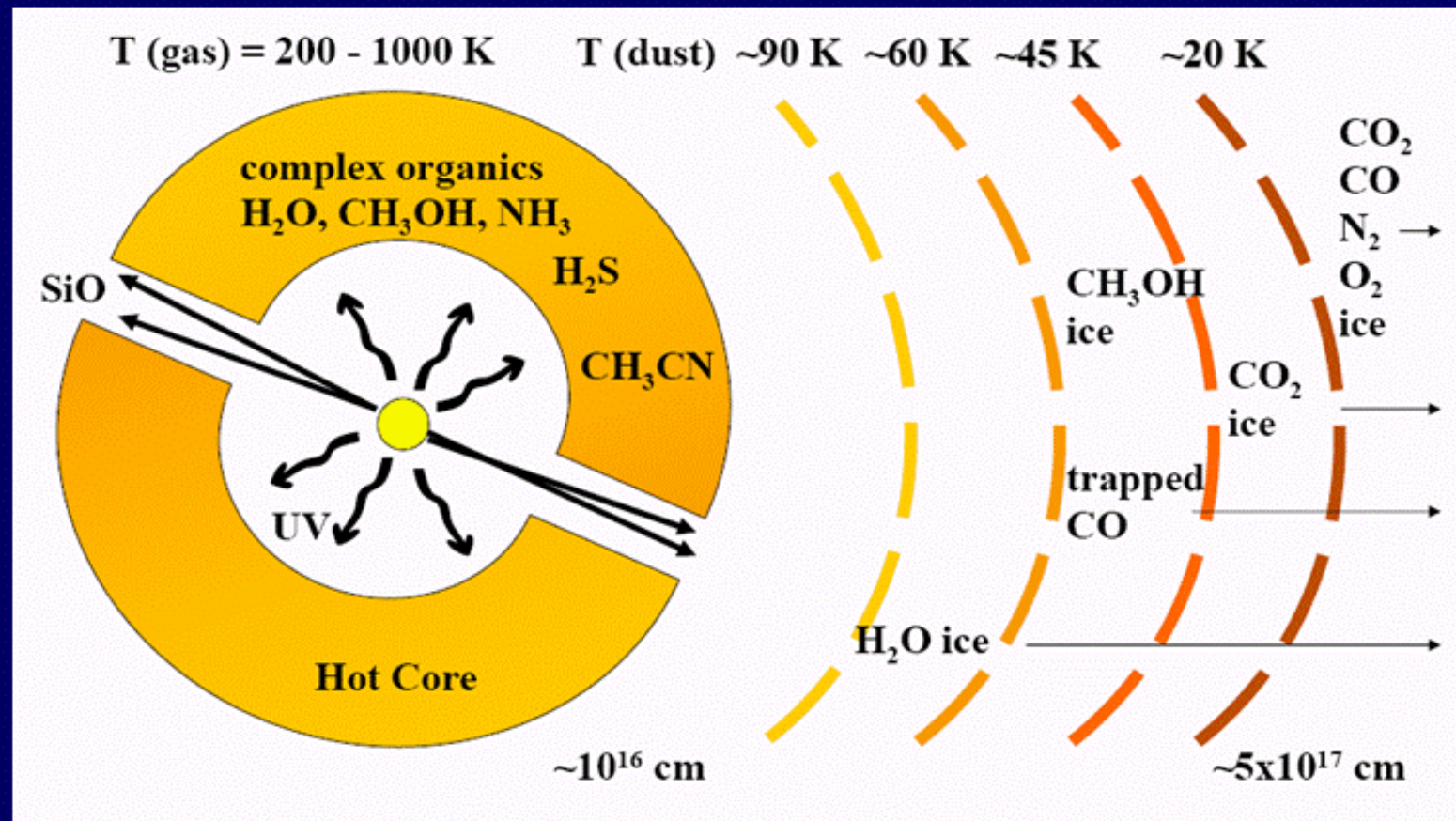


# Cyanoacetylene in the outflow/hot molecular core G331.512-0.103

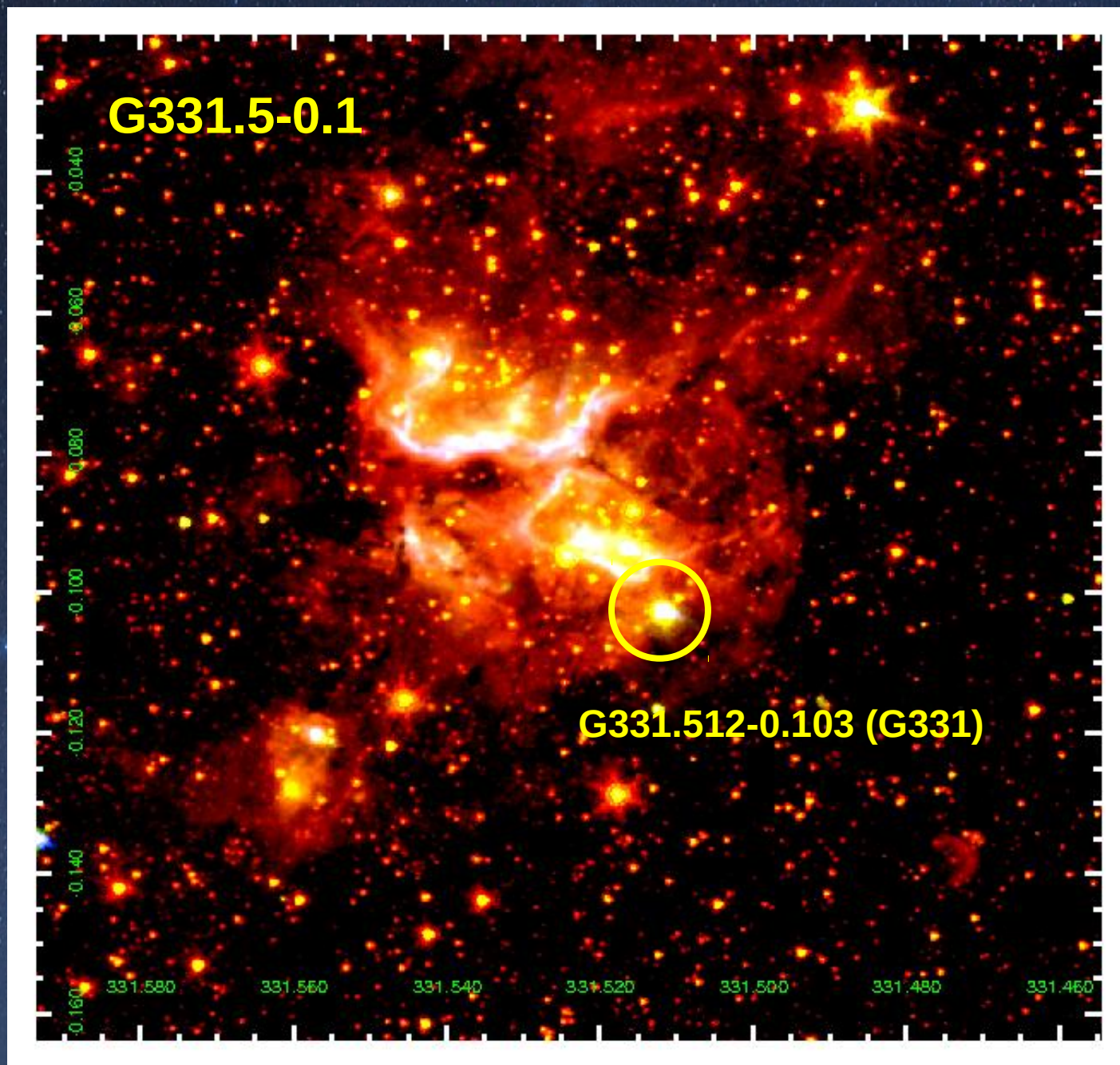
*Duronea N.U.  
Bronfman L.  
Mendoza E.  
Merello M.  
Finger R.  
Reyes N.  
Hervias-Caimapo C.  
Faure A.  
Cappa C.  
Arnal E.M.  
Lépine J.R.D.  
Kleiner I.  
Nyman L-A.*



## Schematic of a Hot Core



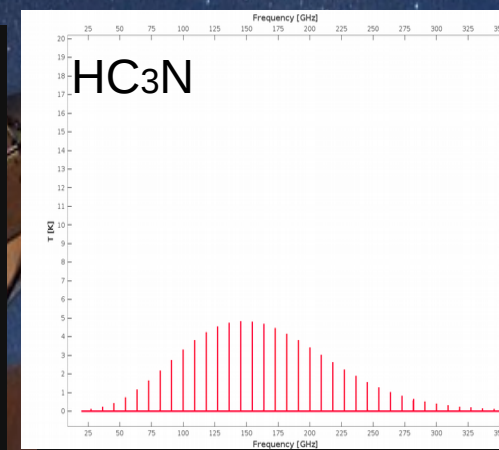
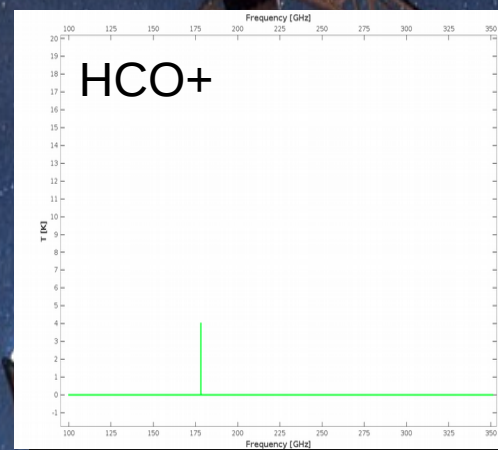
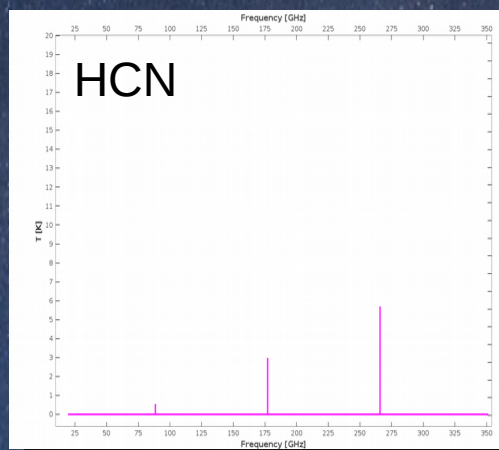
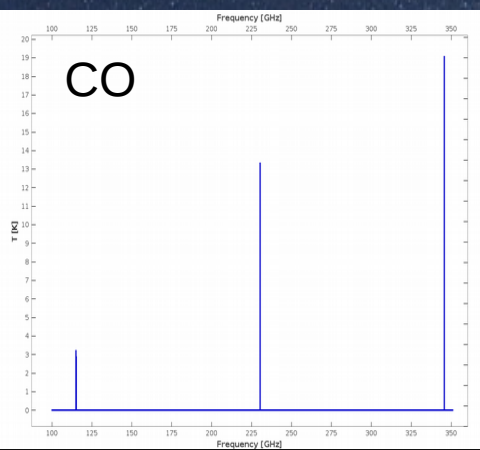
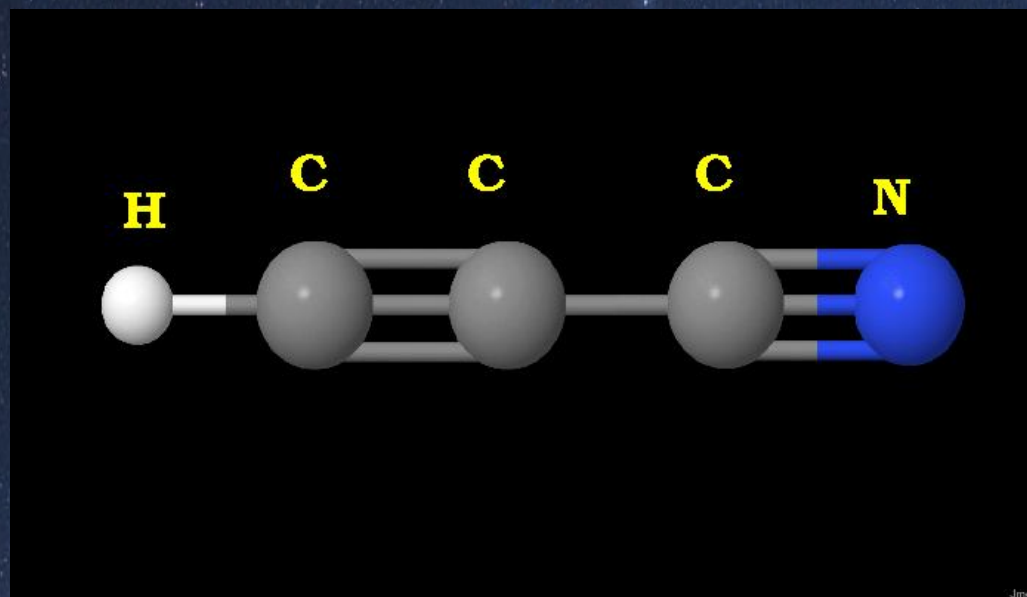


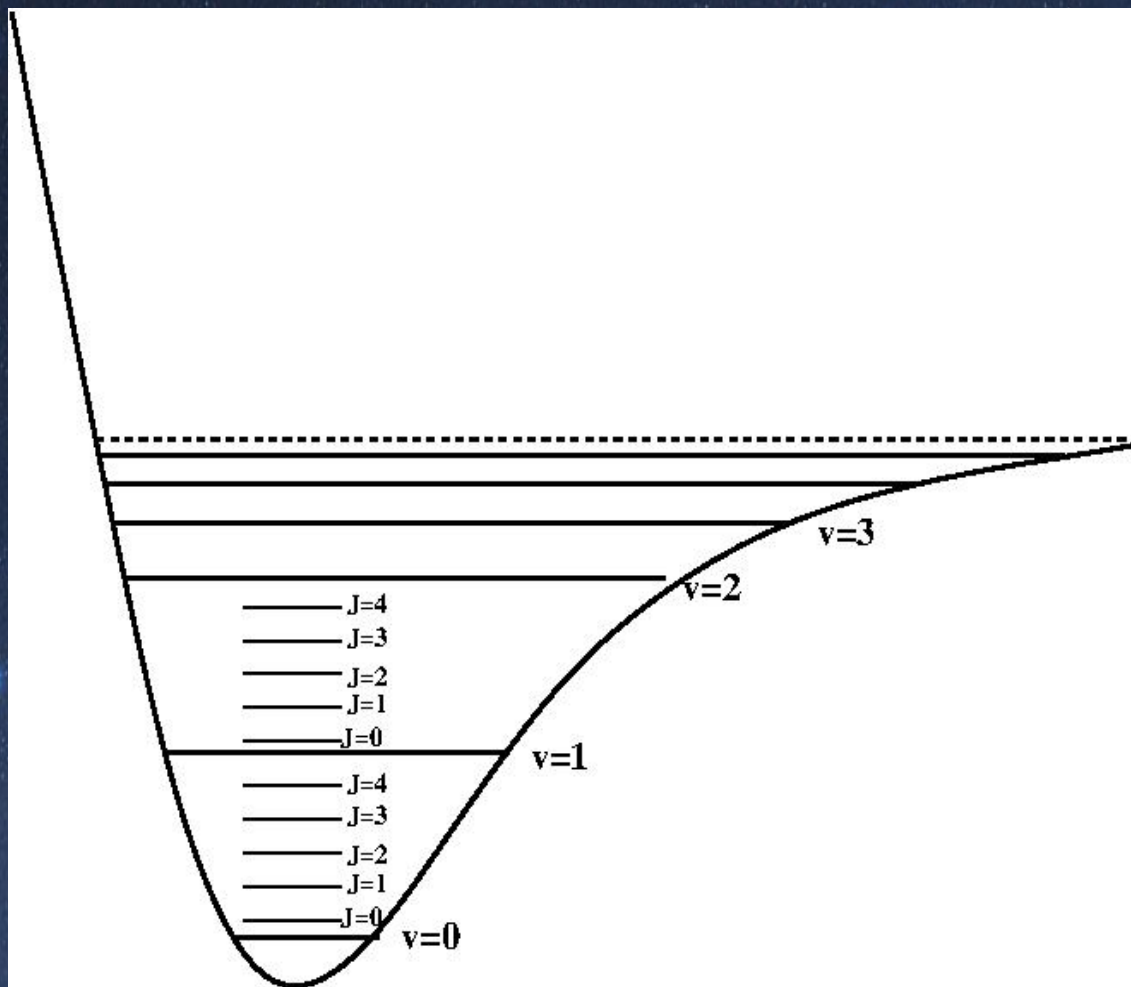




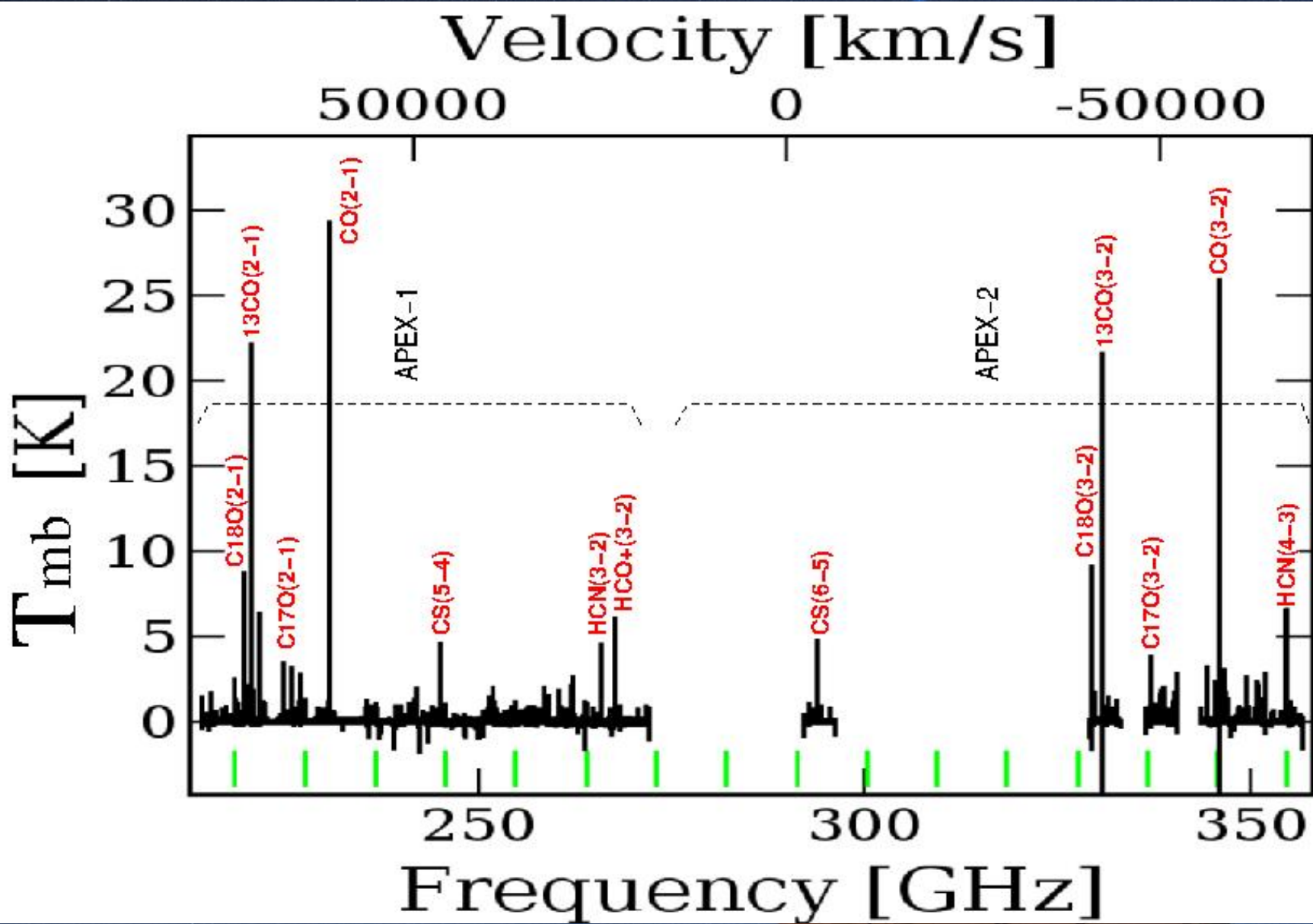


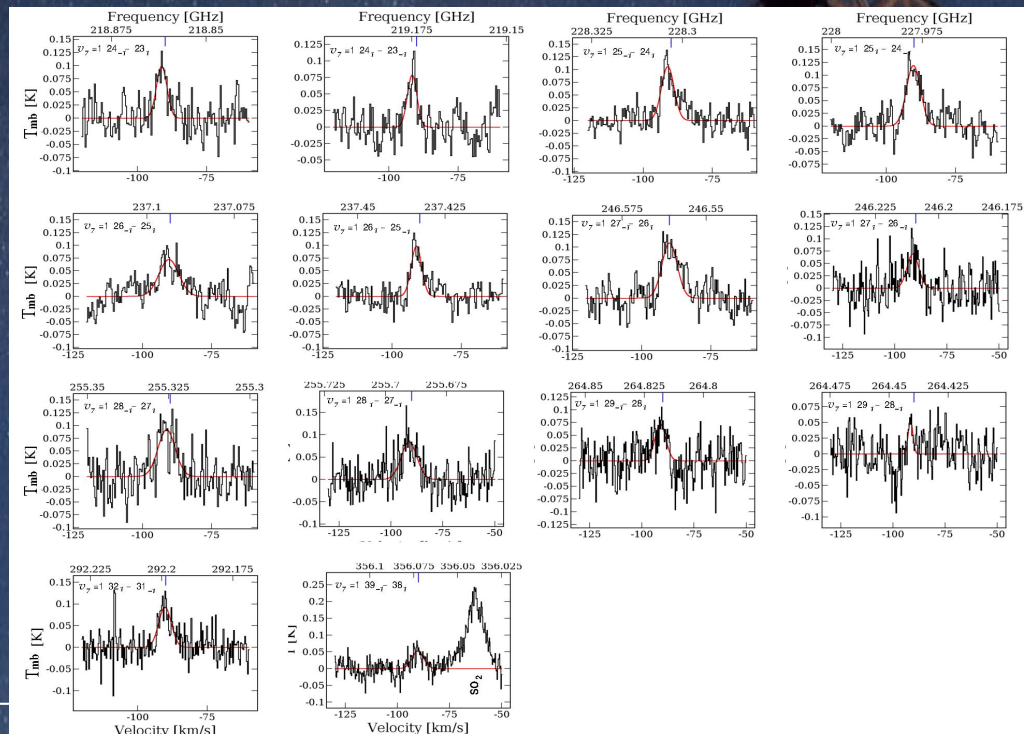
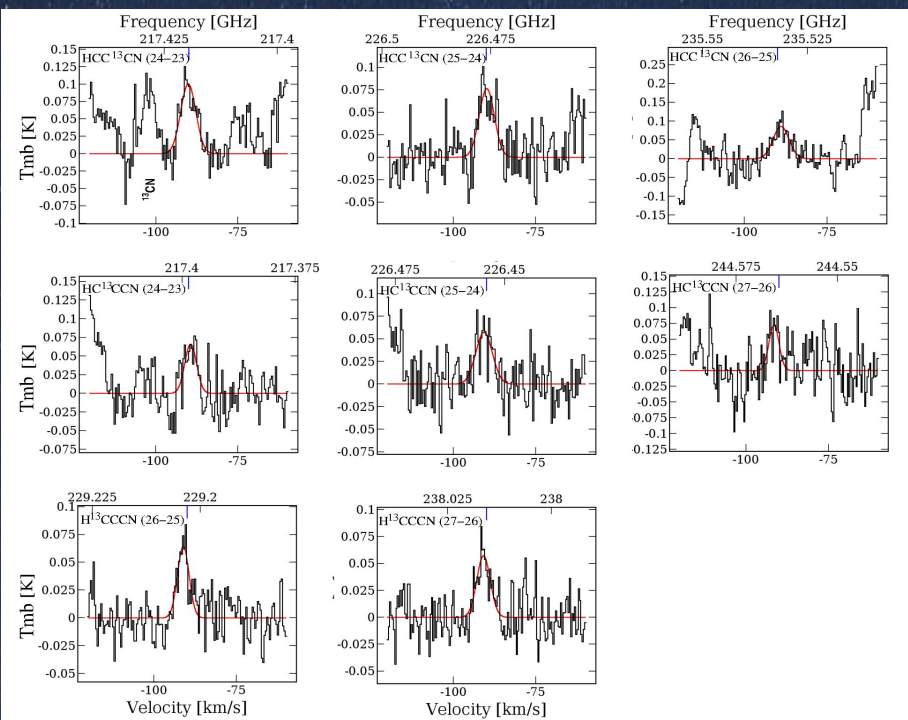
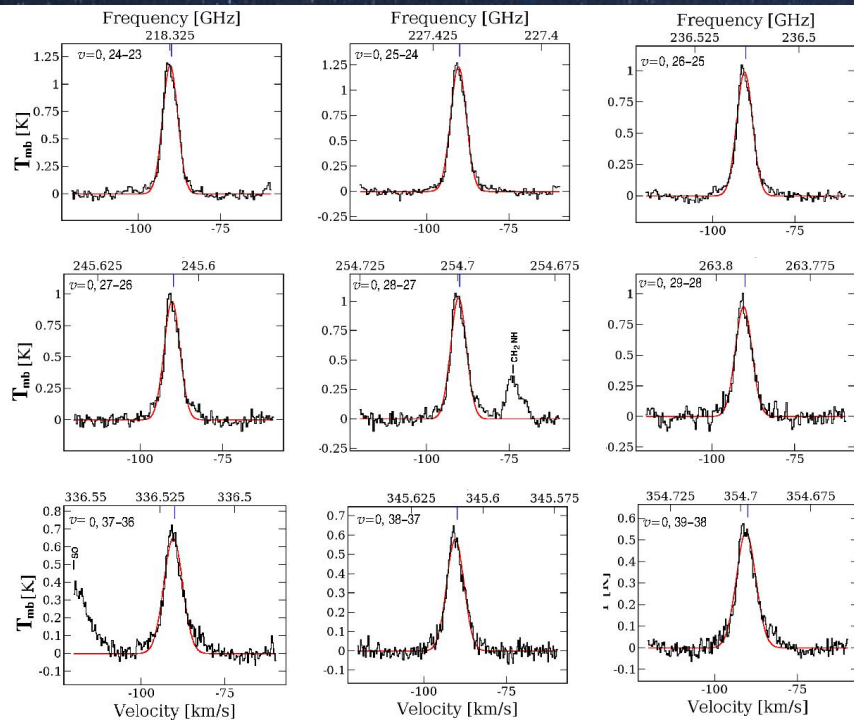














**Table 1.** HC<sub>3</sub>N lines detected in G331 and their parameters obtained from Gaussian fits.

Transition	Frequency (MHz)	$E_u$ (K)	$A_{ul}$ ( $\times 10^{-5} \text{ s}^{-1}$ )	$\int T_{\text{mb}} dv$ (K km s <sup>-1</sup> )	$V_{\text{lsr}}$ (km s <sup>-1</sup> )	$T_{\text{peak}}$ (K)	FWHM (km s <sup>-1</sup> )	$\tau$	Remark <sup>§</sup>
$v = 0$									
24–23	218324.72	130.98	82.6	$6.94 \pm 0.72$	$-90.35 \pm 0.05$	$1.17 \pm 0.05$	$5.39 \pm 0.11$	0.298*	cl
25–24	227418.91	141.89	93.5	$7.49 \pm 0.75$	$-90.37 \pm 0.05$	$1.23 \pm 0.05$	$5.57 \pm 0.11$	0.278*	cl
26–25	236512.78	153.24	105.2	$6.20 \pm 0.62$	$-90.35 \pm 0.05$	$0.99 \pm 0.04$	$5.55 \pm 0.12$	0.260*	cl
27–26	245606.31	165.03	117.9	$6.02 \pm 0.61$	$-90.37 \pm 0.07$	$0.94 \pm 0.06$	$5.63 \pm 0.17$	0.248*	cl
28–27	254699.51	177.25	131.6	$6.47 \pm 0.66$	$-90.37 \pm 0.07$	$1.02 \pm 0.06$	$5.58 \pm 0.15$	0.235*	pbw <sup>33</sup> SO <sub>2</sub> nl CH <sub>2</sub> NH
29–28	263792.31	189.91	146.3	$5.85 \pm 0.59$	$-90.49 \pm 0.07$	$0.89 \pm 0.06$	$5.93 \pm 0.16$	0.206*	pbw CH <sub>3</sub> OH
37–36	336520.08	306.91	304.8	$4.86 \pm 0.50$	$-90.50 \pm 0.08$	$0.65 \pm 0.05$	$6.67 \pm 0.19$	0.082*	nl SO
38–37	345609.01	323.49	330.2	$3.87 \pm 0.39$	$-90.57 \pm 0.06$	$0.58 \pm 0.04$	$6.16 \pm 0.14$	0.077*	pbw CH <sub>3</sub> OH
39–38	354697.46	340.51	357.1	$4.14 \pm 0.43$	$-90.54 \pm 0.08$	$0.53 \pm 0.04$	$6.92 \pm 0.18$	0.060*	cl
<sup>13</sup> C Isotopologues									
H <sup>13</sup> CCCN									
26–25	229203.09	148.51	95.7	$0.28 \pm 0.04$	$-91.1 \pm 0.2$	$0.06 \pm 0.02$	$4.1 \pm 0.4$	0.024 <sup>†</sup>	cl
27–26	238015.68	159.93	197.3	$0.30 \pm 0.04$	$-90.9 \pm 0.2$	$0.06 \pm 0.02$	$4.8 \pm 0.5$	0.022 <sup>†</sup>	cl
HC <sup>13</sup> CCN									
24–23	217398.56	130.42	81.5	$0.28 \pm 0.05$	$-89.4 \pm 0.4$	$0.07 \pm 0.02$	$4.2 \pm 0.8$	0.025 <sup>†</sup>	cl
25–24	226454.18	141.29	92.3	$0.32 \pm 0.05$	$-90.7 \pm 0.4$	$0.06 \pm 0.02$	$5.9 \pm 1.0$	0.024 <sup>†</sup>	cl
27–26	244564.44	164.33	116.4	$0.32 \pm 0.06$	$-91.5 \pm 0.4$	$0.07 \pm 0.03$	$3.6 \pm 0.8$	0.027 <sup>†</sup>	pbw CH <sub>3</sub> OH
HCC <sup>13</sup> CN									
24–23	217419.57	130.44	81.6	$0.51 \pm 0.06$	$-90.2 \pm 0.2$	$0.10 \pm 0.02$	$5.4 \pm 0.4$	0.035 <sup>†</sup>	pbw CH <sub>3</sub> OH nl <sup>13</sup> CN
25–24	226476.04	141.31	92.3	$0.43 \pm 0.06$	$-89.9 \pm 0.4$	$0.08 \pm 0.03$	$5.4 \pm 0.7$	0.031 <sup>†</sup>	cl
26–25	235532.20	152.61	103.9	$0.50 \pm 0.07$	$-88.9 \pm 0.3$	$0.09 \pm 0.02$	$5.6 \pm 0.6$	0.037 <sup>†</sup>	cl
$v_7 = 1$									
24 <sub>-1</sub> –23 <sub>1</sub>	218860.81	452.15	82.7	$0.58 \pm 0.07$	$-91.3 \pm 0.3$	$0.10 \pm 0.03$	$4.9 \pm 0.5$	0.015*	cl
24 <sub>1</sub> –23 <sub>-1</sub>	219173.75	452.34	83.0	$0.34 \pm 0.05$	$-91.6 \pm 0.3$	$0.08 \pm 0.02$	$4.1 \pm 0.6$	0.018*	cl
25 <sub>1</sub> –24 <sub>-1</sub>	227977.27	463.09	93.5	$0.69 \pm 0.08$	$-90.2 \pm 0.2$	$0.12 \pm 0.02$	$6.0 \pm 0.5$	0.013*	cl
25 <sub>-1</sub> –24 <sub>1</sub>	228303.17	463.29	93.4	$0.70 \pm 0.09$	$-90.8 \pm 0.3$	$0.10 \pm 0.02$	$6.8 \pm 0.6$	0.011*	cl
26 <sub>-1</sub> –25 <sub>1</sub>	237093.38	474.47	105.2	$0.53 \pm 0.07$	$-90.5 \pm 0.4$	$0.07 \pm 0.02$	$8.4 \pm 1.2$	0.009*	cl
26 <sub>1</sub> –25 <sub>-1</sub>	237432.26	474.69	105.7	$0.57 \pm 0.07$	$-91.0 \pm 0.2$	$0.10 \pm 0.03$	$5.3 \pm 0.5$	0.014*	cl
27 <sub>1</sub> –26 <sub>-1</sub>	246209.14	486.29	118.0	$0.45 \pm 0.08$	$-91.4 \pm 0.5$	$0.07 \pm 0.03$	$9.0 \pm 1.9$	0.011*	cl
27 <sub>-1</sub> –26 <sub>1</sub>	246560.95	486.52	118.5	$0.78 \pm 0.10$	$-89.3 \pm 0.4$	$0.10 \pm 0.03$	$8.1 \pm 0.9$	0.009*	cl
28 <sub>-1</sub> –27 <sub>1</sub>	255324.55	498.54	131.7	$0.58 \pm 0.10$	$-91.5 \pm 0.5$	$0.09 \pm 0.03$	$6.7 \pm 1.1$	0.011*	cl
28 <sub>1</sub> –27 <sub>-1</sub>	255689.29	498.79	132.2	$0.72 \pm 0.11$	$-91.3 \pm 0.6$	$0.08 \pm 0.02$	$8.9 \pm 1.6$	0.008*	cl
29 <sub>1</sub> –28 <sub>-1</sub>	264439.58	511.23	146.4	$0.20 \pm 0.04$	$-91.6 \pm 0.3$	$0.05 \pm 0.03$	$2.6 \pm 0.7$	0.029*	cl
29 <sub>-1</sub> –28 <sub>1</sub>	264817.24	511.50	147.1	$0.40 \pm 0.07$	$-91.1 \pm 0.5$	$0.07 \pm 0.02$	$6.2 \pm 1.1$	0.012*	cl
32 <sub>1</sub> –31 <sub>-1</sub>	292198.64	552.26	197.9	$0.50 \pm 0.08$	$-90.2 \pm 0.3$	$0.09 \pm 0.02$	$4.9 \pm 0.6$	0.014*	cl
39 <sub>-1</sub> –38 <sub>1</sub>	356072.44	662.68	359.2	$0.31 \pm 0.06$	$-90.3 \pm 0.4$	$0.05 \pm 0.02$	$6.6 \pm 1.0$	0.008*	nlo SO <sub>2</sub>

\*Obtained iteratively from the opacity correction (Sect 4.2.1) <sup>†</sup>Obtained from Eq.8 (Sect. 4.2.3)

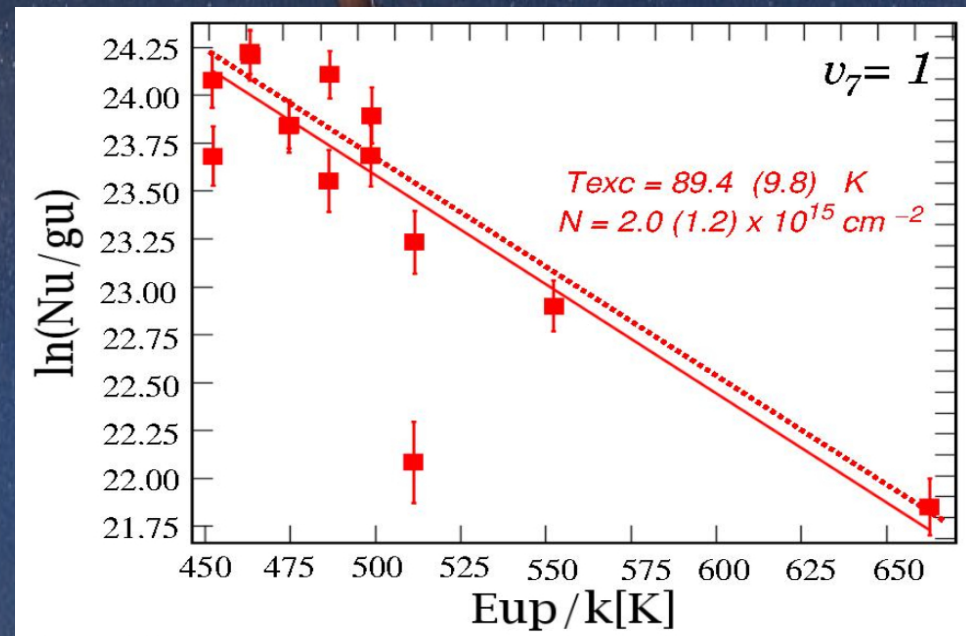
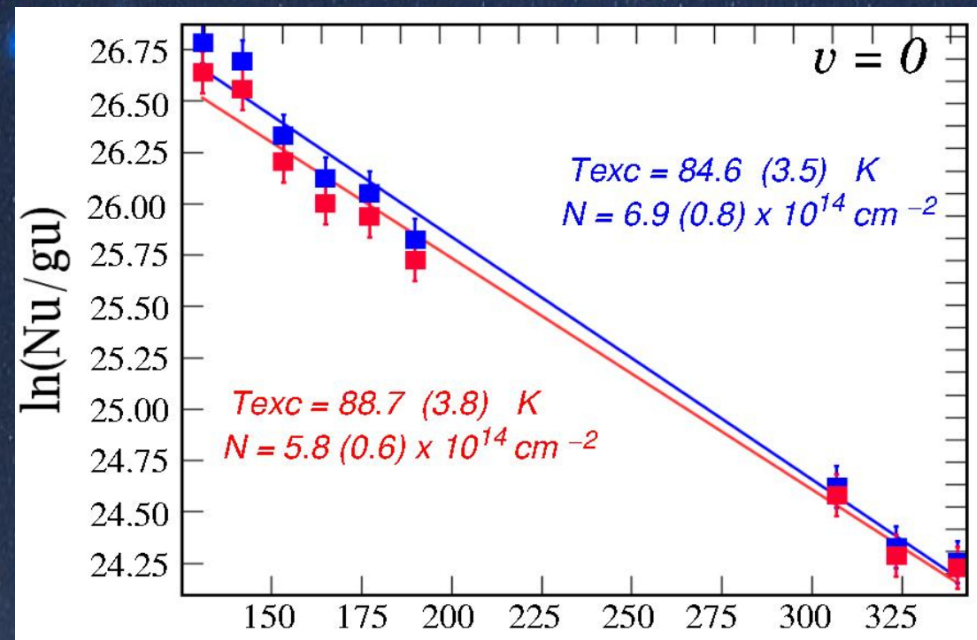


# LTE analysis

$$N_u = \frac{8\pi k\nu^2}{hc^3 A_{ul}} \times \int T_{\text{mb}} dv$$

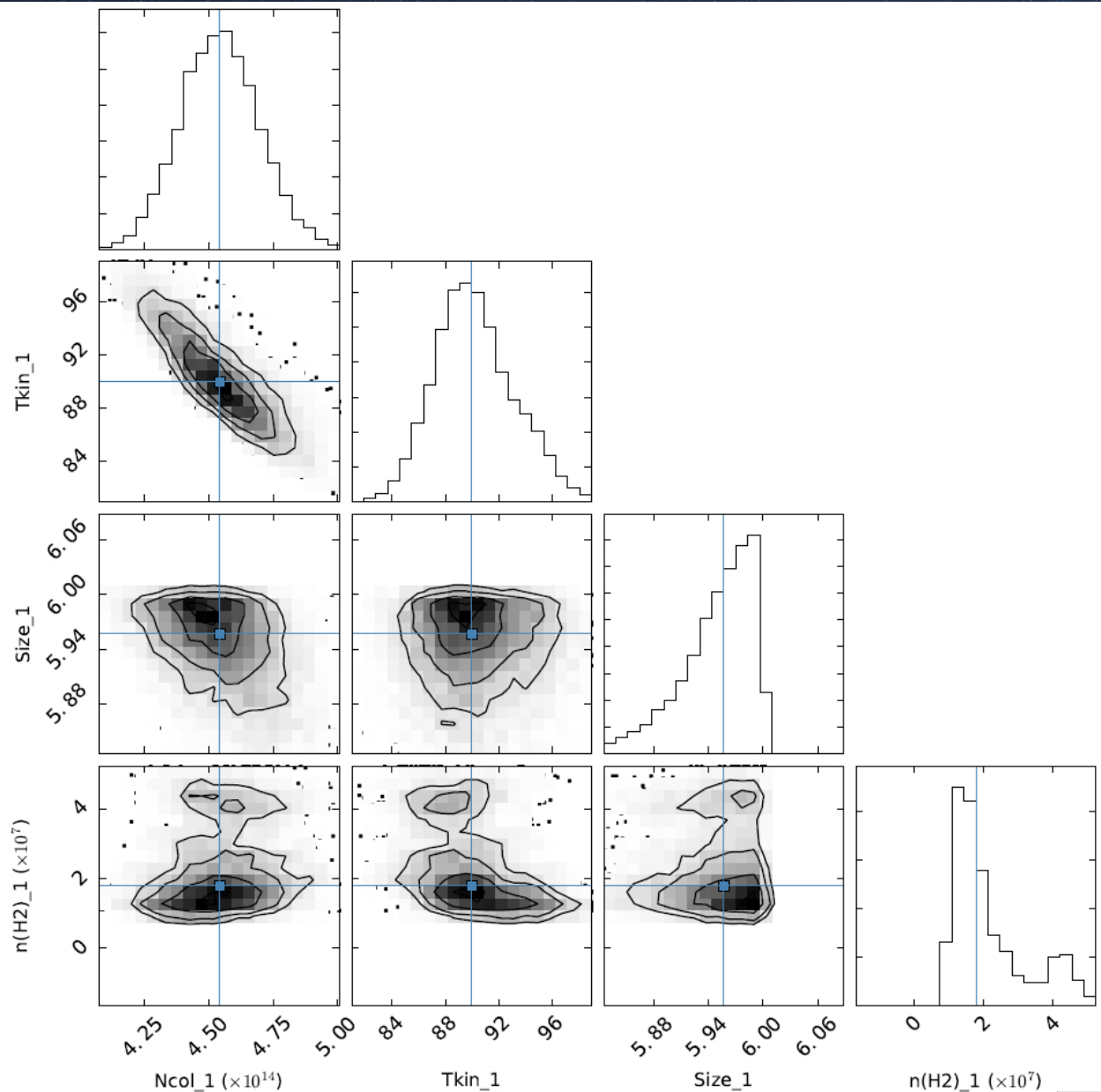
$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N_{\text{tot}}}{Q(T_{\text{exc}})}\right) - \frac{E_u}{kT_{\text{exc}}}$$

$$y = B + Ax$$





# Non-LTE analysis



$$N(\text{HC}_3\text{N}) = 4.5 \times 10^{14} \text{ cm}^{-2}$$

$$T_{\text{kin}} = 90 \text{ K}$$

$$n(\text{H}_2) = 2 \times 10^7 \text{ cm}^{-3}$$

(size  $\leq 6''$ )



## <sup>13</sup>C Isotopologues

$$\tau = -\ln \left[ 1 - \frac{T_{\text{mb}}}{f [J(T_{\text{exc}}) - J(T_{\text{bg}})]} \right] \quad (8)$$

being

$$J(T) = \frac{h\nu}{k} \left[ e^{\left(\frac{h\nu}{kT}\right)} - 1 \right]^{-1}, \quad (9)$$

and

$$N = \tau \frac{3h\Delta\nu}{8\pi^3} \sqrt{\frac{\pi}{4 \ln 2}} \frac{Q}{\mu^2(J_l + 1)} e^{\left(\frac{E_l}{kT_{\text{exc}}}\right)} \left[ 1 - e^{\left(-\frac{h\nu}{kT_{\text{exc}}}\right)} \right]^{-1} \quad (10)$$

Isotopologue	$N$ [ $\times 10^{13} \text{ cm}^{-2}$ ]	$X$ [ $\times 10^{-11}$ ]	$^{12}\text{C}/^{13}\text{C}$
HC <sub>3</sub> N	$69 \pm 8^\dagger$	79 – 62	-
HCC <sup>13</sup> CN	$6.7 \pm 0.9$	7.8 – 5.9	$\sim 10$
HC <sup>13</sup> CCN	$3.8 \pm 0.8$	4.7 – 3.1	$\sim 18$
H <sup>13</sup> CCCN	$3.7 \pm 0.6$	4.4 – 3.2	$\sim 19$
<sup>13</sup> C HC <sub>3</sub> N	$3.3 \pm 0.2^\ddagger$	3.6 – 3.2	$\sim 21$



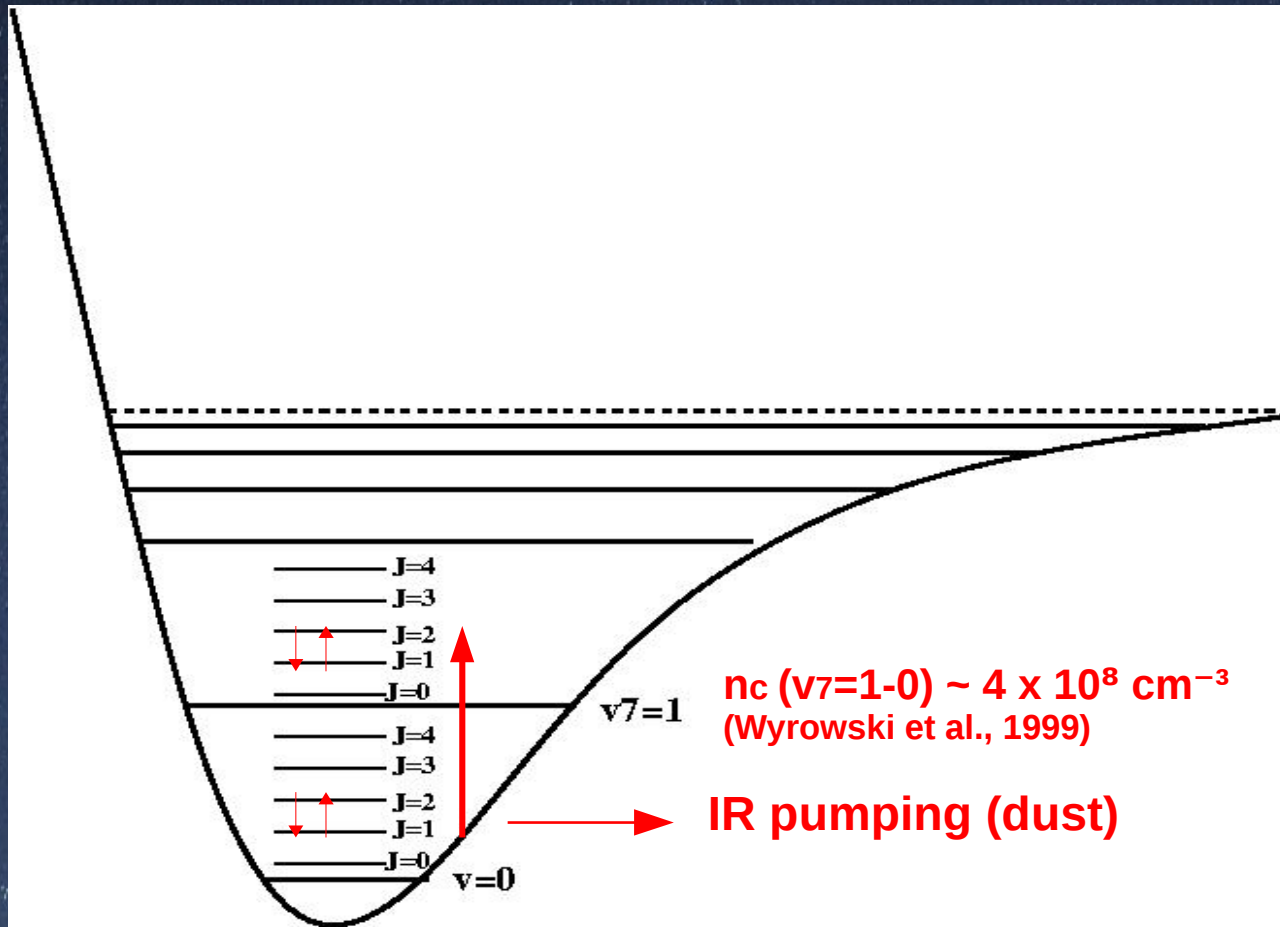
## Excitation of the $v=0$ and $v_7=1$ lines

$$n_c^{J,J-1} \approx \frac{A_{(J,J-1)}}{\gamma(J, J-1)}$$

$J=38-37$   $n_c$  (80-100 K)  $\sim 1.5 \times 10^7 \text{ cm}^{-3}$

$n(\text{RADEX}) \sim 2 \times 10^7 \text{ cm}^{-3}$

→ rotational transitions in LTE





## Excitation of the $v=0$ and $v_7=1$ lines

$$T_{\text{dust}} \sim T_{\text{vib}}$$

$$\frac{W_{(v_7=1)}}{W_{(v=0)}} = \exp \left( \frac{-\Delta E_{70}}{kT_{\text{vib}}} \right)$$

$$T_{\text{vib}} = 140 \text{ K}$$

$$\frac{L_{\text{hc}}}{L_{\odot}} = 1.8625 \times 10^{-5} \left( \frac{r}{10^{16} \text{ cm}} \right)^2 T_{\text{dust}}^4$$

$$L \sim 4 \times 10^6 L_{\odot}$$

→ < O4 (ZAMS)



# Isotopologue abundances

Isotopologue	$N$ [ $\times 10^{13} \text{ cm}^{-2}$ ]	$X$ [ $\times 10^{-11}$ ]	$^{12}\text{C}/^{13}\text{C}$
$\text{HC}_3\text{N}$	$69 \pm 8^\dagger$	$79 - 62$	-
$\text{HCC}^{13}\text{CN}$	$6.7 \pm 0.9$	$7.8 - 5.9$	$\sim 10$
$\text{HC}^{13}\text{CCN}$	$3.8 \pm 0.8$	$4.7 - 3.1$	$\sim 18$
$\text{H}^{13}\text{CCCN}$	$3.7 \pm 0.6$	$4.4 - 3.2$	$\sim 19$
$^{13}\text{C HC}_3\text{N}$	$3.3 \pm 0.2^\ddagger$	$3.6 - 3.2$	$\sim 21$

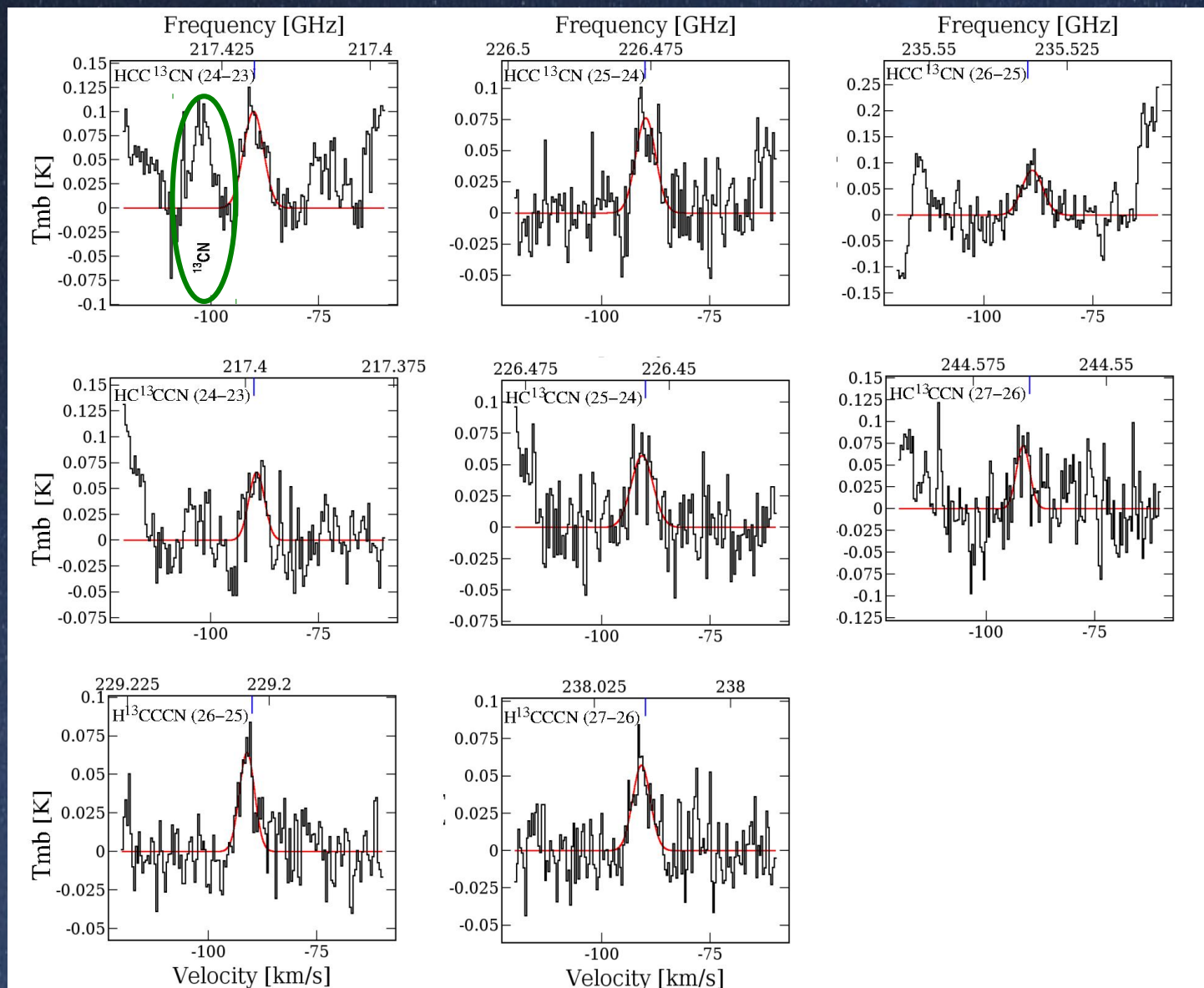
$$[\text{HCC}^{13}\text{CN}]:[\text{HC}^{13}\text{CCN}]:[\text{H}^{13}\text{CCCN}] = 1.8(\pm 0.5):1.0:1.0(\pm 0.4)$$



$$[\text{HCC}^{13}\text{CN}]:[\text{HC}^{13}\text{CCN}]:[\text{H}^{13}\text{CCCN}] = a:b:c, \text{ with } a > b \approx c$$



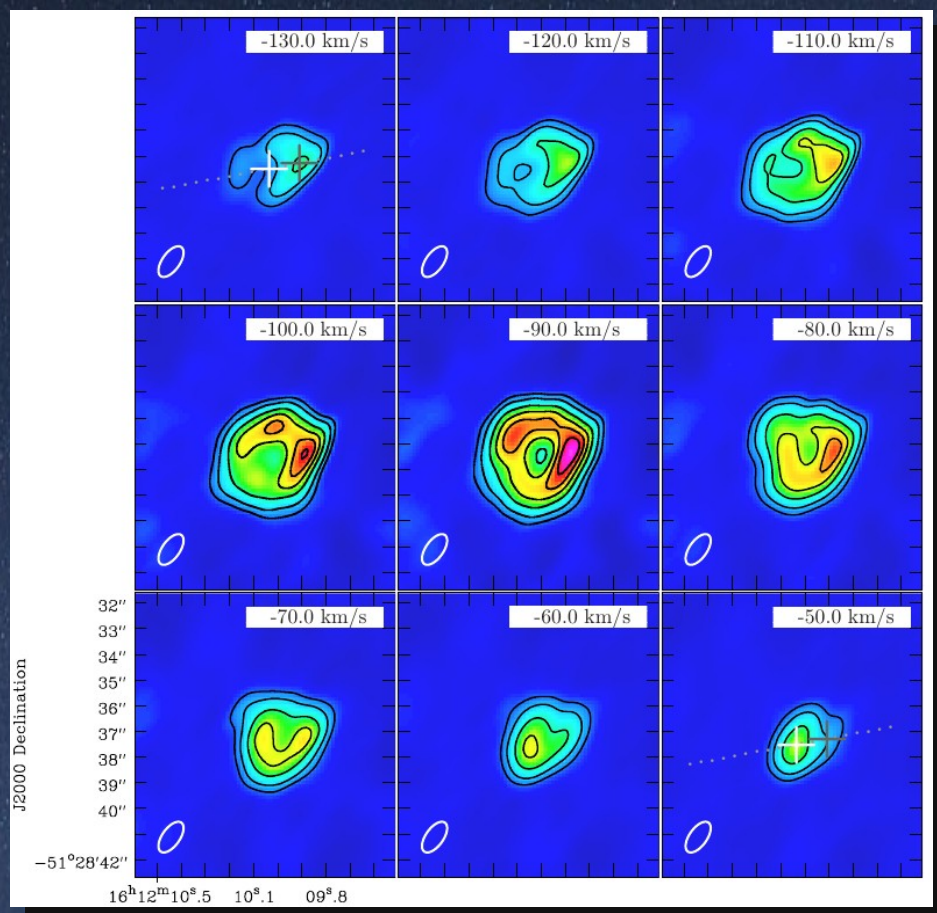
# Isotopologue abundances





# Emission of $\text{HC}_3\text{N}$

Merello et al. 2013



Hervias-Caimapo et al. 2019

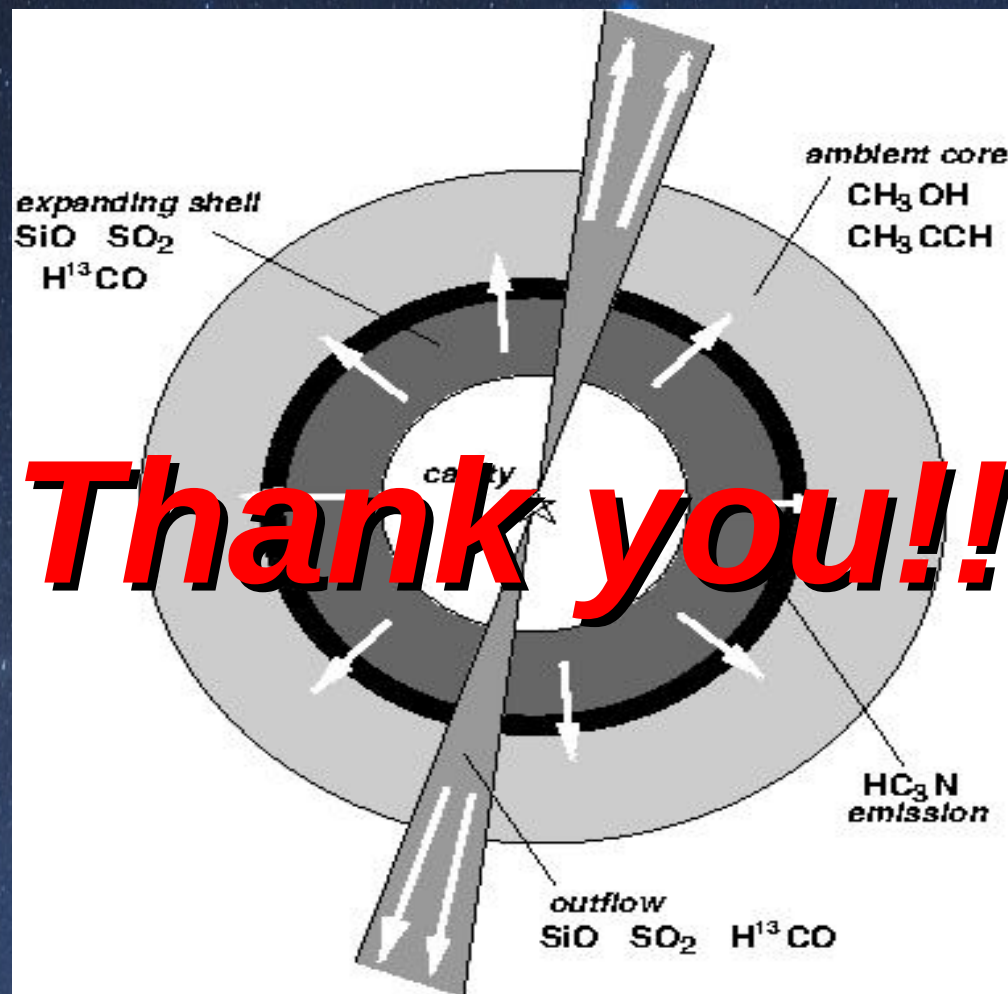
$\text{SiO}$   
 $\text{S}^{18}\text{O}$   
 $\text{HCO}^+$   
 $\text{H}^{13}\text{CN}$   
 $\text{HC}_3\text{N}$

“Broad” lines ( $\sim 160\text{--}200\text{ K}$ )  
(Shocked gas and outflow)

$\text{CH}_3\text{OH}$   
 $\text{CH}_3\text{CCH}$   
 $\text{H}^{13}\text{CO}$

“Narrow” lines ( $\sim 70\text{ K}$ )  
(colder ambient core)





***Thank you!!***