INTERPRETING OBSERVATIONS I: STAR FORMING REGIONS

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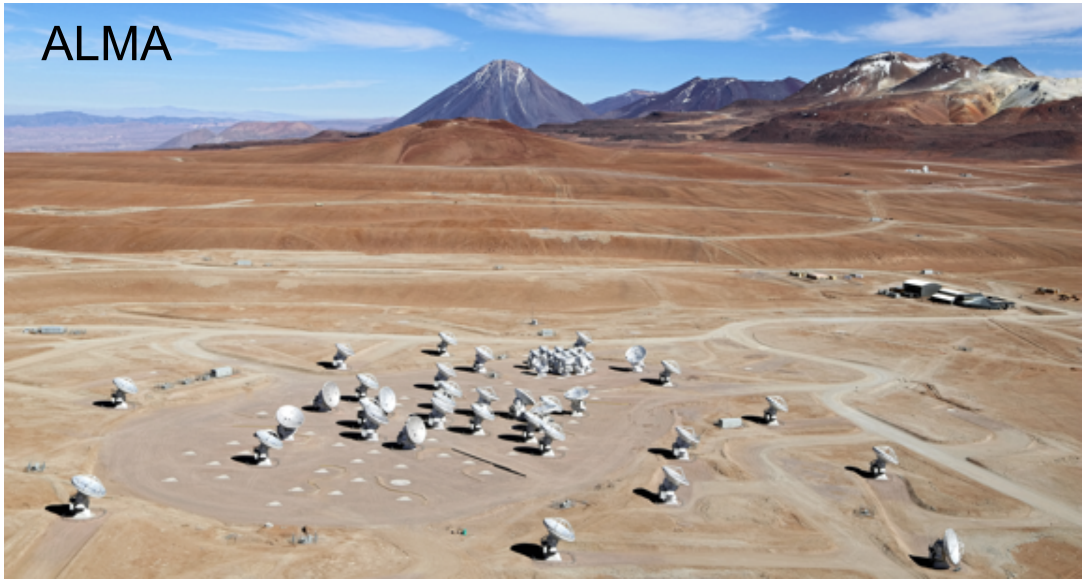
(based on talk by B. Tercero)

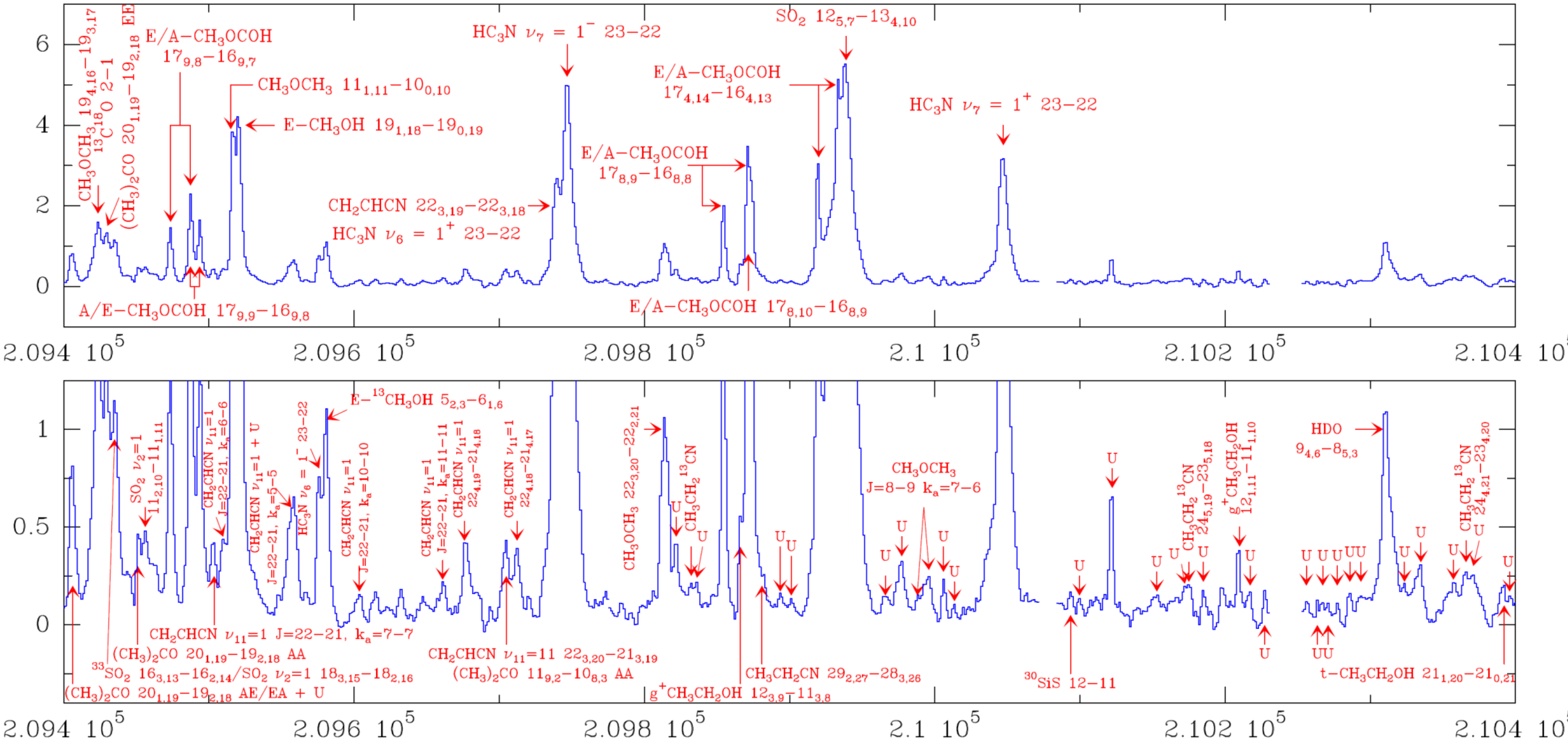
Molecules are found in all places of the Universe where the temperatures are below 2000-2500 K and the density large enough to allow chemical reactions


ALMA

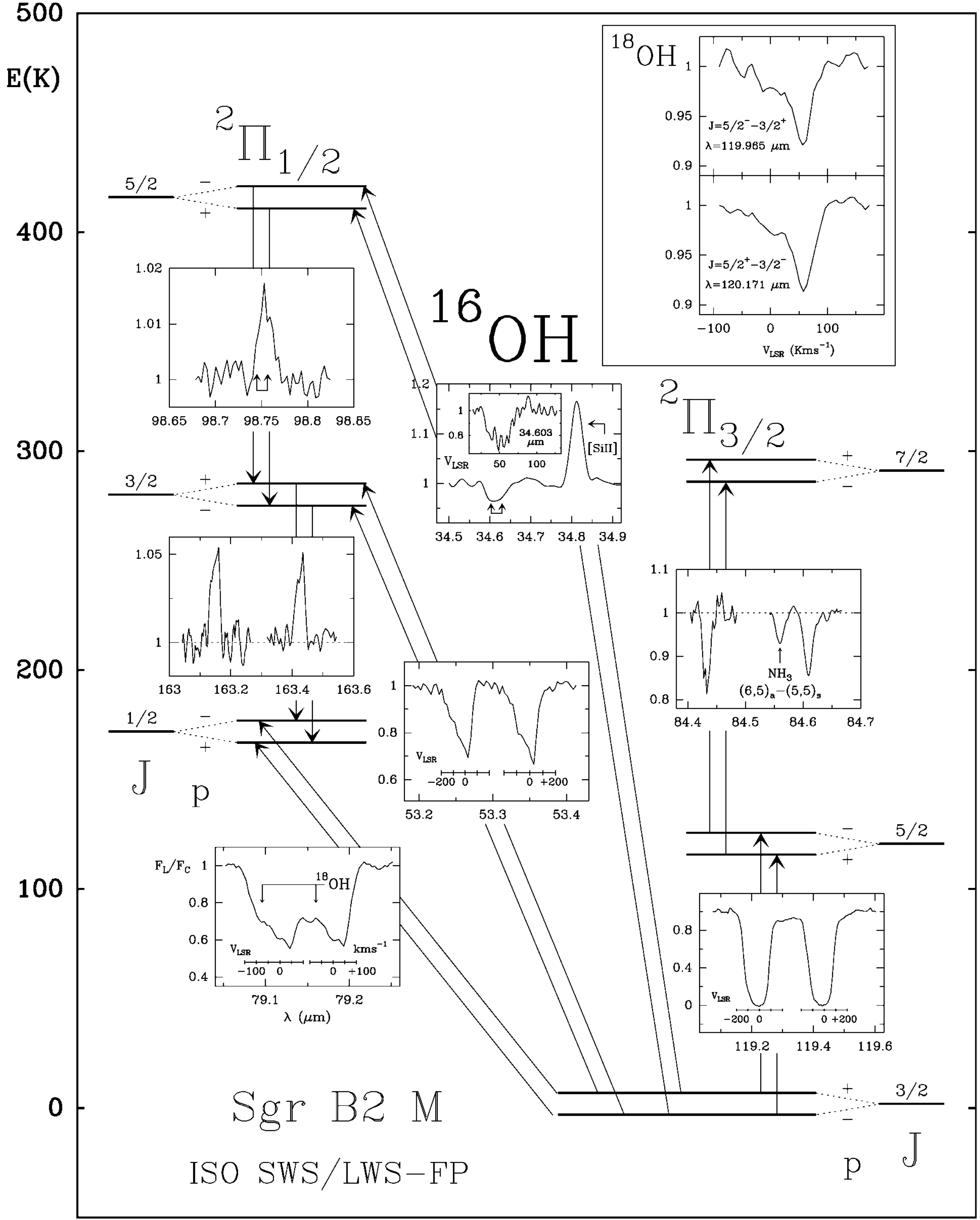

GTM


IRAM


NOEMA



Orion KL,
Tercero et al. (2010)



Sgr B2,
Goicoechea &
Cernicharo (2002)

Prestellar cores
Agúndez et al. 2015

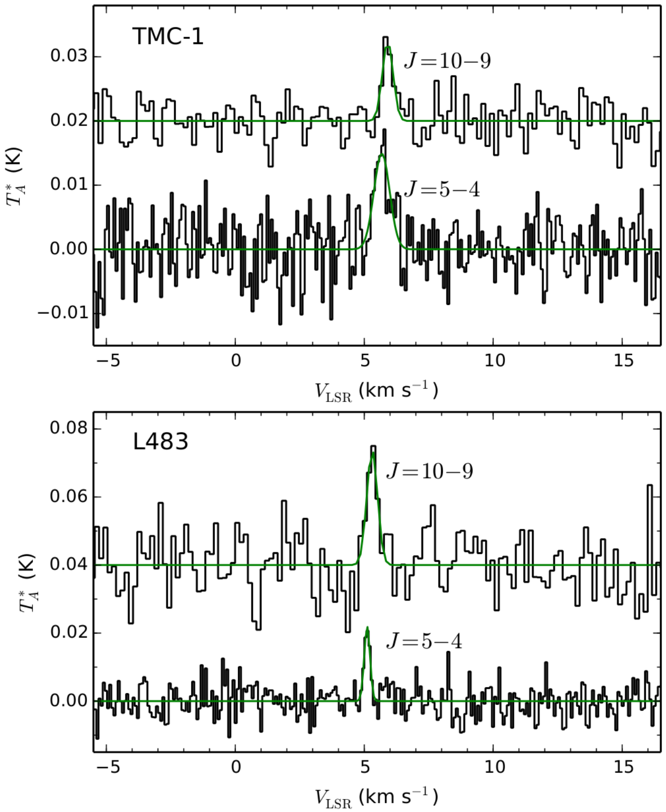
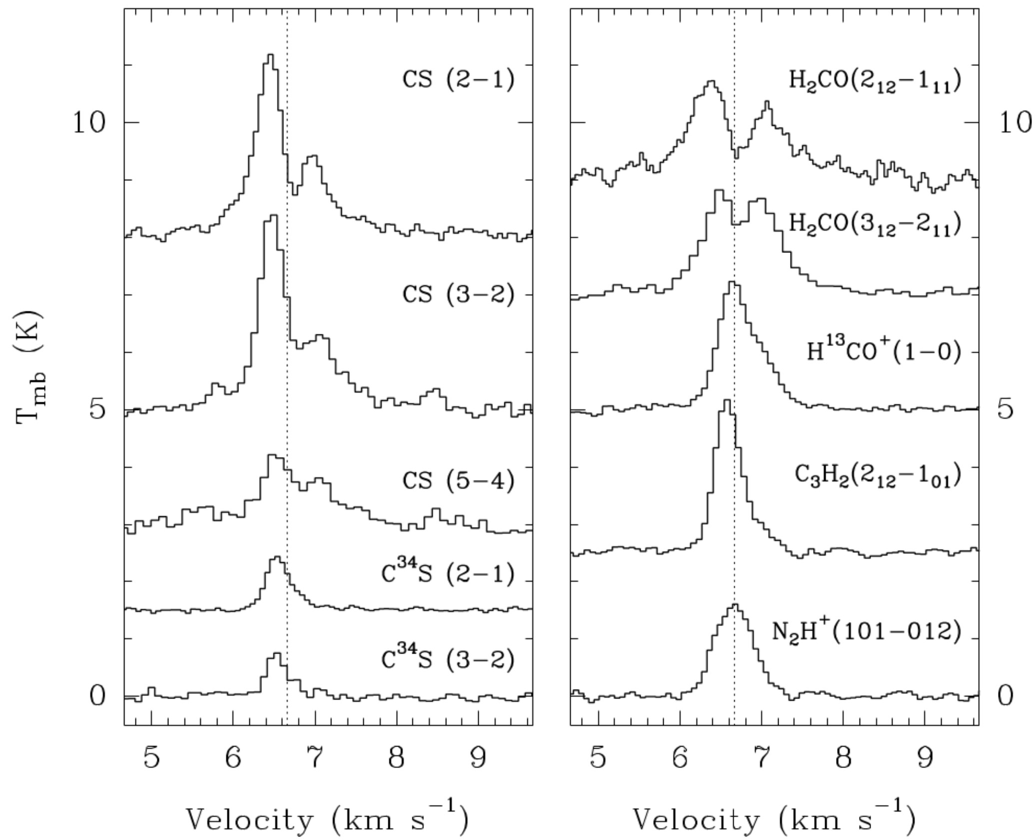
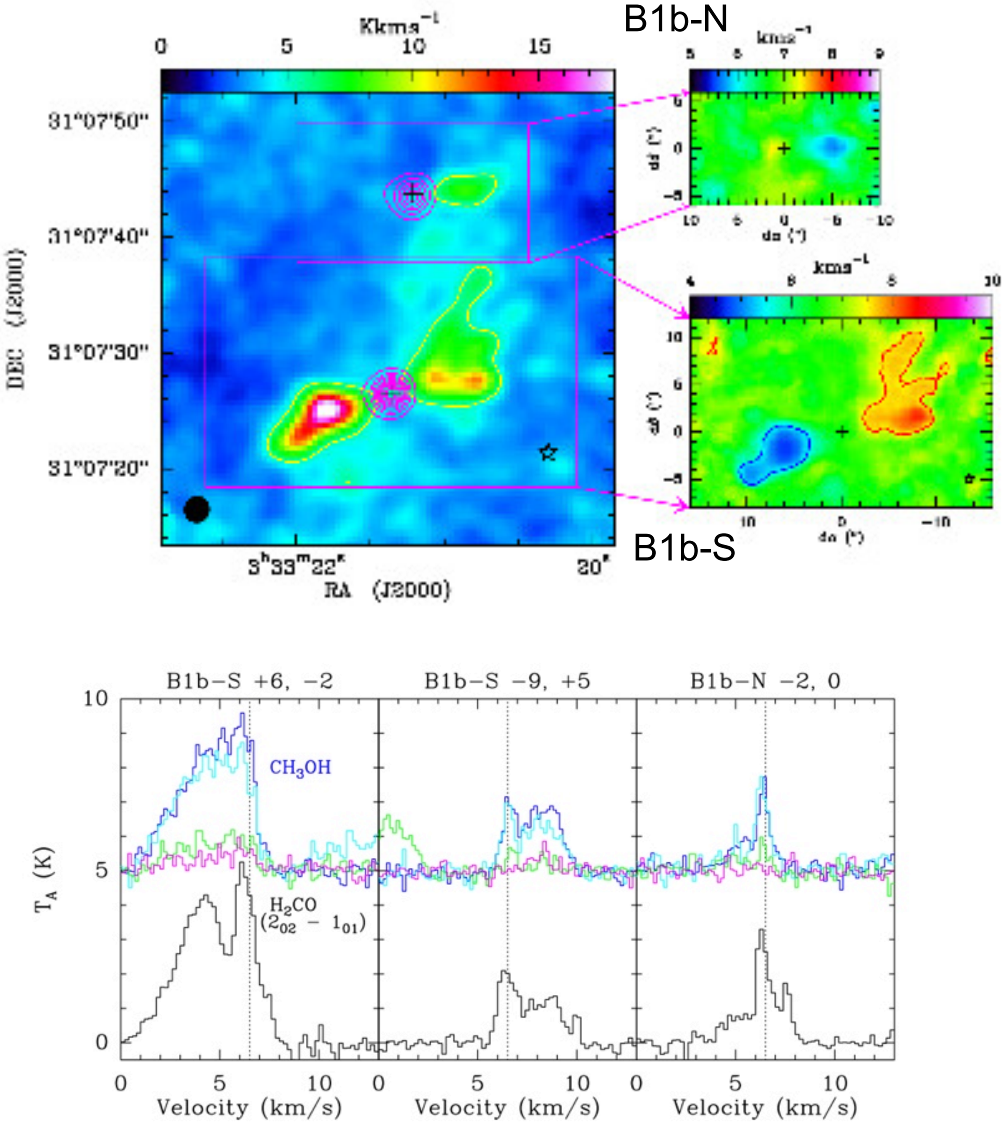


Fig. 1. Spectra of TMC-1 and L483 showing the emission lines assigned to the J = 5–4 and J = 10–9 rotational transitions of $NCCNH^+$, ly-

IRAM 04191+1522
Class 0 protostar
Belloche et al. 2002



Infall and outflow spectral signatures !

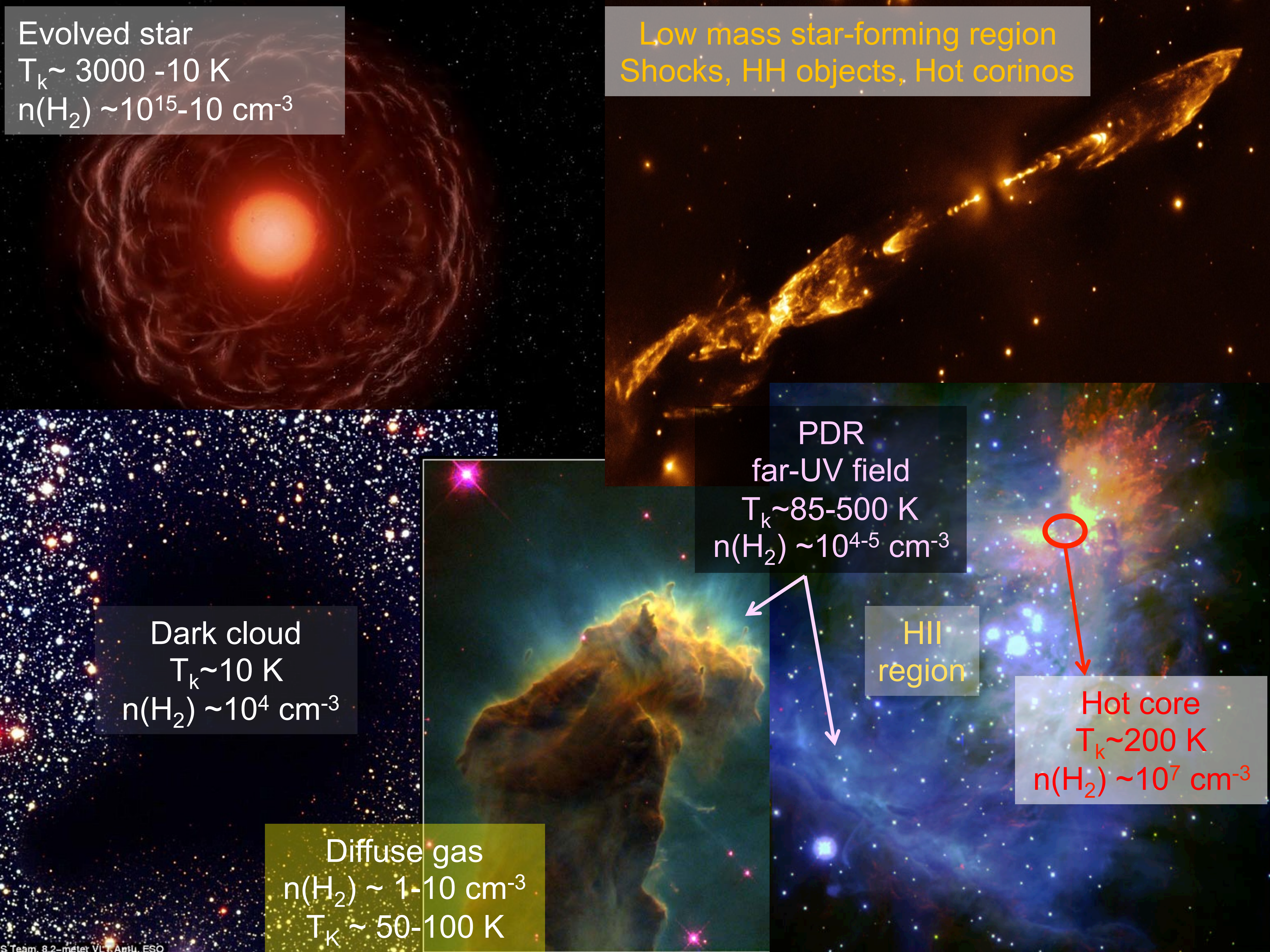


Barnard 1b
Gerin et al. 2015

HOW TO INTERPRET YOUR DATA

STEPS:

1. An idea of your source
2. A deep knowledge of your telescope
3. What kind of information you will get?
4. Line identification
5. Observed line parameters
6. Physical conditions and column densities: different sets of data will provide more constrained parameters
7. Physical model and Chemical model



Evolved star
T_k~ 3000 -10 K
$n(H_2)$ ~10^{15}-10 cm^{-3}
Low mass star-forming region
Shocks, HH objects, Hot corinos
PDR
far-UV field
T_k~85-500 K
$n(H_2)$ ~10^{4-5} cm^{-3}
Dark cloud
T_k~10 K
$n(H_2)$ ~10^4 cm^{-3}
HII
region
Hot core
T_k~200 K
$n(H_2)$ ~10^7 cm^{-3}
Diffuse gas
$n(H_2)$ ~ 1-10 cm^{-3}
T_K ~ 50-100 K
S Team, 8.2-meter VLT Antu, ESO

1. An idea of your source

Species	(1)	(2)	(3)	Species	(1)	(2)	(3)
CS	4	3	3	HC_5N	46	6	30
HCS^+	1	0	0	HC_7N	34	0	0
SO	2	1	1	HC_9N	16	0	0
OCS	1	0	0	H_2C_3	4	0	0
NH_3	6	0	0	H_2C_4	12	0	0
HNCO	5	0	0	H_2CO	1	0	0
l-C_3H	6	0	0	H_2CCO	3	0	0
C_4H	27	0	0	H_2CS	2	1	1
C_5H	16	0	0	CH_2CN	38	0	0
C_6H	42	0	0	CH_3CN	5	0	0
C_3N	12	0	0	CH_3C_3N	8	0	0
CCO	1	0	0	CH_3CCH	3	0	0
C_3O	2	0	0	CH_3C_4H	8	0	0
CCS	11	1	3	CH_3OH	1	0	0
C_3S	8	1	1	CH_3CHO	2	0	0
HC_3N	47	5	27	HCCCHO	1	0	0
HCCNC	5	0	0	CH_2CHCN	12	0	0
HNCCC	4	0	0	*c*-C_3H	6	0	0
HC_3NH^+	2	0	0	*c*-C_3H_2	10	2	6

TMC-1
Dark cloud
Kaifu et al. (2004)
8.8 – 50 GHz

1. An idea of your source

Orion KL
High mass star forming region
Blake et al. (1987)
215 - 263 GHz

Source	v_{LSR} (km s^{-1})	Δv (km s^{-1})	T_{rot} (K)	n (cm^{-3})	θ_{source}	N_{H_2} (cm^{-2})	Molecules Detected
Extended ridge	9	4	55–60	$\sim 10^5$	Extended	3×10^{23}	CN, CO, CS, NO, SO, CCH, C_3H_2, CH_3CCH, HCO^+, HCS^+, HCN, HNC, HC_3N
Compact ridge	7–8	3–5	80–140	$\gtrsim 10^6$	$\lesssim 30''$	...	PN(?), OCS, HDO, H_2CO, H_2CS, HCOOH, CH_3CHO(?), CH_3CN, H_2CCO, CH_3OH, $HCOOCH_3$, CH_3OCH_3
Plateau	7–8	$\gtrsim$20–25	95–150	$\gtrsim 10^6$	$\lesssim 20''$	$\lesssim 1 \times 10^{23}$	CO, CS, SiO, SO, SO_2, OCS, H_2S, HDO, H_2CO, HCN, HC_3N
Hot core	3–5	5–10	150–300	$\gtrsim 10^7$	$\lesssim 10''$	1×10^{24}	CO, HDO, H_2CO, HNCO, HCN, HC_3N, CH_3CN, C_2H_3CN, C_2H_5CN

Different components of the gas within the region

1. An idea of your source

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Blake et al. (1987)
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COM's
N-rich; O-rich; Organic saturated

1. An idea of your source

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Shock chemistry

1. An idea of your source

Species
CH_3CN v=0
CH_3CN v_8=1
$CH_3{}^{13}CN$ v=0
CH_3NC^*
CD_3CN^*
CH_3OH v_t=0,1
$^{13}CH_3OH$ v=0
$^{13}CH_3OH$ v_t=1
CH_2DOH
CH_3OCHO v=0
CH_3OCHO v_t=1
CH_3OCDO
S-CH_2DOCHO
A-CH_2DOCHO
CH_3CH_2CN
CH_3CH_2CN v_{13}=1 /v_{21}=1
CH_2CHCN v_{11}=0,1
CH_3CH_2OH
CH_3COCH_3
(o+p)-H_2CO
(o+p)-$H_2{}^{13}CO$
(o+p)-D_2CO
OCS
OCS v_2=1
$O^{13}CS$
HC_3N
HC_3N v_7=1
DC_3N^*
SO
$S^{18}O$
SO_2
$^{34}SO_2$
HNCO
$HN^{13}CO$
(o+p)-$H_2{}^{13}CS$
(o+p)-$HDCS^*$
HCOOH
$H^{13}COOH$
$HCOOD^*$
CH_3OCH_3
CH_3CHO v_t=0
CH_3CHO v_t=1
CH_3CHO v_t=2
aGg'-$(CH_2OH)_2$
(o+p)-H_2CCO^*
CH_2OHCHO
NH_2CHO^*

NGC 7129 FIRS 2

Hot core intermediate mass star

Fuente et al. (2014)

218.2 – 221.8 GHz

1. An idea of your source

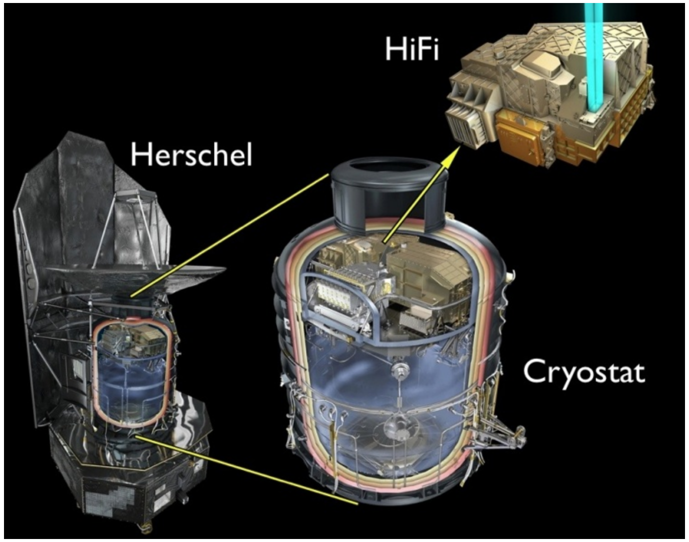
And many more cases…

IMPORTANT: The census of molecules also depends on the frequency range and the telescope sensitivity

2. A deep knowledge of your telescope

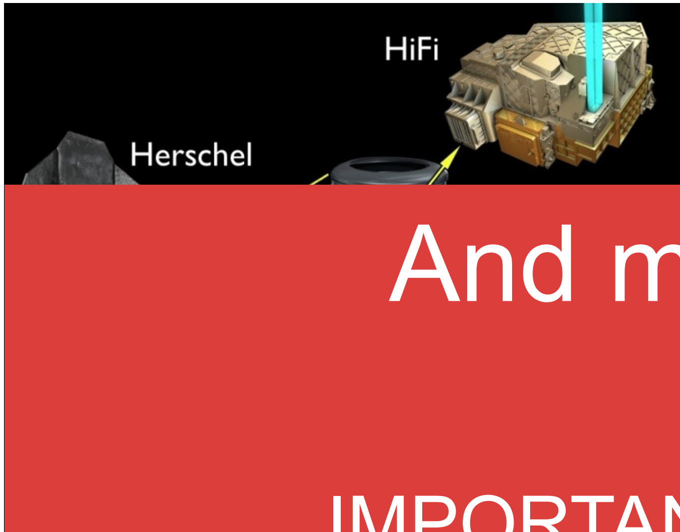
- 30 m diameter → HPBW → beam dilution.
  - 3 mm: HPBW ~ 27″
  - 2 mm: HPBW ~ 17″
  - 1 mm: HPBW ~ 10″
- EMIR receivers at 3, 2, 1.3 mm: 80-115.5 GHz, 123-178 GHz, 200-350 GHz
- Image-band rejection of the receivers
- Spectral resolution
- Observing mode → Wobbler/ position-switching, frequency switching…

2. A deep knowledge of your telescope



Herschel Space Observatory
HIFI / PACS / SPIRE
480−1280, 1426−1535, and 1573−1906 GHz
FarIR wavelengths; Light hydrides

2. A deep knowledge of your telescope



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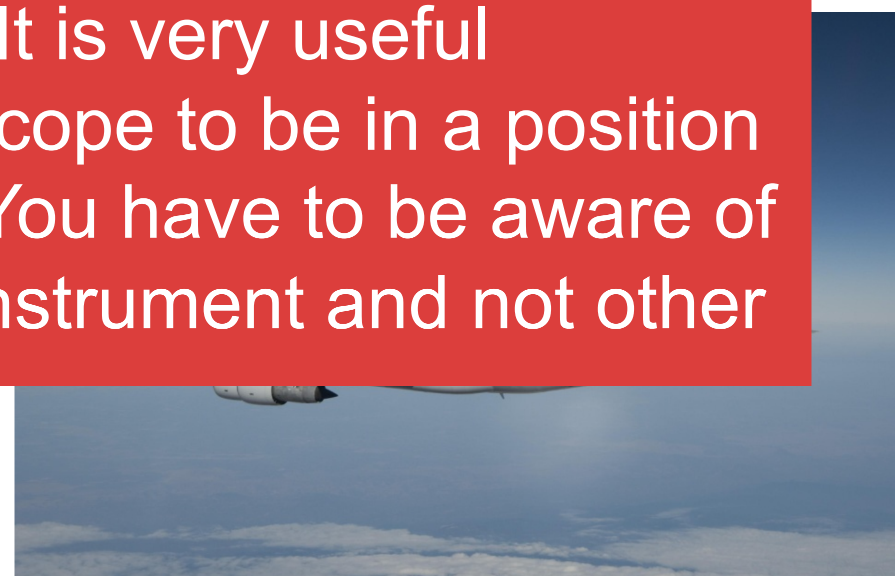
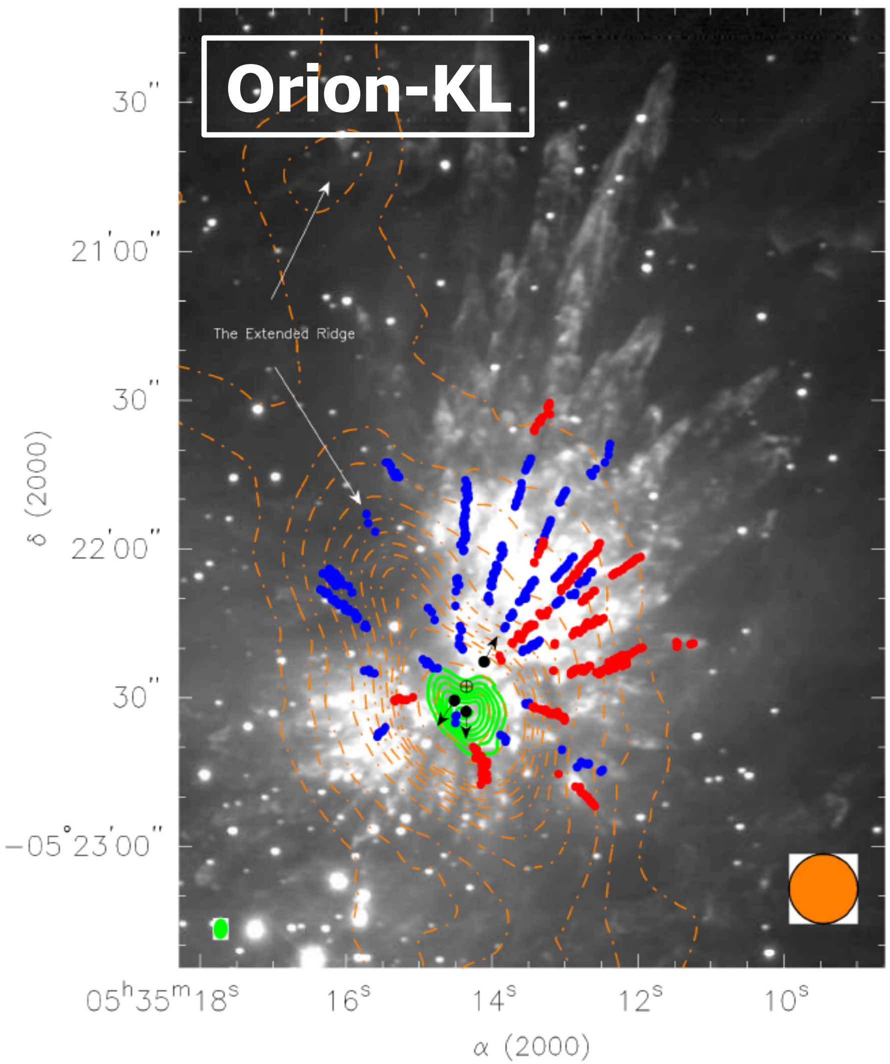
HIFI / PACS / SPIRE



And many more…

IMPORTANT: It is very useful to understand the telescope to be in a position of evaluating the data. You have to be aware of why you are using an instrument and not other

3. What kind of information you will get?



30" HPBW at 80 GHz IRAM 30-m
→ 12500 AU

9" HPBW at 280 GHz IRAM 30-m
→ 3750 AU

2"x1".5 ALMA SV synthetic beam
→ 830 AU

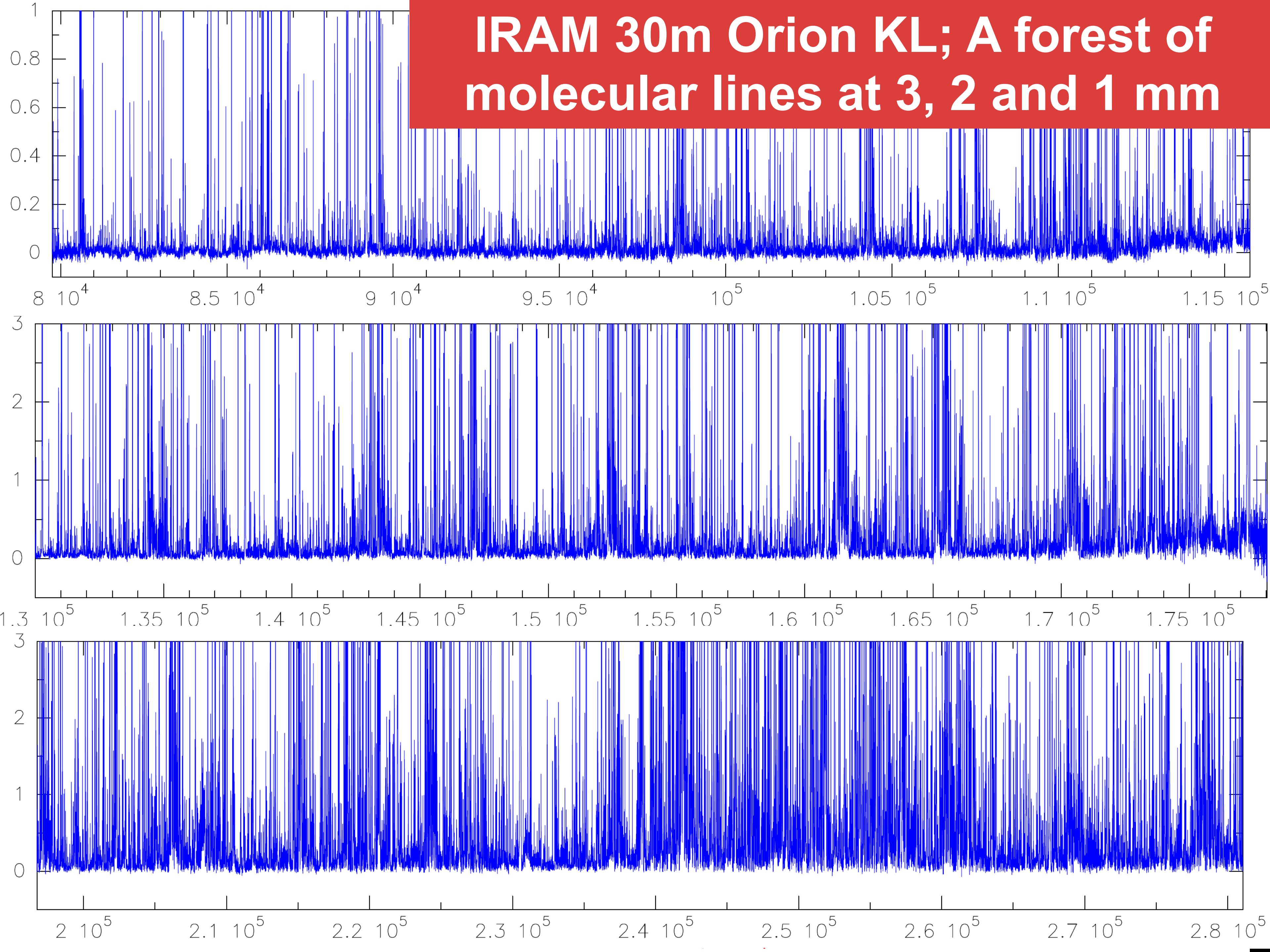
44" HPBW at 480 GHz HIFI
→ 18333 AU

16.5" HPBW at 1280 GHz HIFI
→ 6827 AU

11" HPBW at 1900 GHz HIFI
→ 4583 AU

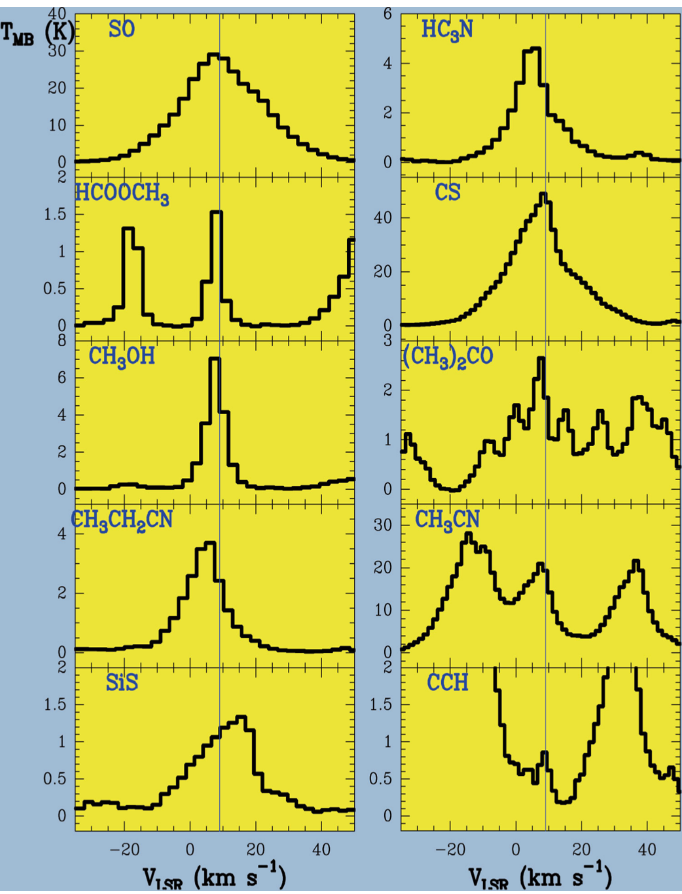
White: H_2; **blue**/**red (SMA)**: CO; **green (SMA)**: CH_3CN; **orange (SCUBA)**: 850 μm; **black**: runaway stars; Zapata et al. 2011.

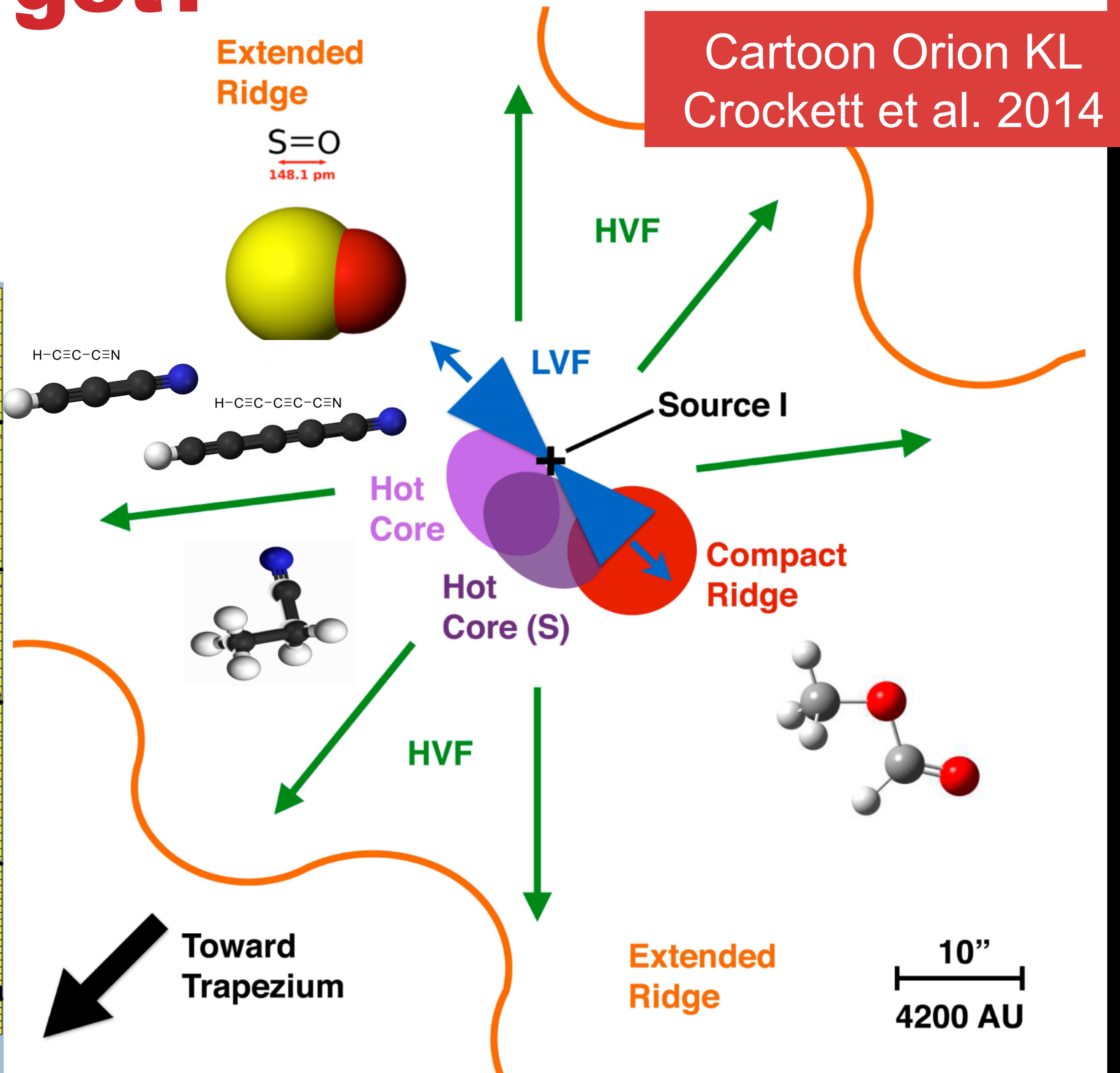
IRAM 30m Orion KL; A forest of molecular lines at 3, 2 and 1 mm



3. What kind of information you will get?

Different gas components
Large variety of molecules
Different v_{LSR} and Δv





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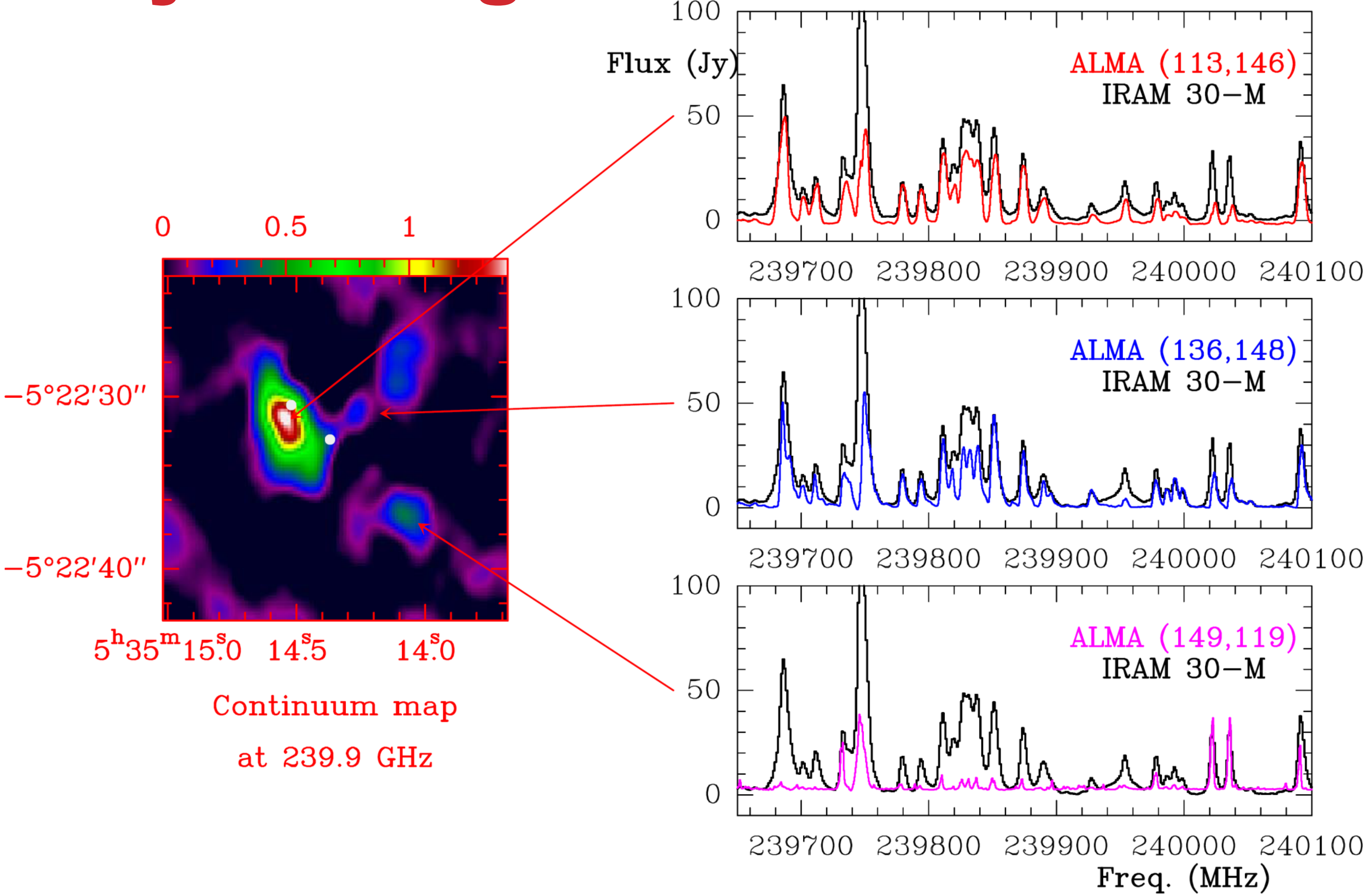

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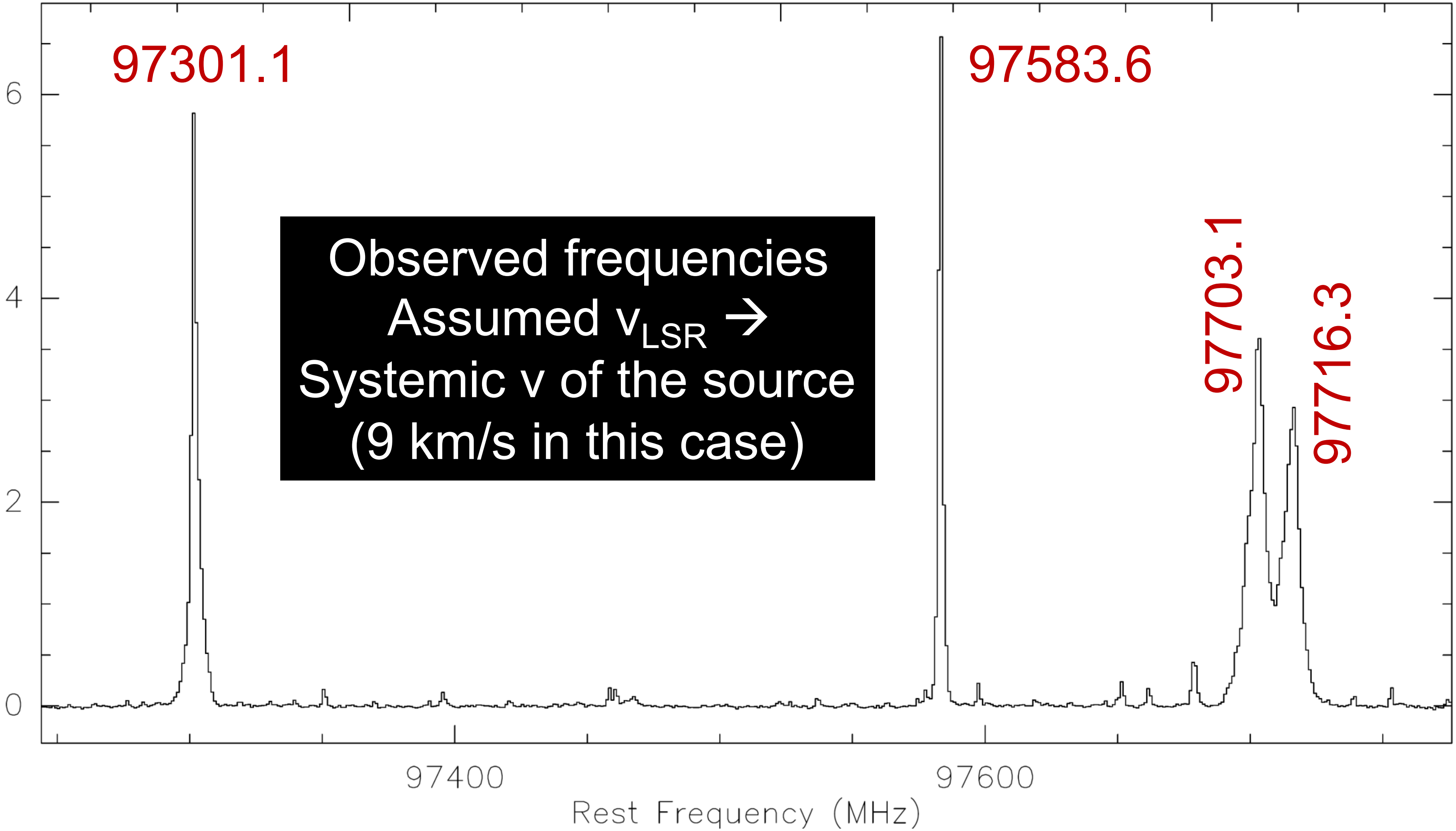


4. Line identification

Prior to go to the catalogs you can try:

- For the most abundant species (more intense lines):
  - Compare your data with other studies of the source
  - Compare your frequency range with other studies in the same frequency range (corrected from v_{LSR})

4. Line identification

Catalogs: CDMS, JPL, Lovas, Splatalogue

97301.1 → OCS; 97301.2085 MHz; J=8-7

97583.6 → CH_3OH

Species	Chemical Name	Ordered Freq (MHz) (rest frame, redshifted)	Resolved QNs	CDMS/JPL Intensity	Lovas/AST Intensity	E_L (cm^{-1})	E_L (K)
$^{34}SO_2$ v=0	Sulfur Dioxide	97580.42780, 97580.42780	47(11,37)-48(10,38)	-5.61220		915.2838	1318.7920
$(CH_3)_2CO$ v=0	Acetone	97582.33750, 97582.33750	4(3, 2)- 3(0, 3) EE	-7.14450		2.4740	3.5595
CH_3OH v_t = 0	Methanol	97582.80400, 97582.80400	2(1, 1)- 1(1, 0) - -	-4.94698	<2.5	11.7330	16.8811
g-CH_3CH_2OH	gauche-Ethanol	97588.85820, 97588.85820	15(3,12)-14(4,11), v_t= 0- 0	-7.72060		113.8145	163.7527

b-type transition: gauche-CH_3CH_2OH → μ_a=1.264D μ_b=0.104D →
b-type transitions of these mol. will be very weak; A_{ul} (Einstein coefficient)

97703.1 → SO_2; 97702.334 MHz; $J_{Ka,Kc}$= $7_{3,5}$-$8_{2,6}$

97716.3 → ^{34}SO; 97715.405 MHz; N_J= 2_3-1_2

4. Line identification

In case of doubt:

- Visit CDMS: http://www.astro.uni-koeln.de/cdms/molecules
  - Has been this species detected? Where?
  - Maybe I have discovered a new molecule in space ?? or I can give the first detection in my source ?

→ Search for all transitions of this species in your data, those that could be detected (models are very useful for COM's)

4. Line identification

CH_2OHCHO → μ_a=0.2620D μ_b=2.330D

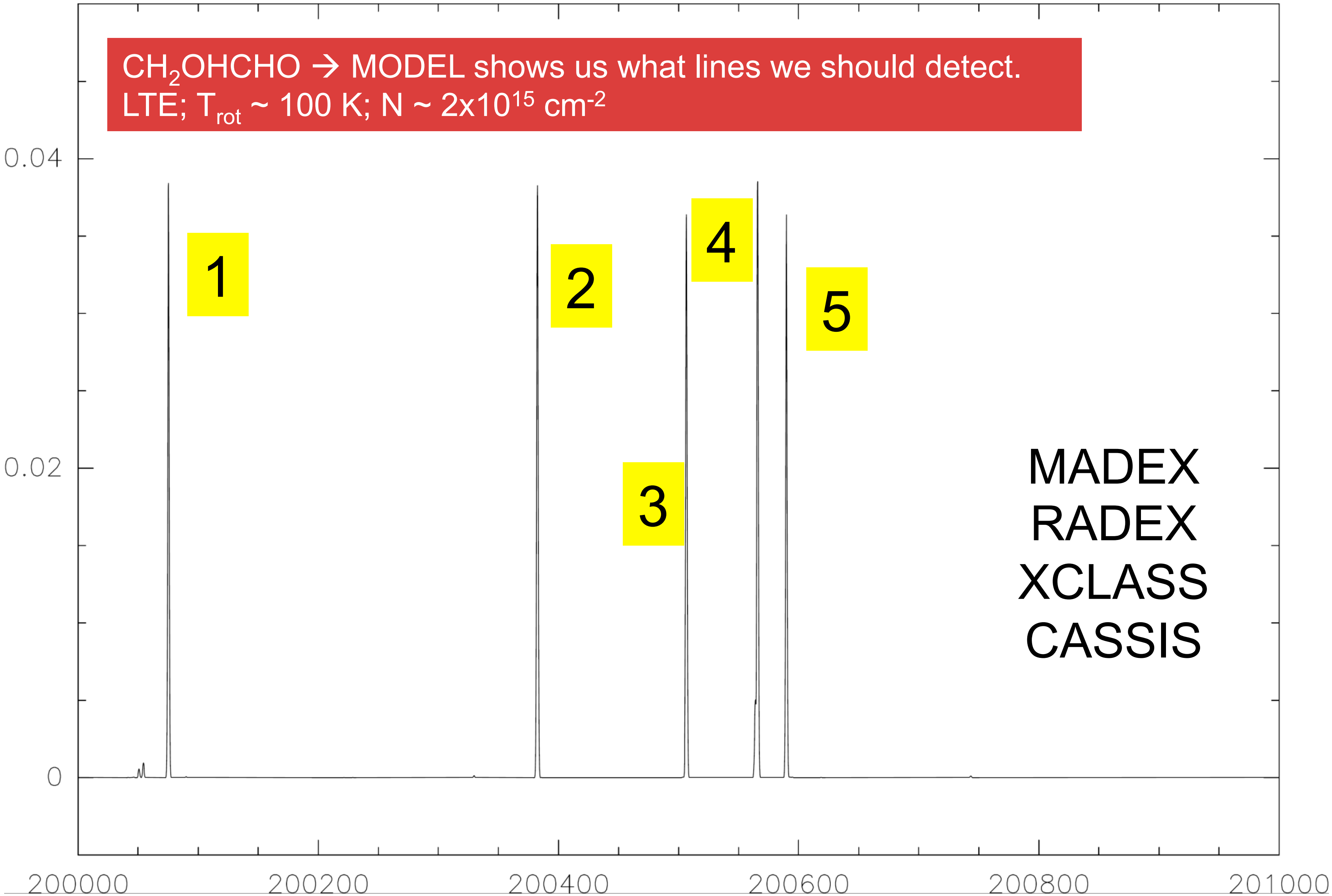
MADEX
Cernicharo
(2012)

LINE	Ju	Ku	ku	Jl	Kl	kl	FREQ(MHz)	Error	Eupp	Aul	Sij	gu	Nu	Nl
3653	33	7	27	33	5	28	200041.12203	.006364	345.2	1.140E-07	1.19421a	67	831	803
1	27	3	24	27	3	25	200045.76982	.015115	217.5	9.564E-08	.82239a	55	524	500
	20	18	3	21	17	4	200050.14667	.013416	313.3	1.873E-06	.15179b	41	749	733
	20	18	2	21	17	5	200050.14667	.013416	313.3	1.873E-06	.15179b	41	750	732
	39	8	32	38	9	29	200053.75918	.022070	477.8	1.482E-05	2.31392b	79	1151	1125
3658	27	3	24	27	2	25	200074.65594	.015100	217.5	8.053E-05	8.75234b	55	524	499
3659	33	9	24	34	6	29	200089.32915	.022090	364.1	4.877E-07	.06455b	67	879	849
3660	9	2	7	8	0	8	200203.76200	.009014	28.4	1.403E-08	.04157a	19	70	47
3661	46	5	41	47	4	44	200220.84827	.084290	615.2	7.460E-07	.13679b	93	1476	1452
3662	46	5	41	47	3	44	200220.85640	.084290	615.2	1.045E-09	.01516a	93	1476	1451
2	46	6	41	47	4	44	200228.15090	.084285	615.2	1.045E-09	.01516a	93	1477	1452
	46	6	41	47	3	44	200228.15902	.084285	615.2	7.461E-07	.13679b	93	1477	1451
	33	24	9	34	23	12	200329.11995	.011321	660.8	6.493E-06	.85631b	67	1587	1556
	33	24	10	34	23	11	200329.11995	.011321	660.8	6.493E-06	.85631b	67	1588	1555
3667	10	3	7	9	2	8	200381.86446	.007616	36.6	4.048E-05	1.67200b	21	89	67
3668	35	6	29	35	6	30	200385.07072	.010620	383.2	1.199E-07	1.32366a	71	921	896
3	7	5	3	7	3	4	200477.94570	.008580	30.7	2.693E-09	.00627a	15	74	50
	46	30	17	47	29	18	200497.50838	.026366	1145.4	9.395E-06	1.71559b	93	2246	2242
	46	30	16	47	29	19	200497.50838	.026366	1145.4	9.395E-06	1.71559b	93	2247	2243
	25	2	23	25	2	24	200502.86600	.018866	180.5	7.450E-08	.58996a	51	435	411
3673	25	2	23	25	1	24	200505.90563	.018864	180.5	5.829E-05	5.83616b	51	435	410
3674	13	4	9	13	1	12	200563.23026	.009551	60.9	4.998E-06	.26472b	27	150	122
4	27	4	24	27	3	25	200565.23907	.014949	217.6	8.111E-05	8.75073b	55	525	500
	25	3	23	25	2	24	200589.17472	.018829	180.5	5.836E-05	5.83600b	51	436	411
	25	3	23	25	1	24	200592.21435	.018827	180.5	7.459E-08	.58992a	51	436	41
	27	4	24	27	2	25	200594.12520	.014933	217.6	9.639E-08	.82203a	55	525	49
3679	32	5	27	32	5	28	200618.03700	.010183	317.3	1.173E-07	1.18232a	65	764	73
3680	26	7	19	27	4	24	200742.66144	.017960	227.2	2.646E-07	.02743b	53	545	52
3681	45	8	37	44	10	34	200921.34545	.029081	631.4	1.623E-08	.22784a	91	1518	1495
3682	42	8	34	42	8	35	201083.26086	.017410	556.1	1.210E-07	1.58273a	85	1333	1316
3683	31	9	22	32	5	27	201110.92938	.019507	327.0	6.593E-10	.00639a	63	786	764

5

Search for all transitions of this species in your data →
BUT ONLY THOSE THAT COULD BE DETECTED

4. Line identification



4. Line identification

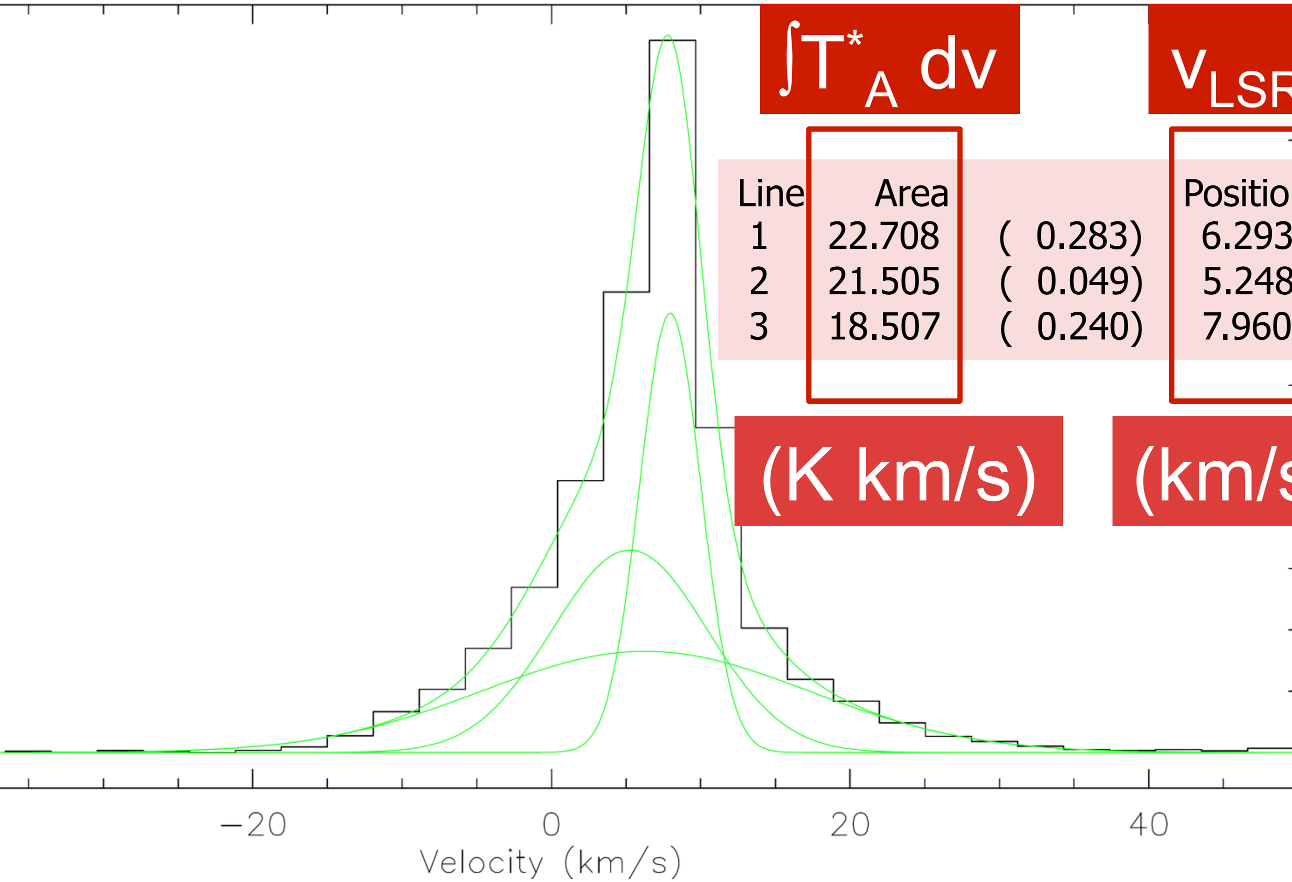
- IMPORTANT:
  Study something about the source

- Study something about the molecules:
  Interpret Einstein coefficients, energies of the upper level, dipole moments and associated transitions

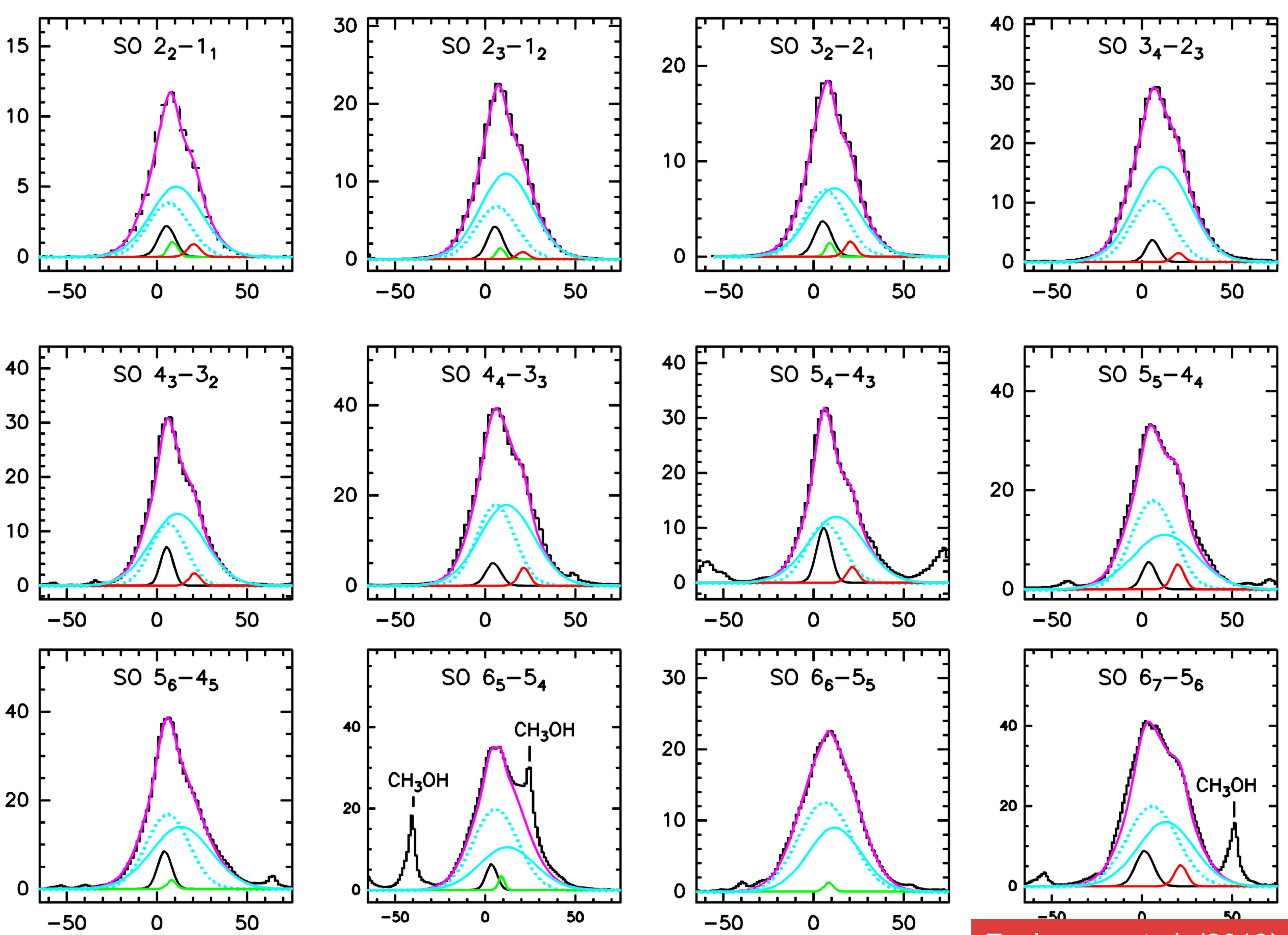
- Models are very useful for identifying the emission of the most complex species → Large number of transitions

5. Observed line parameters

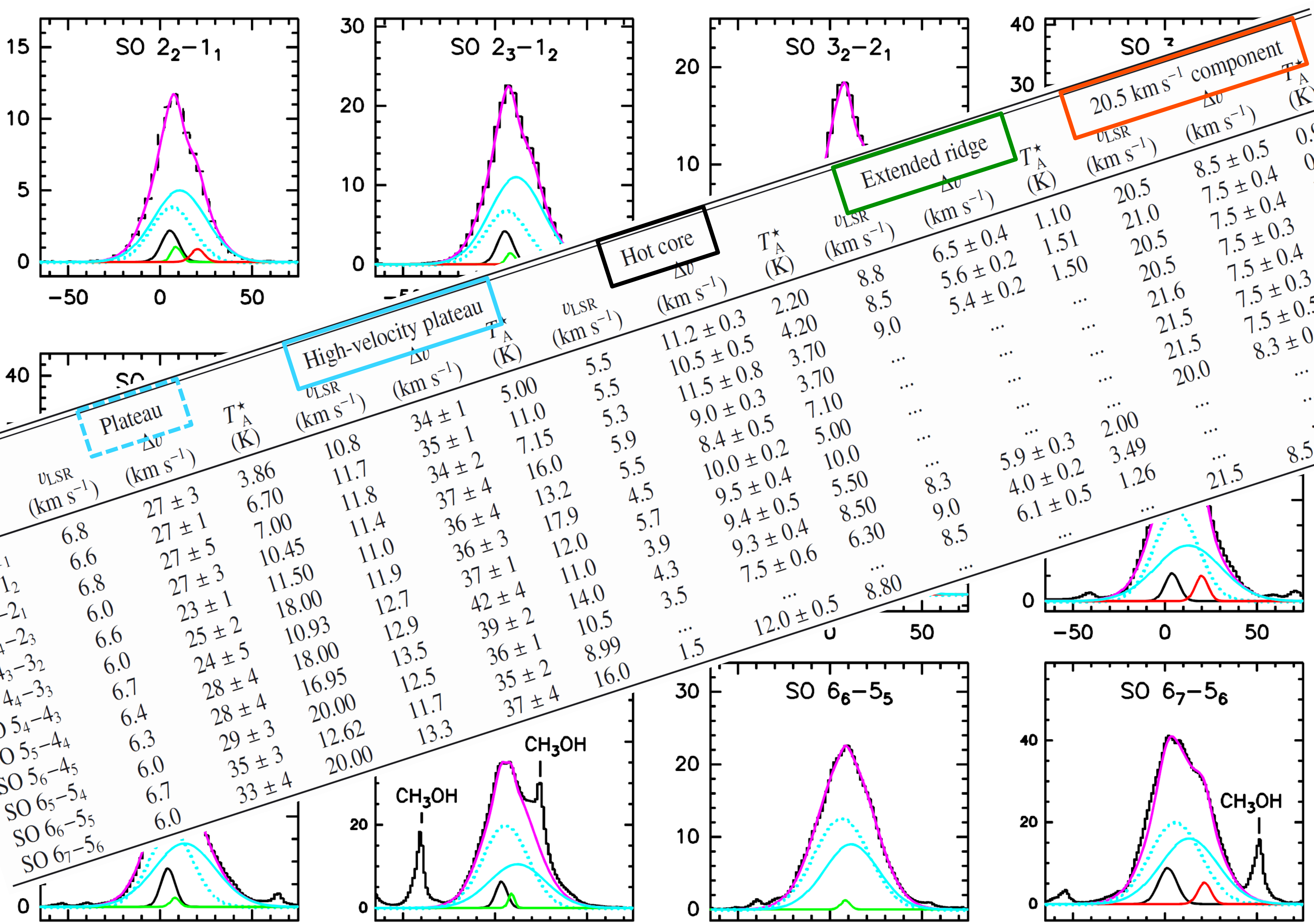
Software: GILDAS package (CLASS)



Line	Area $\int T^*_A\,dv$ (K km/s)		Position v_{LSR} (km/s)		Width Δv (km/s)		Tpeak T^*_A (K)
1	22.708	(0.283)	6.293	(0.223)	25.827	(0.352)	0.82597
2	21.505	(0.049)	5.248	(0.104)	12.225	(0.057)	1.6526
3	18.507	(0.240)	7.960	(0.023)	4.845	(0.037)	3.5883



Esplugues et al. (2013)



	Plateau			High-velocity plateau			Hot core			Extended ridge			20.5 km s^{-1} component		
	v_{LSR} (km s^{-1})	Δv (km s^{-1})	$T^{\star}_{A}$ (K)	v_{LSR} (km s^{-1})	Δv (km s^{-1})	$T^{\star}_{A}$ (K)	v_{LSR} (km s^{-1})	Δv (km s^{-1})	$T^{\star}_{A}$ (K)	v_{LSR} (km s^{-1})	Δv (km s^{-1})	$T^{\star}_{A}$ (K)	v_{LSR} (km s^{-1})	Δv (km s^{-1})	$T^{\star}_{A}$ (K)
$_1$	6.8	27 ± 3	3.86	10.8	34 ± 1	5.00	5.5	11.2 ± 0.3	2.20	8.8	6.5 ± 0.4	1.10	20.5	8.5 ± 0.5	0.9
1_2	6.6	27 ± 1	6.70	11.7	35 ± 1	11.0	5.5	10.5 ± 0.5	4.20	8.5	5.6 ± 0.2	1.51	21.0	7.5 ± 0.4	0
-2_1	6.8	27 ± 5	7.00	11.8	34 ± 2	7.15	5.3	11.5 ± 0.8	3.70	9.0	5.4 ± 0.2	1.50	20.5	7.5 ± 0.4	
-2_3	6.0	27 ± 3	10.45	11.4	37 ± 4	16.0	5.9	9.0 ± 0.3	3.70	...	...	...	20.5	7.5 ± 0.3	
4_3-3_2	6.6	23 ± 1	11.50	11.0	36 ± 4	13.2	5.5	8.4 ± 0.5	7.10	...	...	...	21.6	7.5 ± 0.4	
4_4-3_3	6.0	25 ± 2	18.00	11.9	36 ± 3	17.9	4.5	10.0 ± 0.2	5.00	...	...	...	21.5	7.5 ± 0.3	
O 5_4-4_3	6.7	24 ± 5	10.93	12.7	37 ± 1	12.0	5.7	9.5 ± 0.4	10.0	...	...	...	21.5	7.5 ± 0.5	
O 5_5-4_4	6.4	28 ± 4	18.00	12.9	42 ± 4	11.0	3.9	9.4 ± 0.5	5.50	...	...	...	20.0	8.3 ± 0	
SO 5_6-4_5	6.3	28 ± 4	16.95	13.5	39 ± 2	14.0	4.3	9.3 ± 0.4	8.50	8.3	5.9 ± 0.3	2.00	...	...	
SO 6_5-5_4	6.0	29 ± 3	20.00	12.5	36 ± 1	10.5	3.5	7.5 ± 0.6	6.30	9.0	4.0 ± 0.2	3.49	...	...	
SO 6_6-5_5	6.7	35 ± 3	12.62	11.7	35 ± 2	8.99	...	...	...	8.5	6.1 ± 0.5	1.26	...	...	
SO 6_7-5_6	6.0	33 ± 4	20.00	13.3	37 ± 4	16.0	1.5	12.0 ± 0.5	8.80	...	...	...	21.5	8.5	

Esplugues et al. (2013)

1. A molecule has been identified
2. I observed several lines from different transitions
3. I fit the line profiles to n Gaussians

I can derive physical parameters for each component (Gaussian):

- LTE approximation: T_{rot} and N of the molecule (rotational diagram)
- LVG approximation: T_k and $n(H_2)$ of the region

- LVG: $n(H_2)<10^{6-7}$ cm^{-3}
  but collisional rates are needed !

- LTE: $n(H_2)>10^{7}$ cm^{-3} (most of the hot cores)

e.g.
COM's → collisional rates are not available for most of these species.

But

COM's are typical of hot cores → LTE is a reasonable approximation for the study of COM's in hot cores.

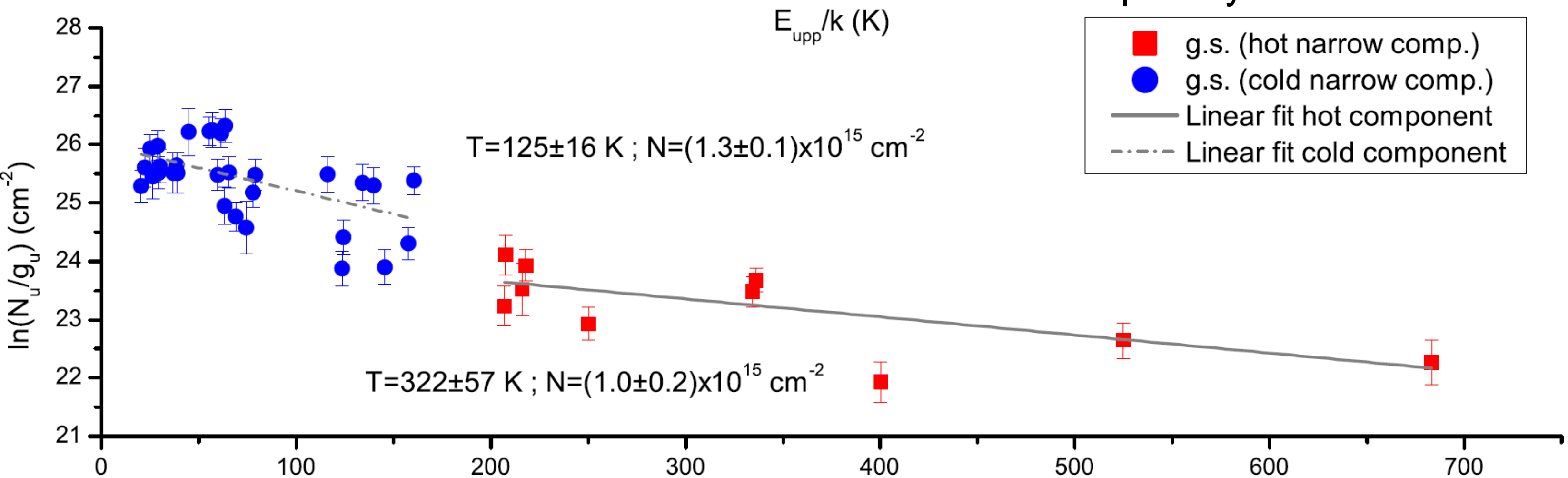
6. T_{rot} and N over the beam

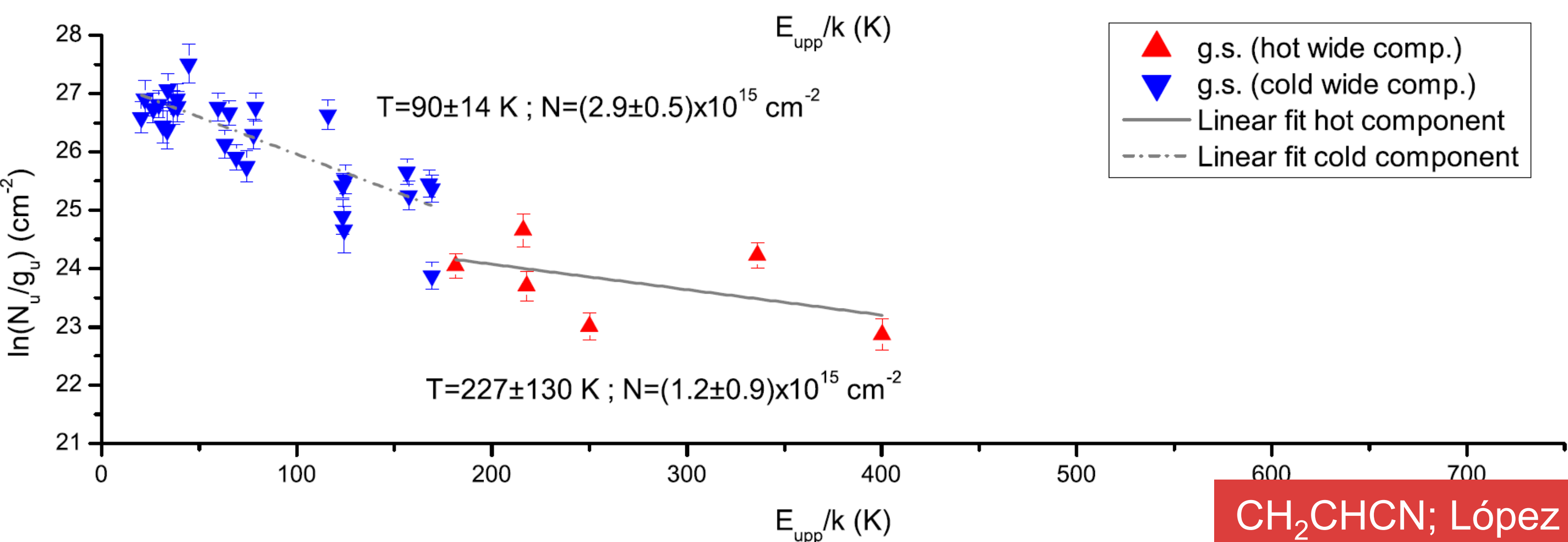
Rotational diagrams

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{8\pi k\nu^2 W_{obs}}{hc^3 A_{ul} g_u}\right) = \ln\left(\frac{N}{Q_{rot}}\right) - \frac{E_{upp}}{kT_{rot}}$$

Rayleigh-Jeans aprox.
LTE
Optically thin

See Turner (1991)





CH_2CHCN; López et al. (2014)

6. T_{rot} and N over the source diameter

Rotational diagrams

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{8\pi k\nu^2 W_{obs}}{hc^3 A_{ul} g_u}\right) = \ln\left(\frac{N}{Q_{rot}}\right) - \frac{E_{upp}}{kT_{rot}} + \ln b$$

$$b = \frac{\Omega_S}{\Omega_A} = \frac{\theta_S^2}{\theta_S^2 + \theta_B^2},$$

See Turner (1991)

But… How can I derive the size of my source?

1. INTERFEROMETRIC OBSERVATIONS → Check previous studies of your source

2. USING OPTICALLY THICK LINES →
(Sometimes optically thick lines are useful)

Region thermalized $T_{ex}=T_k$

$T_b=T_{ex}(1-e^{-\tau})$ → optically thick → $T_b=T_{ex}$

$T_{obs}=T_b(\Omega_{source}/\Omega_{beam})$

6. T_{rot} and N over the source diameter

Rotational diagrams

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{8\pi k \nu^2 W_{obs}}{hc^3 A_{ul} g_u}\right) = \ln\left(\frac{N}{Q_{rot}}\right) - \frac{E_{upp}}{kT_{rot}} + \ln b$$

$$b = \frac{\Omega_S}{\Omega_A} = \frac{\theta_S^2}{\theta_S^2 + \theta_B^2},$$

See Turner (1991)

But… How can I derive th

1. INT

Different sets of data will provide more constrained parameters

…LLY THICK LINES →

…es optically thick lines are useful)

Region thermalized $T_{ex}=T_k$

$T_b=T_{ex}(1-e^{-\tau})$ → optically thick → $T_b=T_{ex}$

$T_{obs}=T_b(\Omega_{source}/\Omega_{beam})$

1. A molecule has been identified
2. I observed several lines from different transitions
3. I fit the line profiles to n Gaussians → → v_{LSR}, Δv, T^*_A for the different spectral components
4. T_{rot} and N from rotational diagrams for each component

MODEL

1. A molecule has been identified
2. I observed several lines from diffe… transitions
3. I fit the line profil… …sians →
→ v_{L}… …e different spectral …
… and N from rotational diagrams for each component

ITERATIVE PROCESS

MODEL

1. A molecule has been identified
2. I observed several lines from diffe
   transitions
3. I fit the line profil sians →

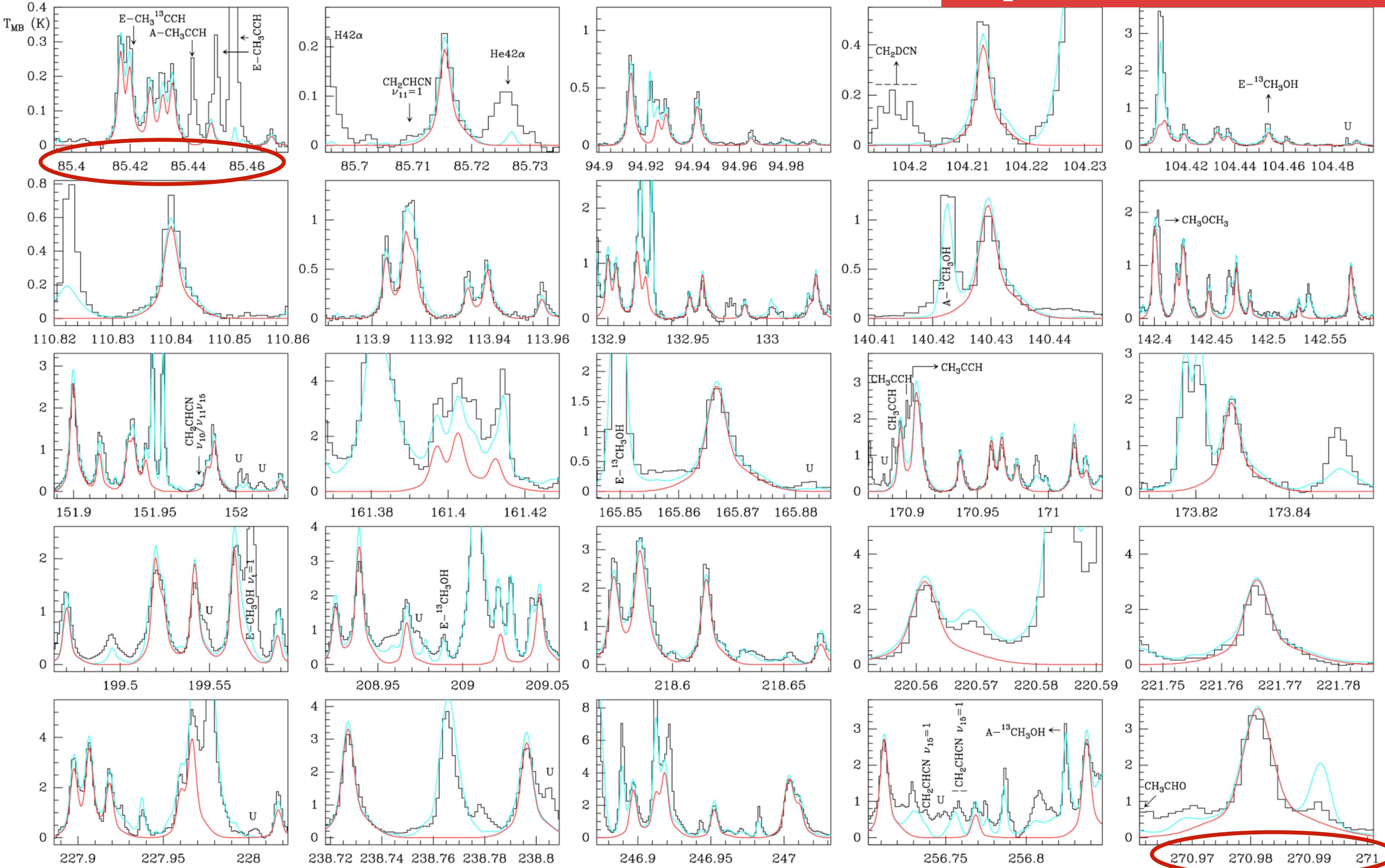
PROCESS

A MODEL WILL HELP
TO IDENTIFY LINES (COM'S AND OTHERS)
AND TO DETERMINE
v_{LSR}, Δv, T^{*}_{A} , T_{rot}, N (and T_k, $n(H_2)$ using LVG)

MODEL

7. Physical and chemical models

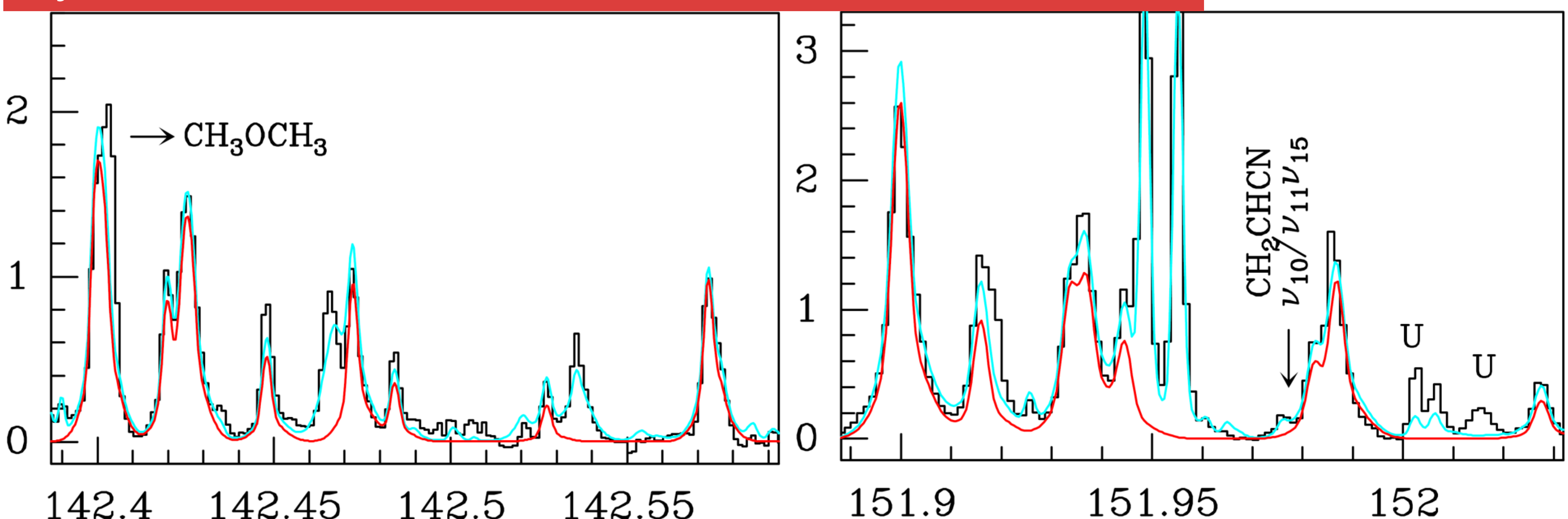
CH$_2$CHCN; López et al. (2014)



7. Physical and chemical models

	Hot narrow comp.	*Cold narrow comp.*	*Hot wide comp.*	*Cold wide comp.*
d_{sou} (")	5	10	5	10
offset (")	2	2	0	0
Δv_{FWHM} ($km\,s^{-1}$)	6(7*)	6(7*)	20	20
v_{LSR} ($km\,s^{-1}$)	5	5	3	3
T_{rot} (K)	*320*	*100*	*200*	*90*
$N_{CH_2CHCN(g.s.)}$ (cm^{-2})	$(3.0 \pm 0.9) \times 10^{15}$	$(1.0 \pm 0.3) \times 10^{15}$	$(9 \pm 3) \times 10^{14}$	$(1.3 \pm 0.4) \times 10^{15}$

Red: CH_2CHCN model → four components
Cyan: Total model



7. Physical and chemical models

	Hot narrow comp.	*Cold narrow comp.*	*Hot wide comp.*	*Cold wide comp.*
d_{sou} ('')	5	10	5	10
offset ('')	2	2	0	0
Δv_{FWHM} (km s^{-1})	6(7*)	6(7*)	20	20
v_{LSR} (km s^{-1})	5	5	3	3
T_{rot} (K)	*320*	*100*	*200*	*90*
$N_{CH_2CHCN(g.s.)}$ (cm^{-2})	$(3.0 \pm 0.9) \times 10^{15}$	$(1.0 \pm 0.3) \times 10^{15}$	$(9 \pm 3) \times 10^{14}$	$(1.3 \pm 0.4) \times 10^{15}$
$N_{CH_2CHCN(v_{11}=1)}$(cm^{-2})	$(9 \pm 3) \times 10^{14}$	$(2.5 \pm 0.8) \times 10^{14}$	...	...
$N_{CH_2CHCN(v_{11}=2)}$(cm^{-2})	$(2 \pm 1) \times 10^{14}$	$(5 \pm 2) \times 10^{13}$	...	...
$N_{CH_2CHCN(v_{11}=3)}$(cm^{-2})	$\leq(2 \pm 1) \times 10^{14}$	$\leq(5 \pm 2) \times 10^{13}$	...	...
$N_{CH_2CHCN(v_{15}=1)}$(cm^{-2})	$(4 \pm 1) \times 10^{14}$	$(1.0 \pm 0.3) \times 10^{14}$	...	...
$N_{CH_2CHCN(v_{10}=1\Leftrightarrow(v_{11}=1,v_{15}=1))}$(cm^{-2})	$(4 \pm 2) \times 10^{14}$	$(8 \pm 4) \times 10^{13}$	...	...

Vibrational Temperatures

$$\frac{N(\mathrm{CH_2CHCN}\ \ v_x)}{N(\mathrm{CH_2CHCN})} = \frac{\exp\left(-\frac{E_{v_x}}{T_{vib}}\right)}{f_v}$$

$$N(\mathrm{CH_2CHCN}) = N_{g.s.} \times f_v$$

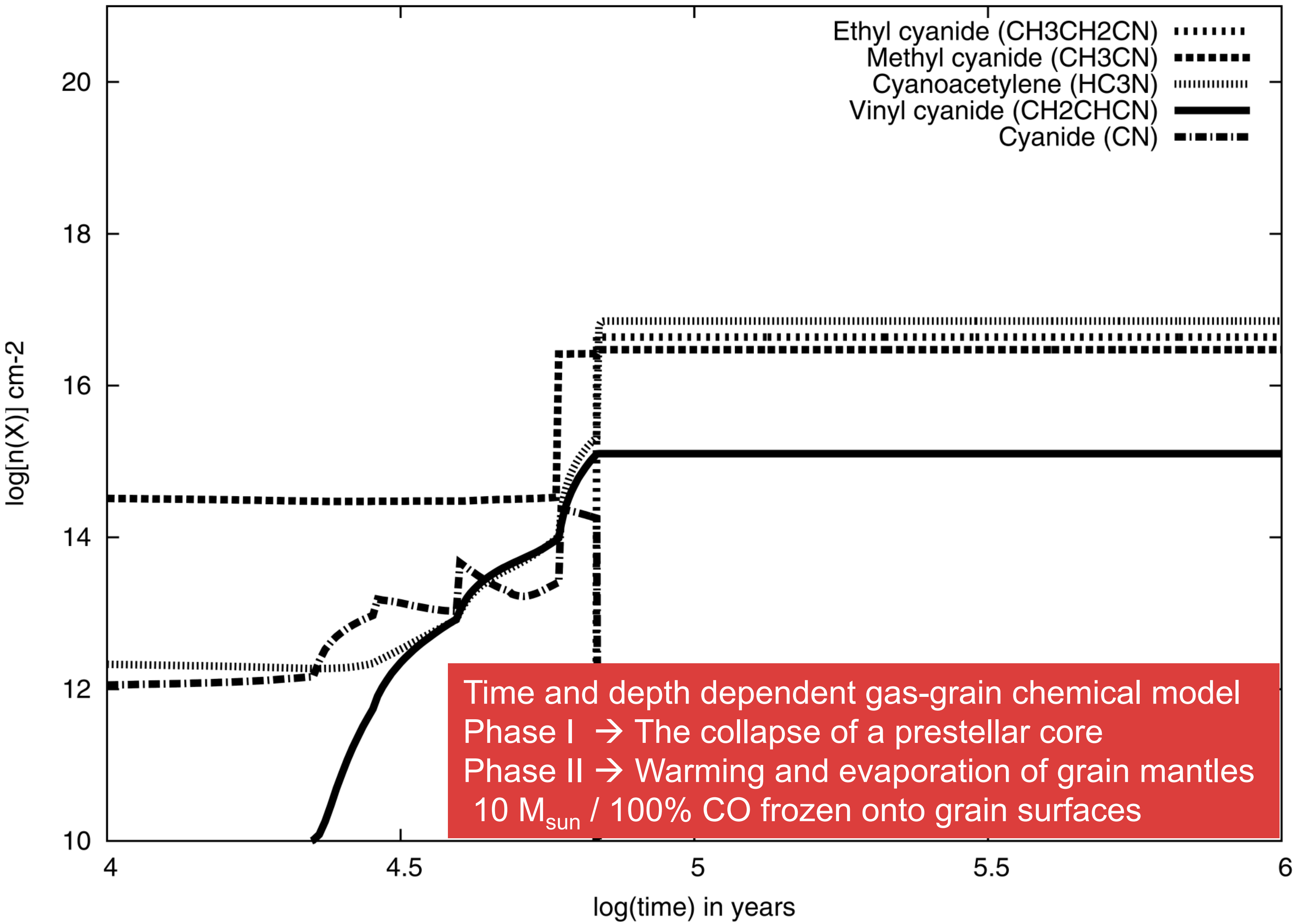
Tvib > Trot → IR pumping, temperature gradient ?

7. Physical and chemical models

	Hot narrow comp.	*Cold narrow comp.*	*Hot wide comp.*	*Cold wide comp.*
d_{sou} (")	5	10	5	10
offset (")	2	2	0	0
Δv_{FWHM} (km s^{-1})	6(7*)	6(7*)	20	20
v_{LSR} (km s^{-1})	5	5	3	3
T_{rot} (K)	*320*	*100*	*200*	*90*
$N_{\mathrm{CH_2CHCN(g.s.)}}$ (cm^{-2})	$(3.0 \pm 0.9) \times 10^{15}$	$(1.0 \pm 0.3) \times 10^{15}$	$(9 \pm 3) \times 10^{14}$	$(1.3 \pm 0.4) \times 10^{15}$
$N_{\mathrm{CH_2CHCN}(v_{11}=1)}$(cm^{-2})	$(9 \pm 3) \times 10^{14}$	$(2.5 \pm 0.8) \times 10^{14}$	...	...
$N_{\mathrm{CH_2CHCN}(v_{11}=2)}$(cm^{-2})	$(2 \pm 1) \times 10^{14}$	$(5 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2CHCN}(v_{11}=3)}$(cm^{-2})	$\leq(2 \pm 1) \times 10^{14}$	$\leq(5 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2CHCN}(v_{15}=1)}$(cm^{-2})	$(4 \pm 1) \times 10^{14}$	$(1.0 \pm 0.3) \times 10^{14}$	...	...
$N_{\mathrm{CH_2CHCN}(v_{10}=1\Leftrightarrow(v_{11}=1,v_{15}=1))}$(cm^{-2})	$(4 \pm 2) \times 10^{14}$	$(8 \pm 4) \times 10^{13}$	...	...
$N_{\mathrm{^{13}CH_2CHCN}}$(cm^{-2})	$(4 \pm 2) \times 10^{14}$	$(5 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2^{13}CHCN}}$(cm^{-2})	$(4 \pm 2) \times 10^{14}$	$(5 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2CH^{13}CN}}$(cm^{-2})	$(4 \pm 2) \times 10^{14}$	$(5 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2CHC^{15}N}}$(cm^{-2})	$\leq(1.0 \pm 0.5) \times 10^{14}$	$\leq(2 \pm 1) \times 10^{13}$	...	...
N_{HCDCHCN}(cm^{-2})	$\leq(4 \pm 2) \times 10^{14}$	$\leq(4 \pm 2) \times 10^{13}$	...	...
N_{DCHCHCN}(cm^{-2})	$\leq(4 \pm 2) \times 10^{14}$	$\leq(4 \pm 2) \times 10^{13}$	...	...
$N_{\mathrm{CH_2CDCN}}$(cm^{-2})	$\leq(3 \pm 1) \times 10^{14}$	$\leq(3 \pm 1) \times 10^{13}$	...	...

Isotope ratios
^{12}C/^{13}C ratio
Lower limits to ^{14}N/^{15}N, H/D

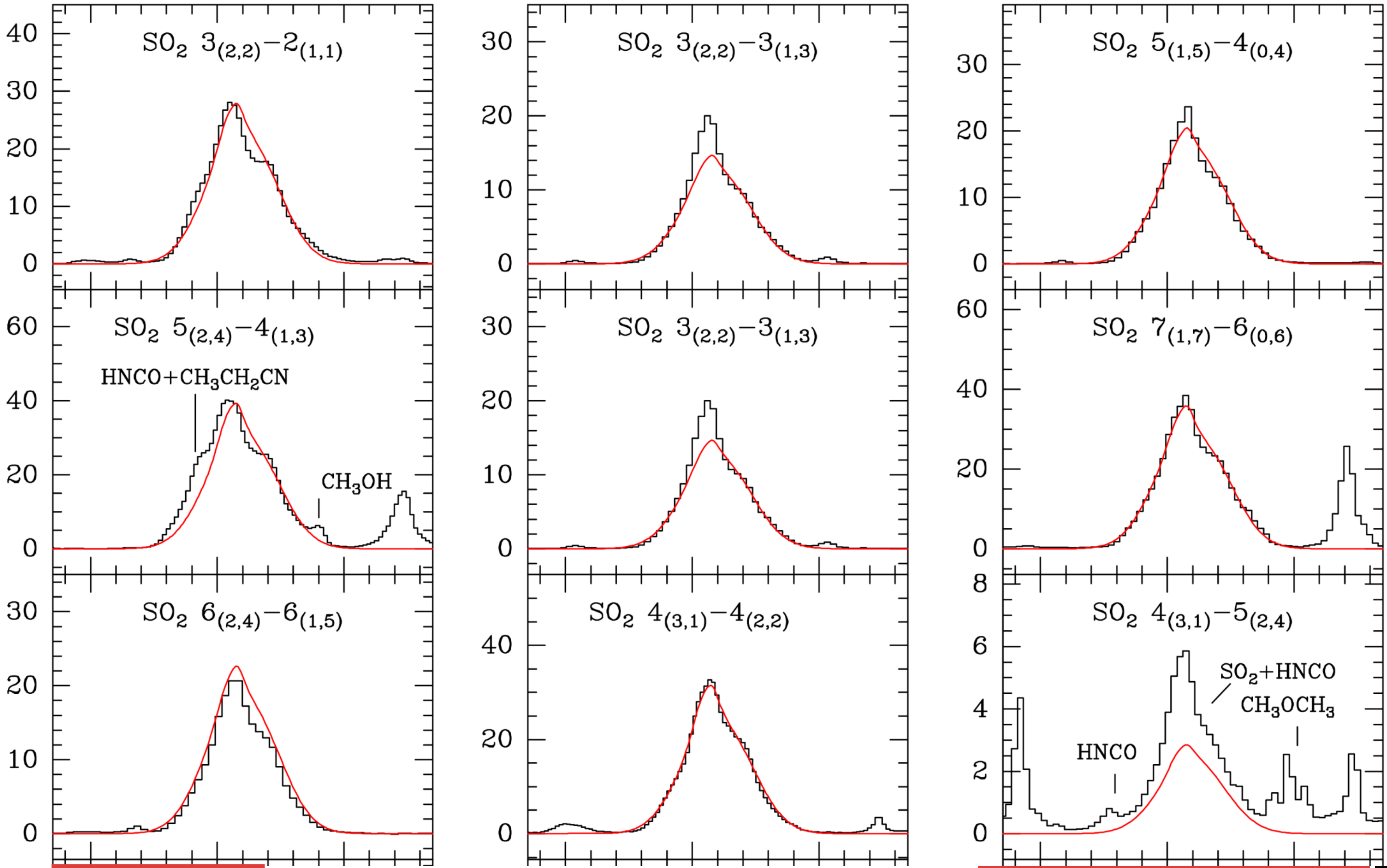
7. Physical and chemical models



7. Physical and chemical models

- We have identified many more molecules
- Other species could trace different regions
- Repeat the procedure for another molecule
- Add the obtained synthetic spectrum to the total model
- Add this new information to your understanding of the source (dense and hot gas, shocks, ambient cold cloud ?)
- Improve the chemical models

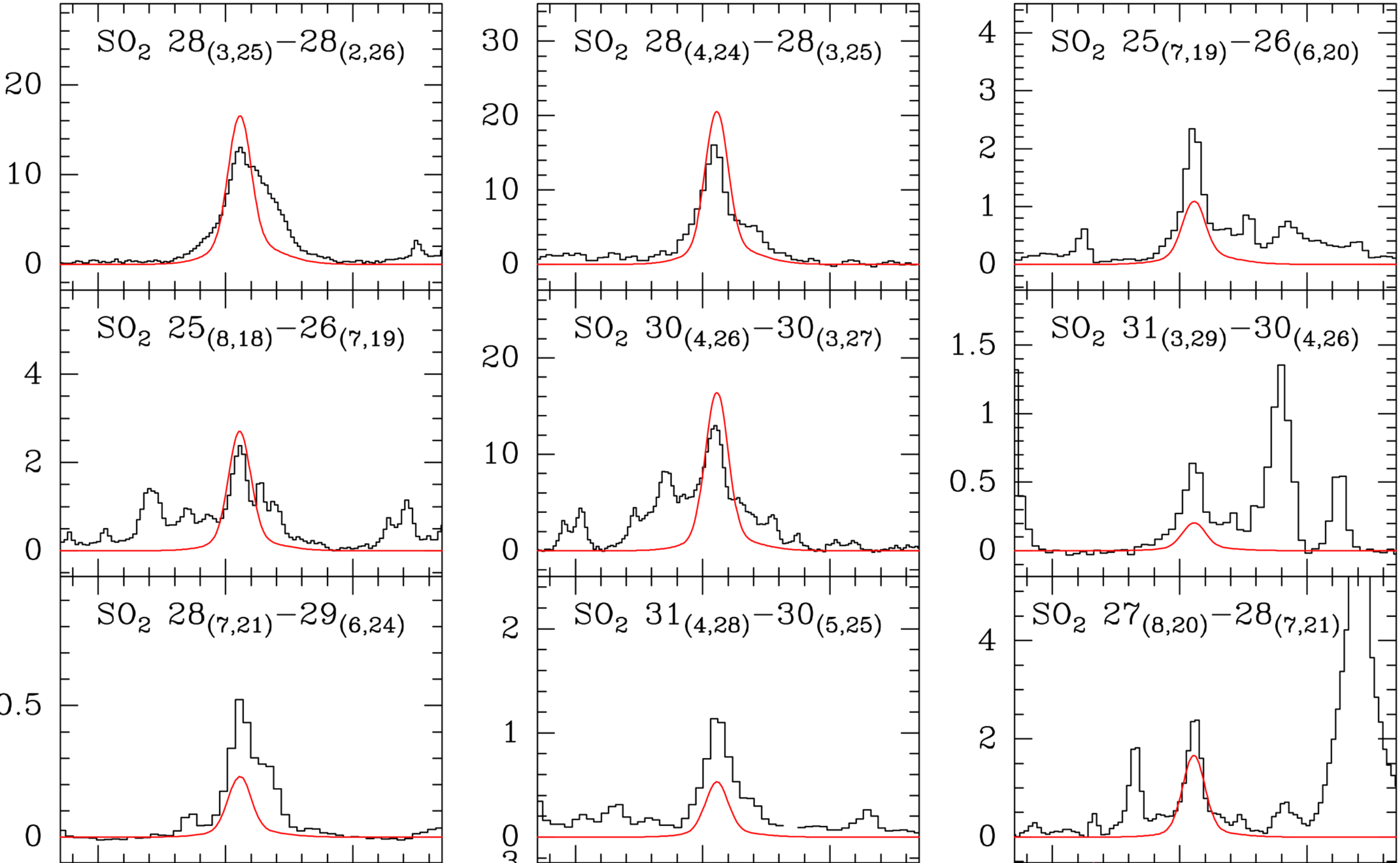
Repeat the procedure for another molecule



E_{up} < 400 K

Esplugues et al. (2013)

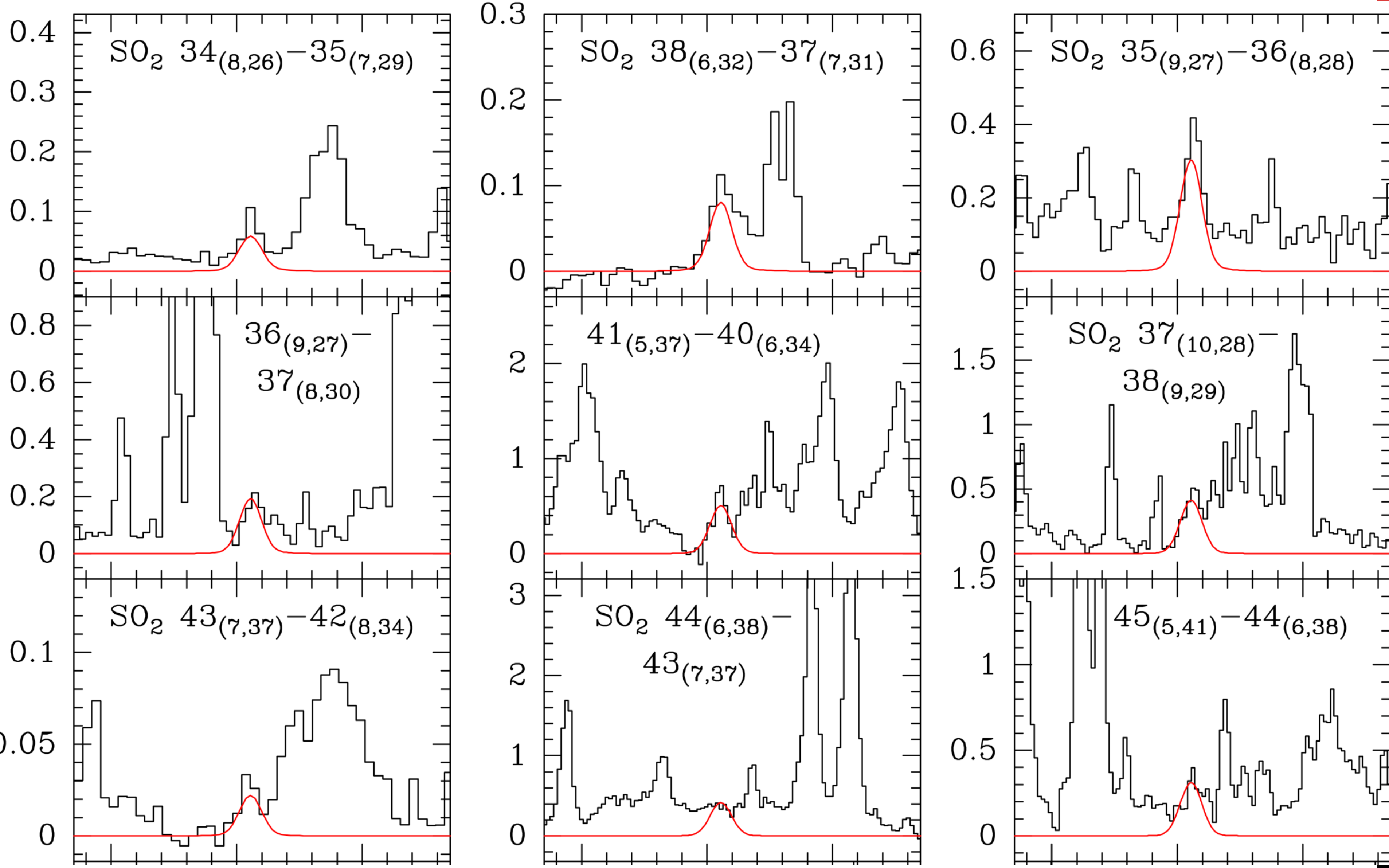
Repeat the procedure for another molecule



400 K <Eup < 700 K

Esplugues et al. (2013)

Repeat the procedure for another molecule



E_{up} > 700 K

Esplugues et al. (2013)

Repeat the procedure for another molecule

Component	Source diameter ($''$)	Offset (IRc2) ($''$)	$n(H_2)$ cm^{-3}	T_K (K)	Δv_{FWHM} (km s^{-1})	v_{LSR} (km s^{-1})
Extended ridge (ER)	120	0	10^5	60	4	8.5
Compact ridge (CR)	15	7	10^6	110	3	8
High-velocity plateau (HVP)	30	4	10^6	100	30	11
Plateau (PL)	20	0	5×10^6	150	25	6
Hot core (HC)	10	2	1.5×10^7	220	10	5.5
20.5 km s^{-1} component	5	2	5×10^6	90	7.5	20.5

Component	SO_2 $N \times 10^{15}$ (cm^{-2})
Extended ridge	0.23 ± 0.06
Compact ridge	1.2 ± 0.4
High-velocity plateau	130 ± 50
Plateau	10 ± 3
Hot core	100 ± 40
20.5 km s^{-1} comp.	0.17 ± 0.06

A single model with
5 components
that reproduces all
SO_2 lines
simultaneously →
166 lines
E_{up} from 15 to 1400 K

Repeat the procedure for another molecule

SO_2 $N \times 10^{15}$ (cm^{-2})	$^{34}SO_2$ $N \times 10^{15}$ (cm^{-2})	$SO_2$$^{(a)}$ $N \times 10^{15}$ (cm^{-2})	$^{33}SO_2$ $N \times 10^{15}$ (cm^{-2})	$SO^{18}O$ $N \times 10^{15}$ (cm^{-2})	$SO^{17}O$ $N \times 10^{15}$ (cm^{-2})	SO_2 $v_2 = 1$ $N \times 10^{15}$ (cm^{-2})	$^{34}SO_2$ $v_2 = 1$ $N \times 10^{15}$ (cm^{-2})
0.23 ± 0.06	0.10 ± 0.04	2.3 ± 0.7	0.04 ± 0.001	0.020 ± 0.007	0.007 ± 0.003	0.013 ± 0.003	...
1.2 ± 0.4	0.5 ± 0.2	12 ± 2	0.07 ± 0.02	0.03 ± 0.01	0.007 ± 0.003	0.20 ± 0.05	0.05 ± 0.02
130 ± 50	7 ± 2	161 ± 46	1.0 ± 0.3	0.9 ± 0.3	0.10 ± 0.04	0.4 ± 0.1	0.06 ± 0.02
10 ± 3	0.6 ± 0.2	14 ± 3	0.5 ± 0.2	0.06 ± 0.02	0.03 ± 0.01	...	...
100 ± 40	10 ± 4	230 ± 60	4 ± 1	1.5 ± 0.5	0.9 ± 0.3	4 ± 1	0.7 ± 0.2
0.17 ± 0.06	0.04 ± 0.01	0.8 ± 0.2	0.009 ± 0.003	...	...	...	...

N (SO_2) using $^{34}SO_2$

Isotopologues ratios

Vibrational Temperatures

How to analyze spectral line surveys?

1. Identify molecular transitions of a given species
2. Identify lines from isotopologues and vibrationally excited states of the same species
3. Model the lines
4. Derive source structure, densities, kinetic temperatures and chemical abundances
5. Repeat for another molecule
6. Identify unknown lines
7. Model the chemistry
8. Ask our physical-chemistry and laboratory colleagues for help