Probing the composition of the planet-building reservoir in protoplanetary disks

what we have learned from comets and ALMA?

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UNIVERSITY OF LEEDS

Our astrochemical origins

Inheritance?

Disk formation?

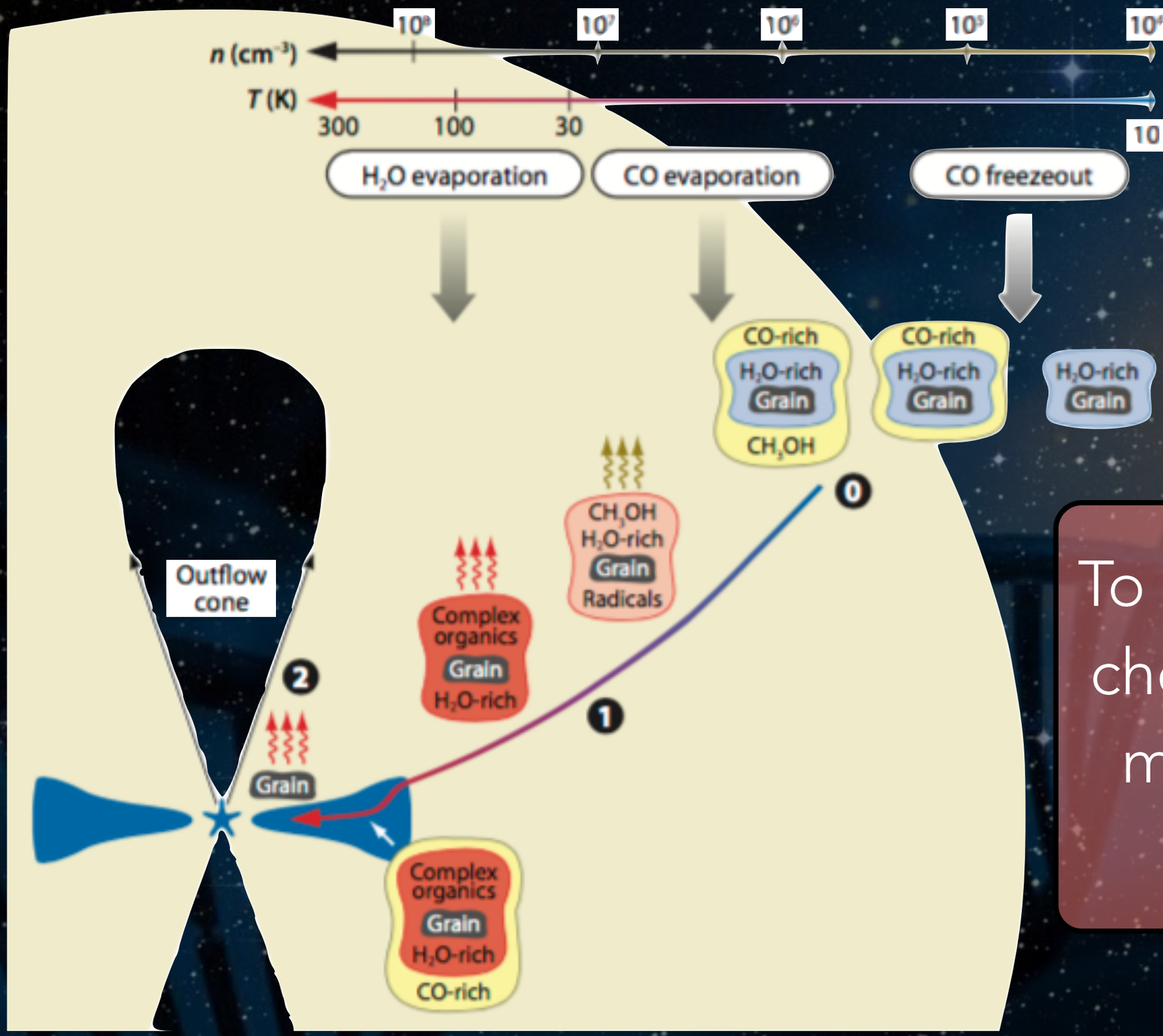
Disk processing?

Delivery?

What is the provenance of planetary system building material?

Credit: B. Saxton (NRAO/AUI/NSF)

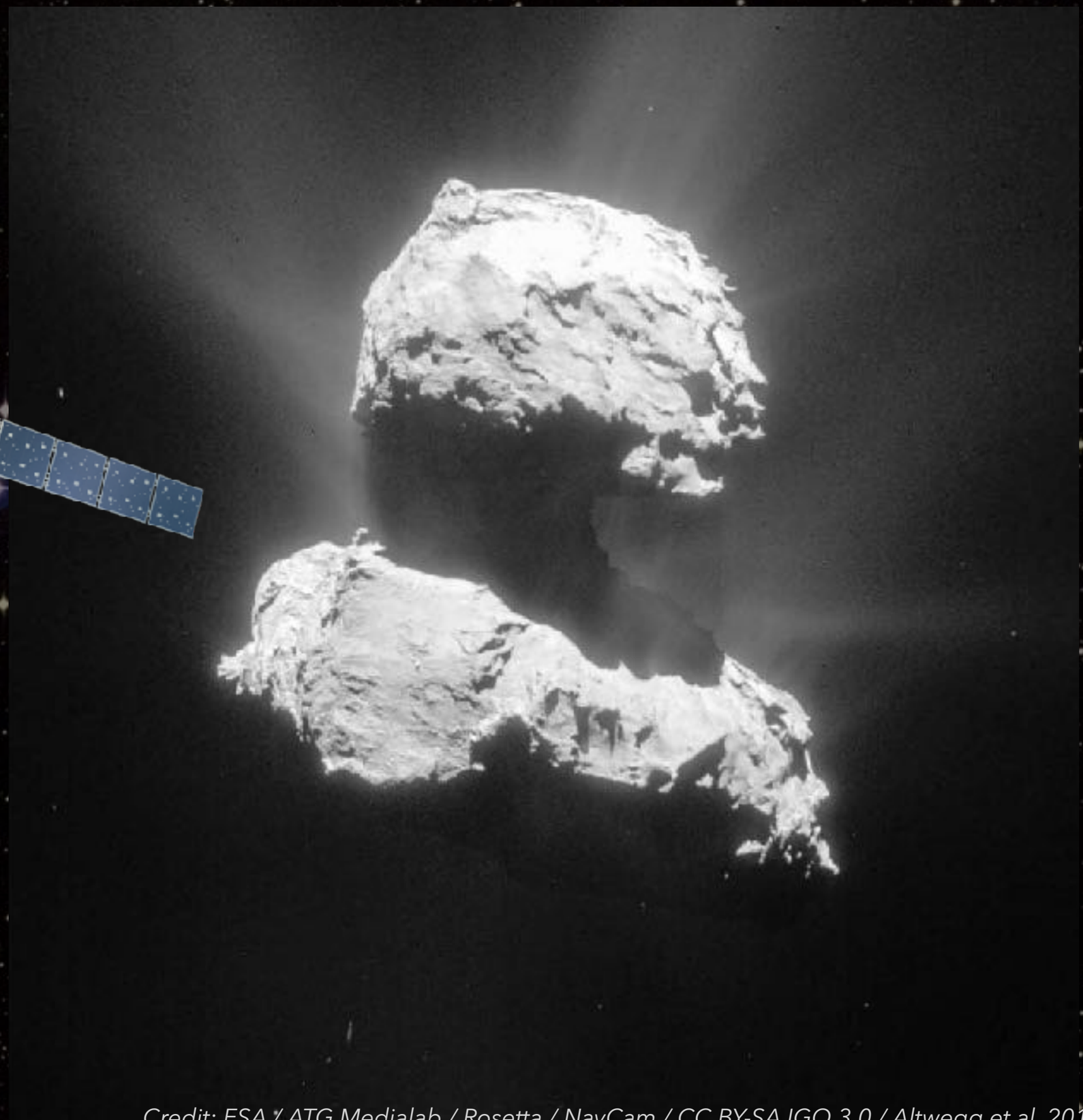
Protoplanetary disks have a history



To what degree does chemical processing modify interstellar material?

Herbst, E. & van Dishoeck, E. F. 2009; Visser, R., et al. 2009, 2011; Drozdovskaya, M. R., et al. 2014, 2016; Jorgensen, J. K., et al. 2016

From clouds to disks to comets



Comets are frozen relics of planet-building material in the Solar System

Credit: ESA / ATG Medialab / Rosetta / NavCam / CC BY-SA IGO 3.0 / Altwegg et al. 2016

Our astrochemical origins

Is chemistry useful?

What can chemistry tell us about physics?

Can I trust chemistry?
Its complicated!

Credit: ESO/T. Preibisch

Our astrochemical origins

2 atoms		3 atoms		4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	≥ 10 atoms
H_2	HD	C_3	AlNC	*c*-C_3H	C5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N
AlF	FeO ?	C_2H	SiNC	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$
AlCl	O_2	C_2O	HCP	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$
C_2	CF^+	C_2S	CCP	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO
CH	SiH ?	CH_2	AlOH	C_3S	*c*-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	HC_9N
CH^+	PO	HCN	H_2O^+	C_2H_2	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3C_6H
CN	AlO	HCO	H_2Cl^+	NH_3	CH_4	CH_3SH	*c*-C_2H_4O	*l*-HC_6H	CH_3CONH_2	C_2H_5OCHO
CO	OH^+	HCO^+	KCN	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO ?	C_8H^-	CH_3OCOCH_3
CO^+	CN^-	HCS^+	FeCN	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6	*c*-C_6H_6
CP	SH^+	HOC^+	O_2H	HNCO	HCOOH	NH_2CHO		H_2NCH_2CN	CH_3CH_2SH	*n*-C_3H_7CN
SiC	SH	H_2O	TiO_2	HNCS	H_2CNH	C_5N		CH_3CHNH		*i*-C_3H_7CN
HCl	HCl^+	H_2S	C_2N	$HOCO^+$	H_2C_2O	*l*-HC_4H				C_{60}
KCl	TiO	HNC	Si_2C	H_2CO	H_2NCN	*l*-HC_4N				C_{70}
NH	ArH^+	HNO		H_2CN	HNC_3	*c*-H_2C_3O				
NO	NO^+ ?	MgCN		H_2CS	SiH_4	H_2CCNH ?				
NS		MgNC		H_3O^+	H_2COH^+	C_5N^-				
NaCl		N_2H^+		*c*-SiC_3	C_4H^-	HNCHCN				
OH		N_2O		CH_3	HCOCN					
PN		NaCN		C_3N^-	HNCNH					
SO		OCS		PH_3	CH_3O					
SO^+		SO_2		HCNO	NH_4^+					
SiN		*c*-SiC_2		HSCN	H_2NCO^+ ?					
SiO		CO_2		H_2O_2	$HCCNH^+$					
SiS		NH_2		C_3H^+						
CS		H_3^+		HMgNC						
HF		SiCN		HCCO						

Protoplanetary disk molecules/volatiles?

25* and counting …

* not including isotopologues

Adapted from the Cologne Database for Molecular Spectroscopy: http://www.astro.uni-koeln.de/cdms

Our astrochemical origins

Quantity	Example Tracers
Mass	$^{x}C^{y}O$, HD
Temperature	$^{x}C^{y}O$, CH_3CN
Density	CS, H_2CO, HC_3N
Kinematics	$^{x}C^{y}O$, HCO^+
Photodissociation	CN, HCN, C_2H
Ionisation	HCO^+, N_2H^+, CH^+
Deuteration	DCO^+, N_2D^+, DCN
Turbulence	$^{x}C^{y}O$, CS, HC_3N
C/N/O fractionation	$^{x}C^{y}O$, $^{x}C^{z}N$, $H^{x}C^{z}N$
Snow lines	$^{x}C^{y}O$, N_2H^+, DCO^+, HCO^+
Grain-surface processes	Complex molecules

x = 12,13; y = 16,17,18; z = 14,15

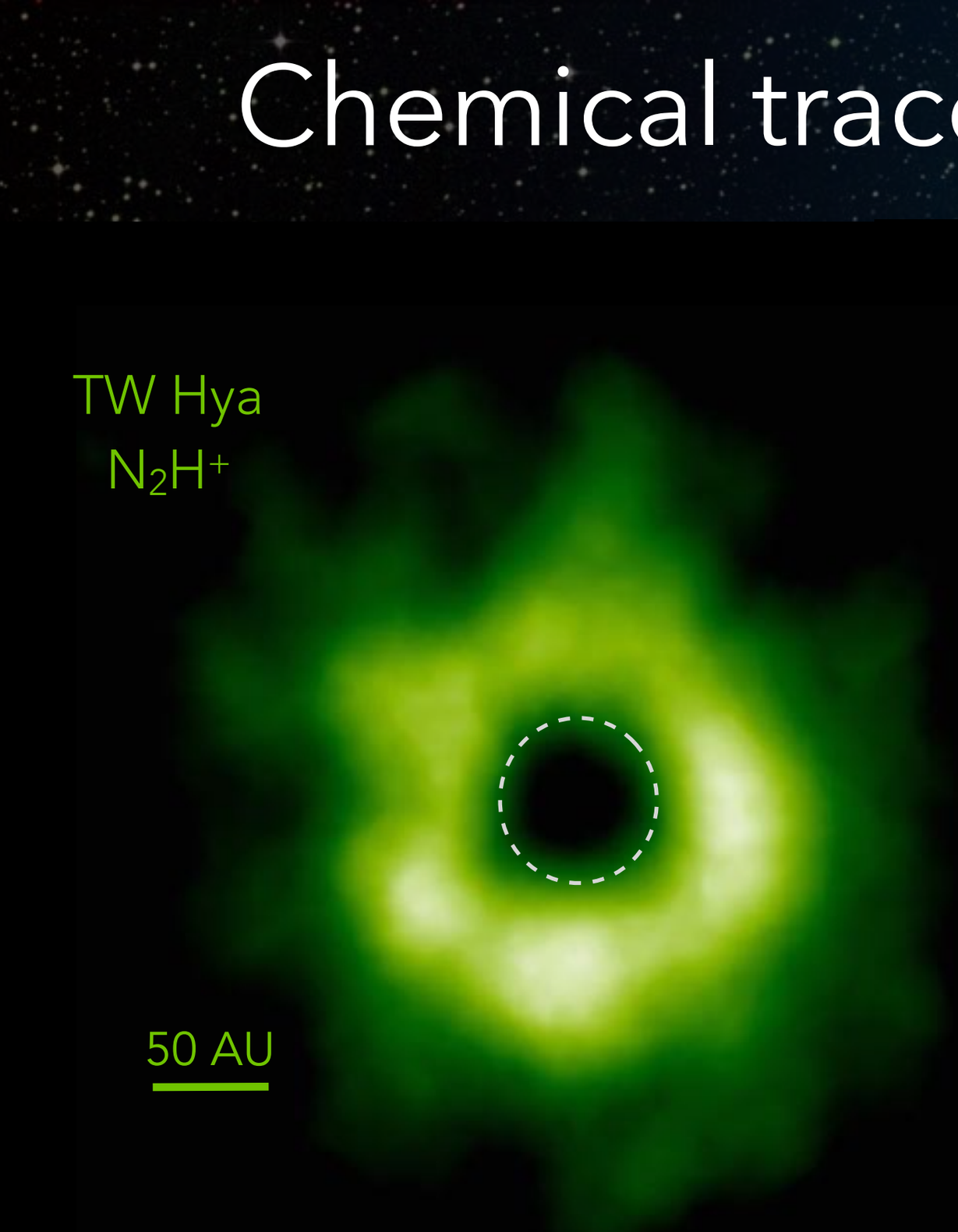
Adapted from Henning & Semenov 2013, Chem. Rev., 113, 9016

What has ALMA revealed about disk composition and chemistry?

Chemical tracers of snowlines

TW Hya

N_2H^+



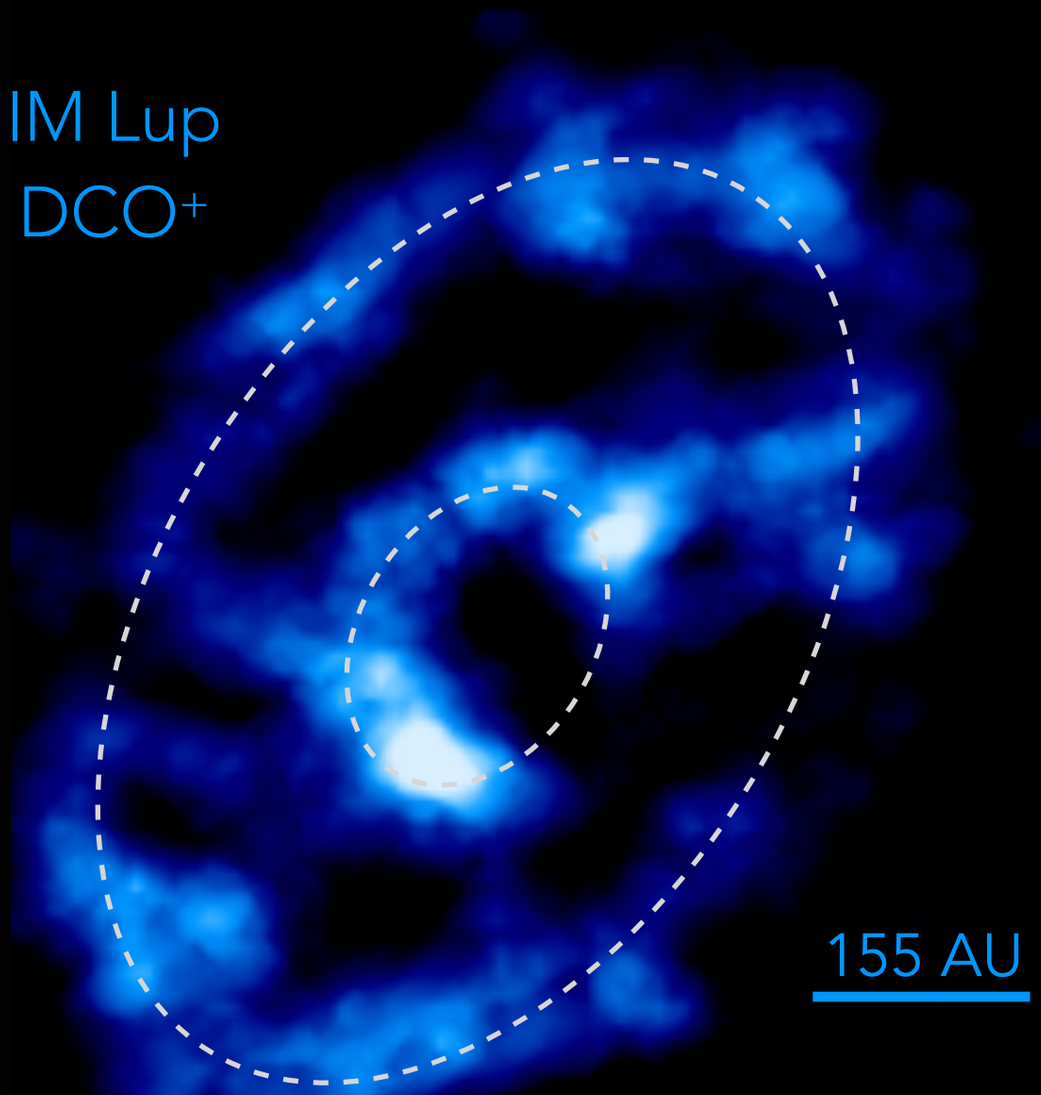
50 AU

$N_2 + H_3^+ \rightarrow N_2H^+ + H_2$

$CO + N_2H^+ \rightarrow HCO^+ + N_2$

IM Lup

DCO^+



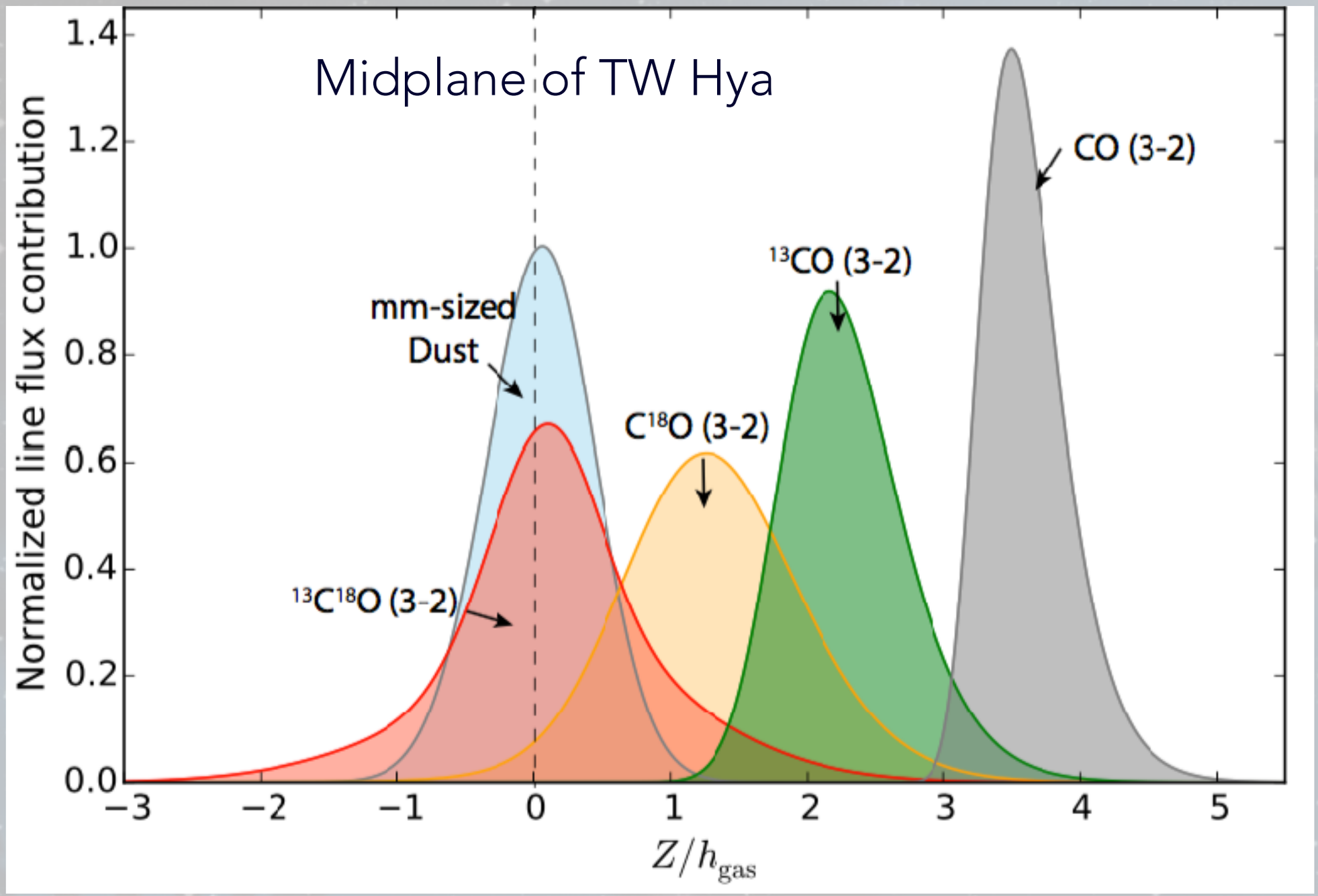
155 AU

$HD + H_3^+ \rightarrow H_2D^+ + H_2$

$CO + H_2D^+ \rightarrow DCO^+ + H_2$

Qi, C., et al. 2013; Öberg, K. I., et al. 2015; van 't Hoff et al. 2017

Chemical tracers of snowlines

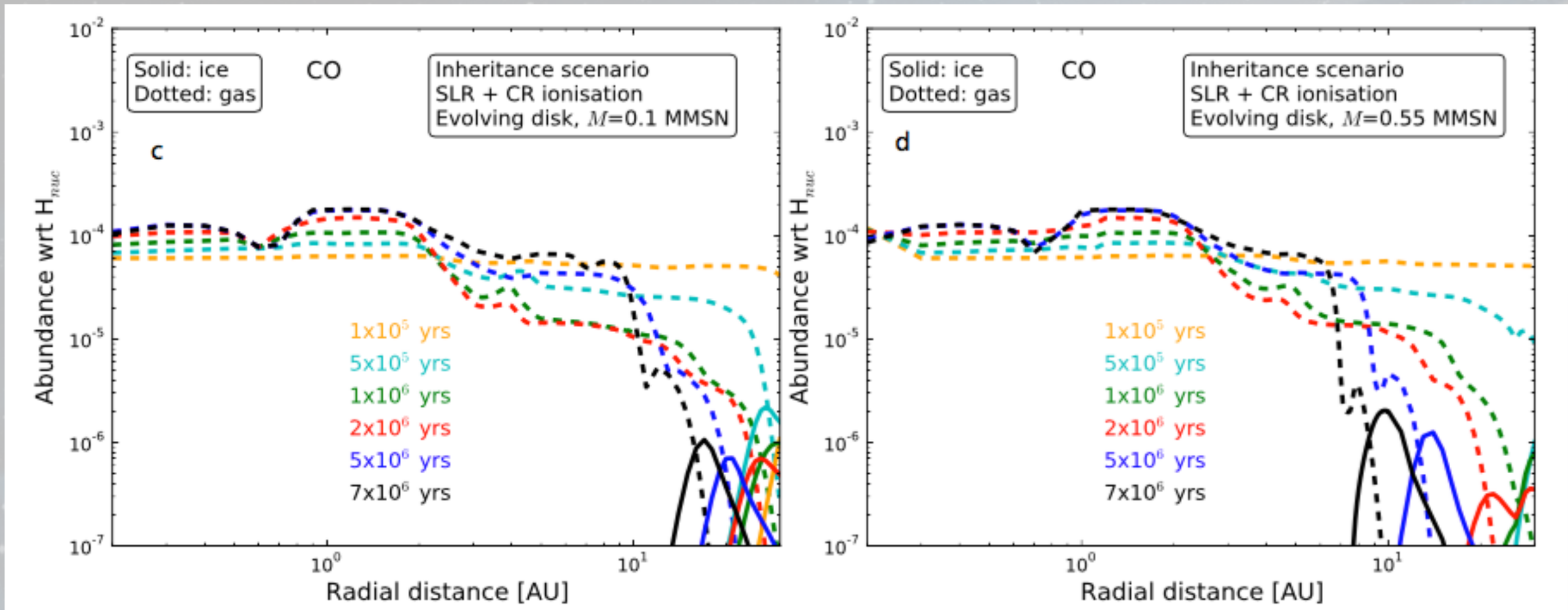


R_{snow} = 20.5 ± 1.3 au; T_{snow} = 27 ± 3 K; $CO/H_2 \sim 10^{-6}$

Schwarz, K., et al. 2016; Zhang, Ke, et al. 2017

Chemical tracers of snowlines

Chemical models of disk midplanes with gas and ice chemistry predict a chemical conversion of CO into a less volatile form: CO_2, C_xH_y, COMs



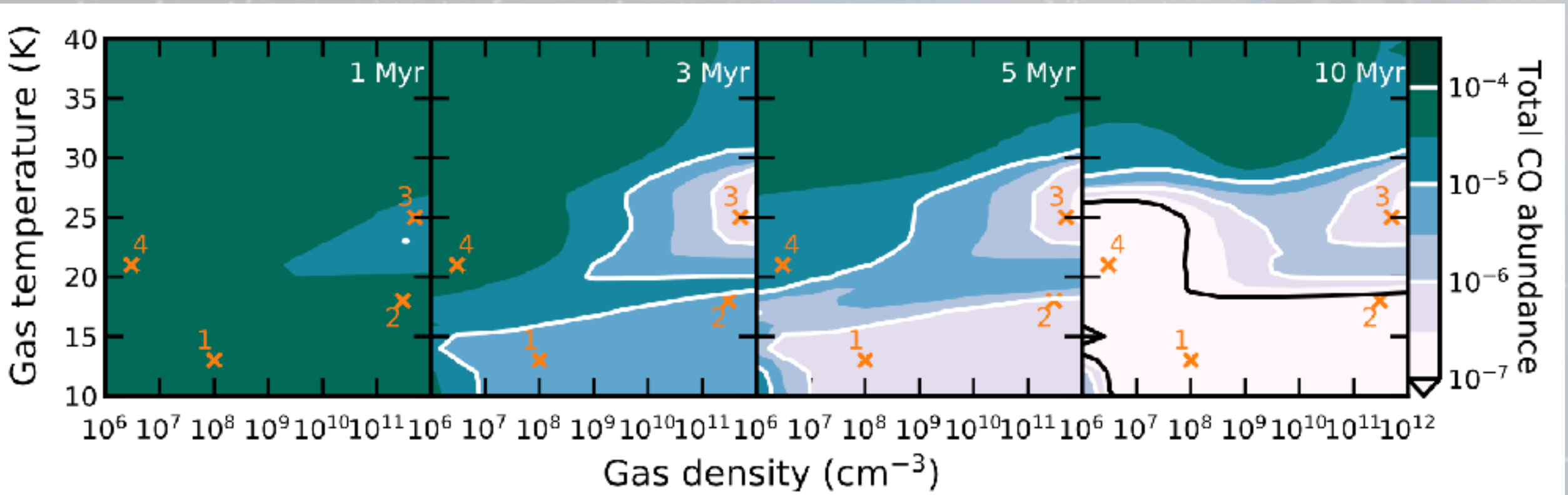
Results in a "fake" CO snowline which evolves in time

The gas-phase CO in the outer disk is also depleted over time

Aikawa, Y., et al. 1997; Helling, C., et al. 2014; Reboussin, L., et al. 2015; Eistrup, C., et al. 2016, 2018; Yu, M., et al. 2016, 2017

What is happening to the CO?

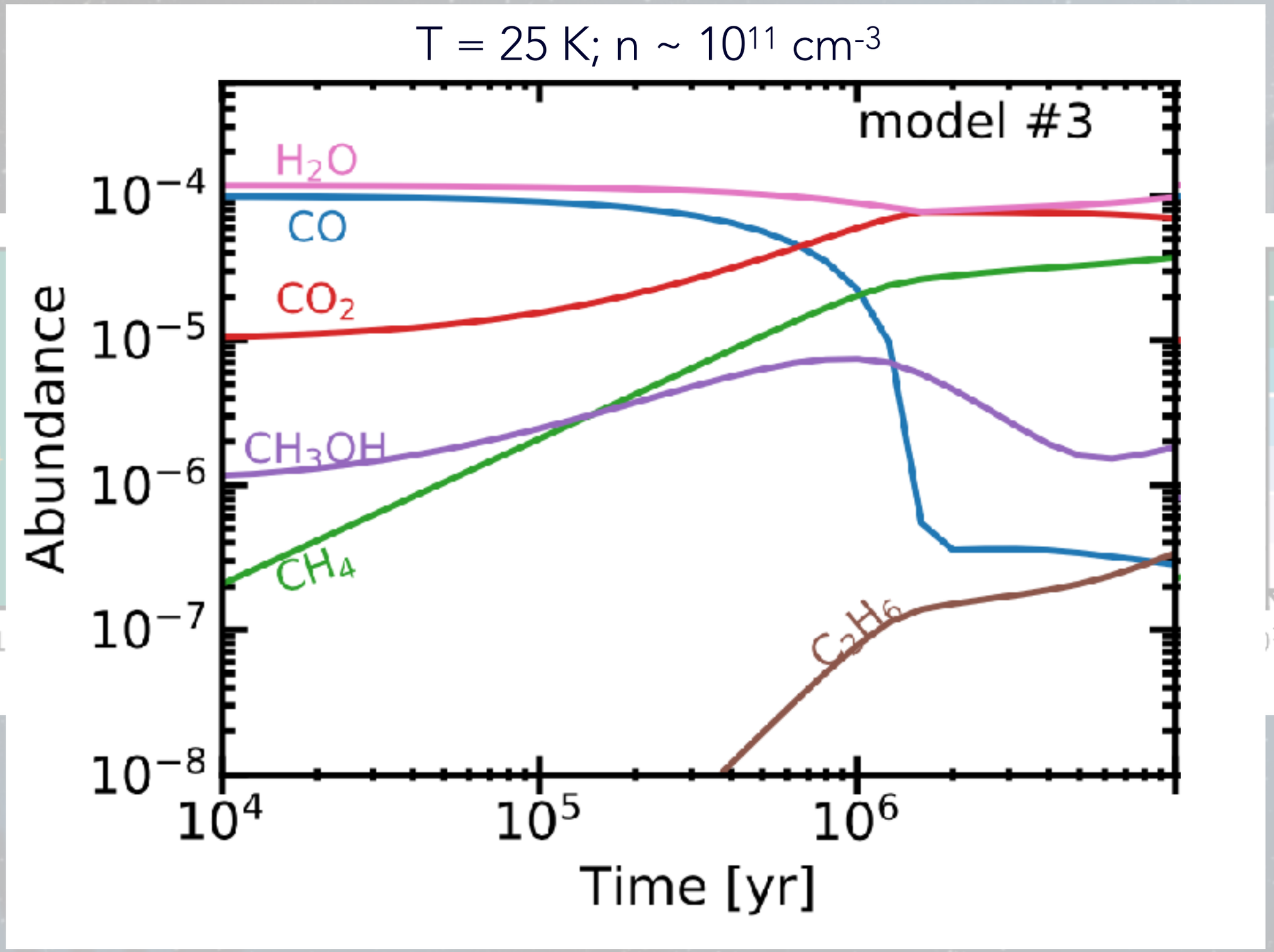
What does a systematic exploration using single-point chemical models tell us?



If the gas and dust are moderately warm, CO is chemically converted to other species on ~ 1 Myr timescales

Bosman et al. 2018; Schwarz et al. 2018

What is happening to the CO?

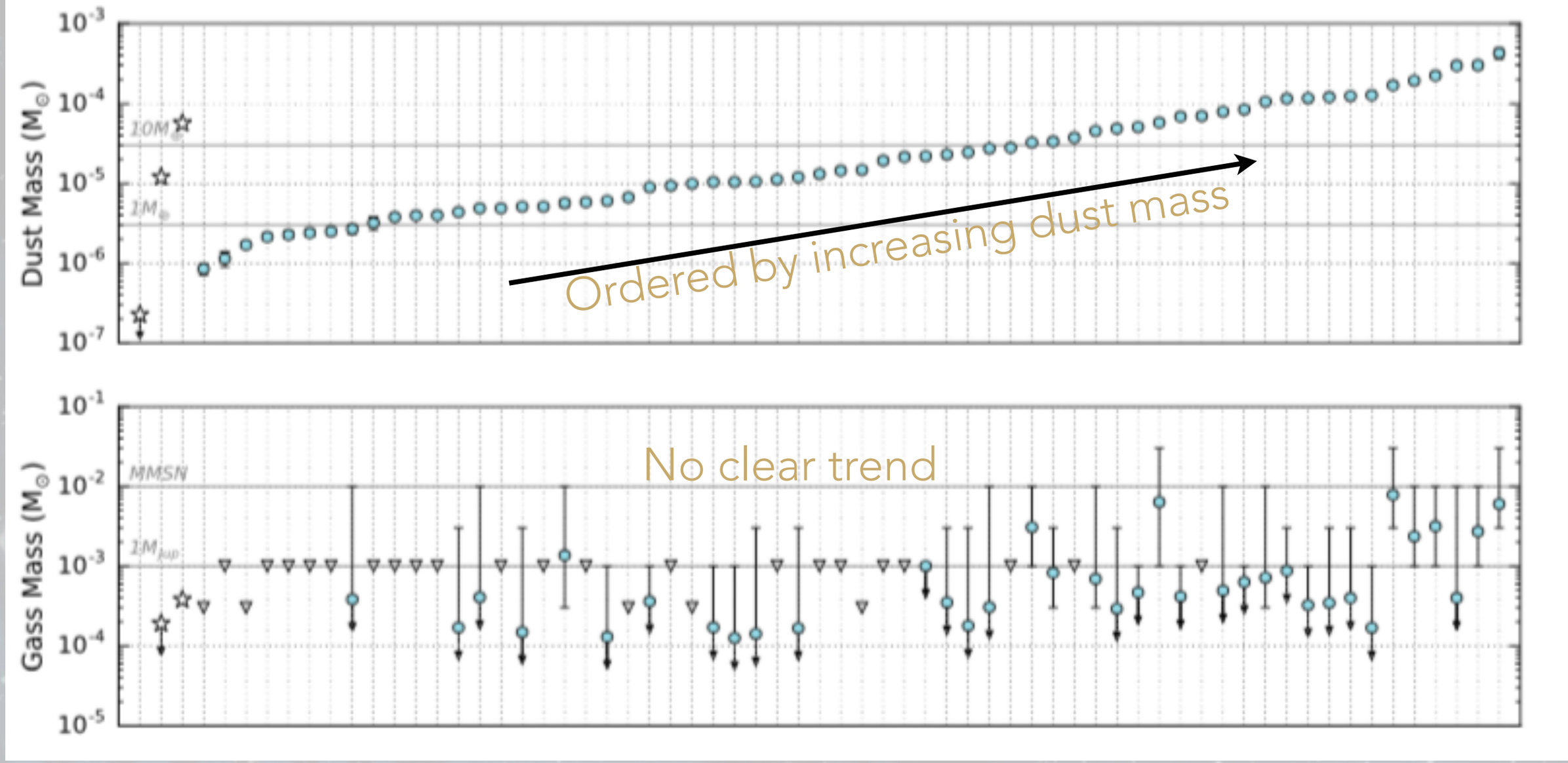


Bosman et al. 2018; Schwarz et al. 2018

CO as a tracer of gas mass?

ALMA survey of Lupus star-forming region

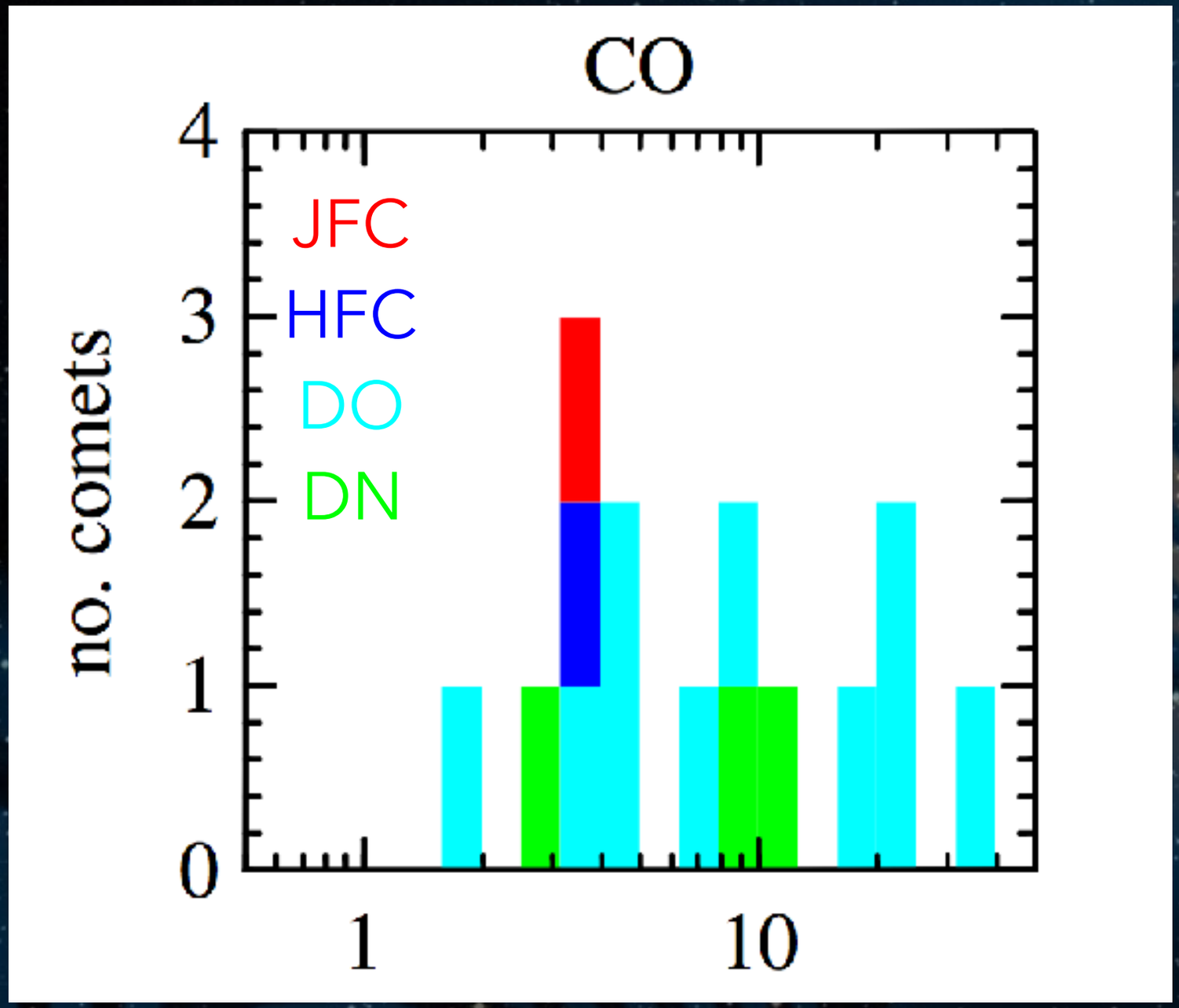
Low gas-to-dust mass ratios? Or low CO/H_2 abundance ratios?



Low disk gas masses also inferred for Chameleon I and Upper Sco

Ansdell, M., et al. 2016; Barenfeld, S. A., et al. 2017; Long, F., et al. 2017; Miotello, A., et al. 2017

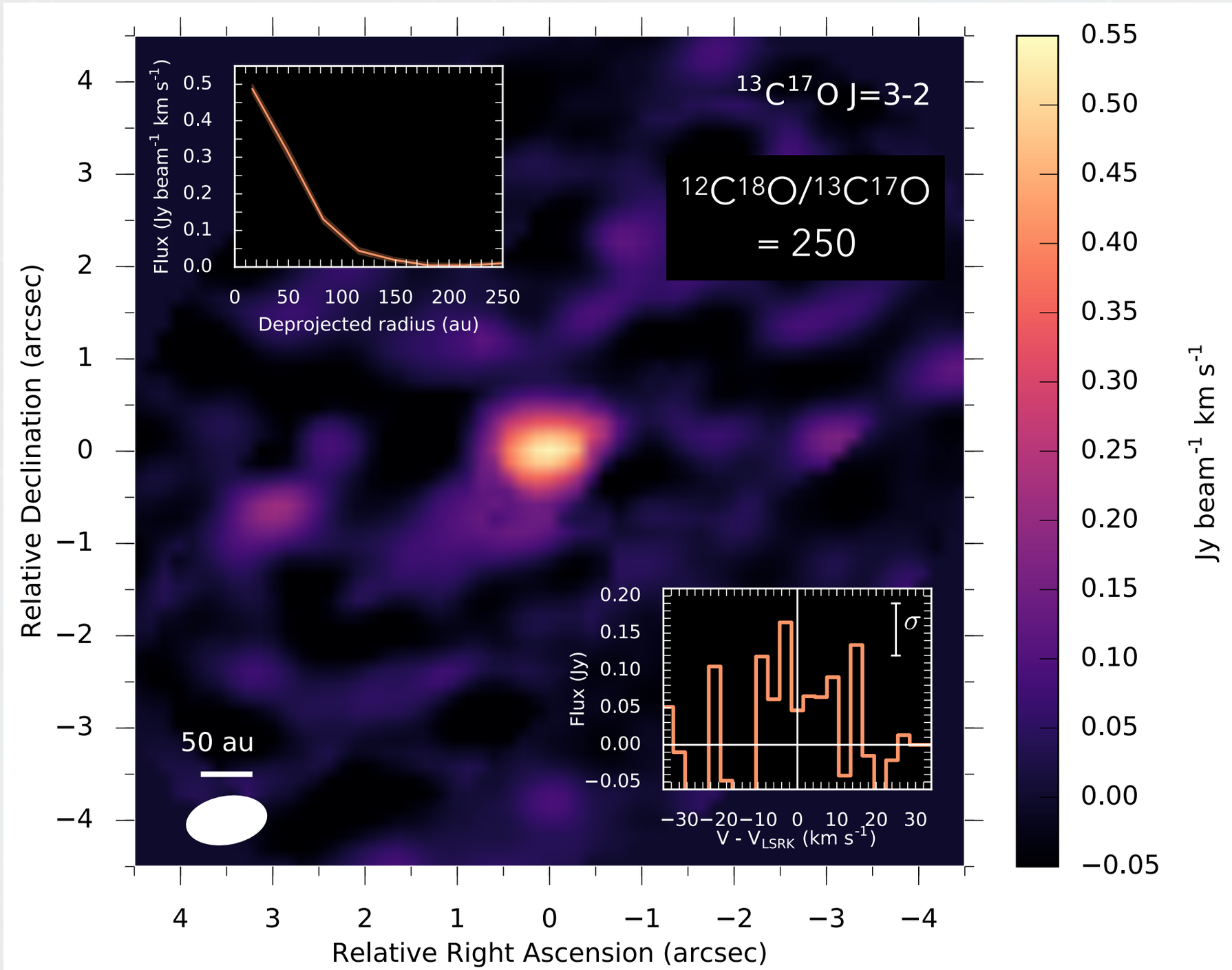
How does this compare with comets?



% abundance relative to H_2O
Based on radio observations

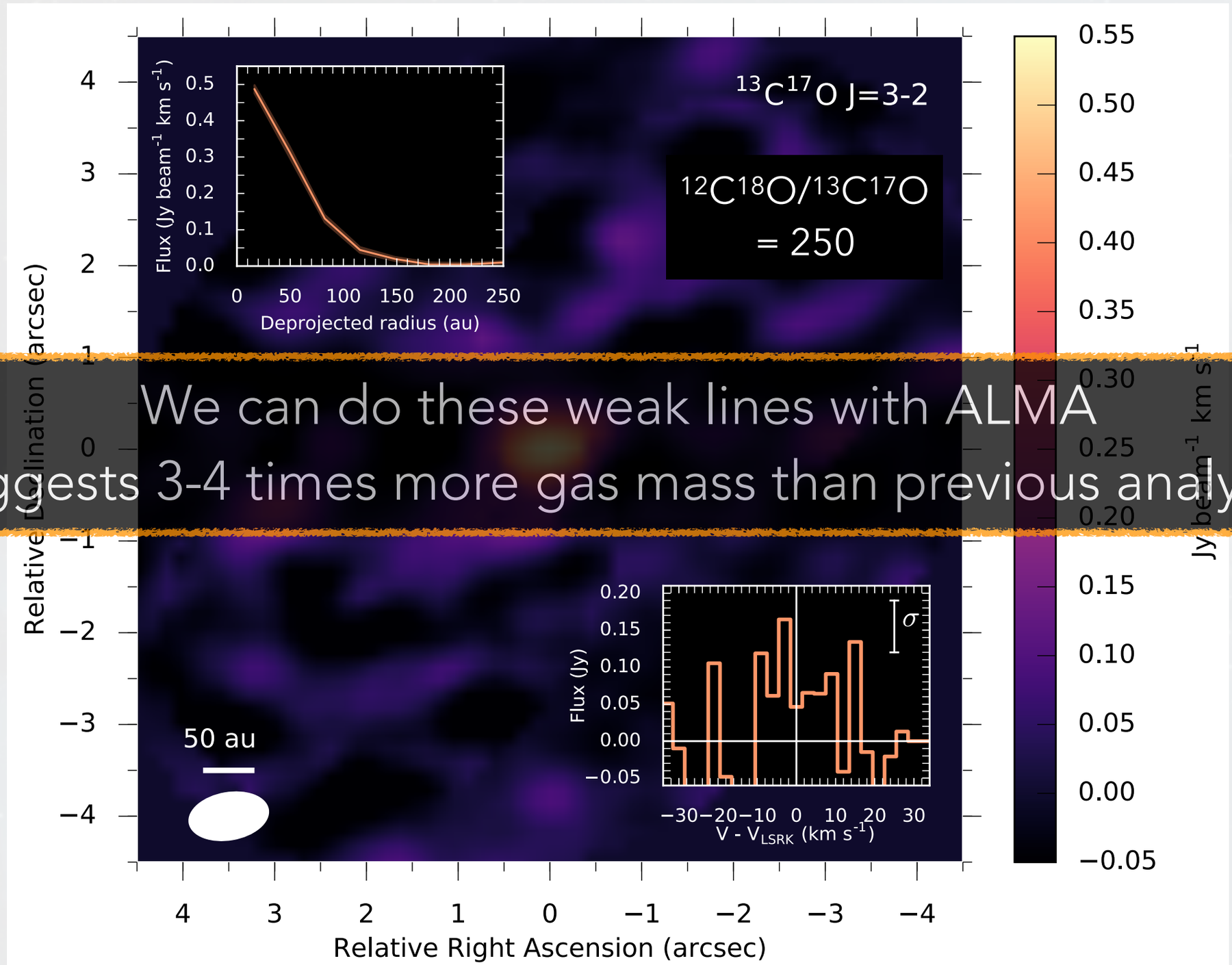
Bockelee-Morvan & Biver 2017

First detection of $^{13}C^{17}O$



Booth, A., Walsh, C., et al. 2019, in prep

First detection of $^{13}C^{17}O$



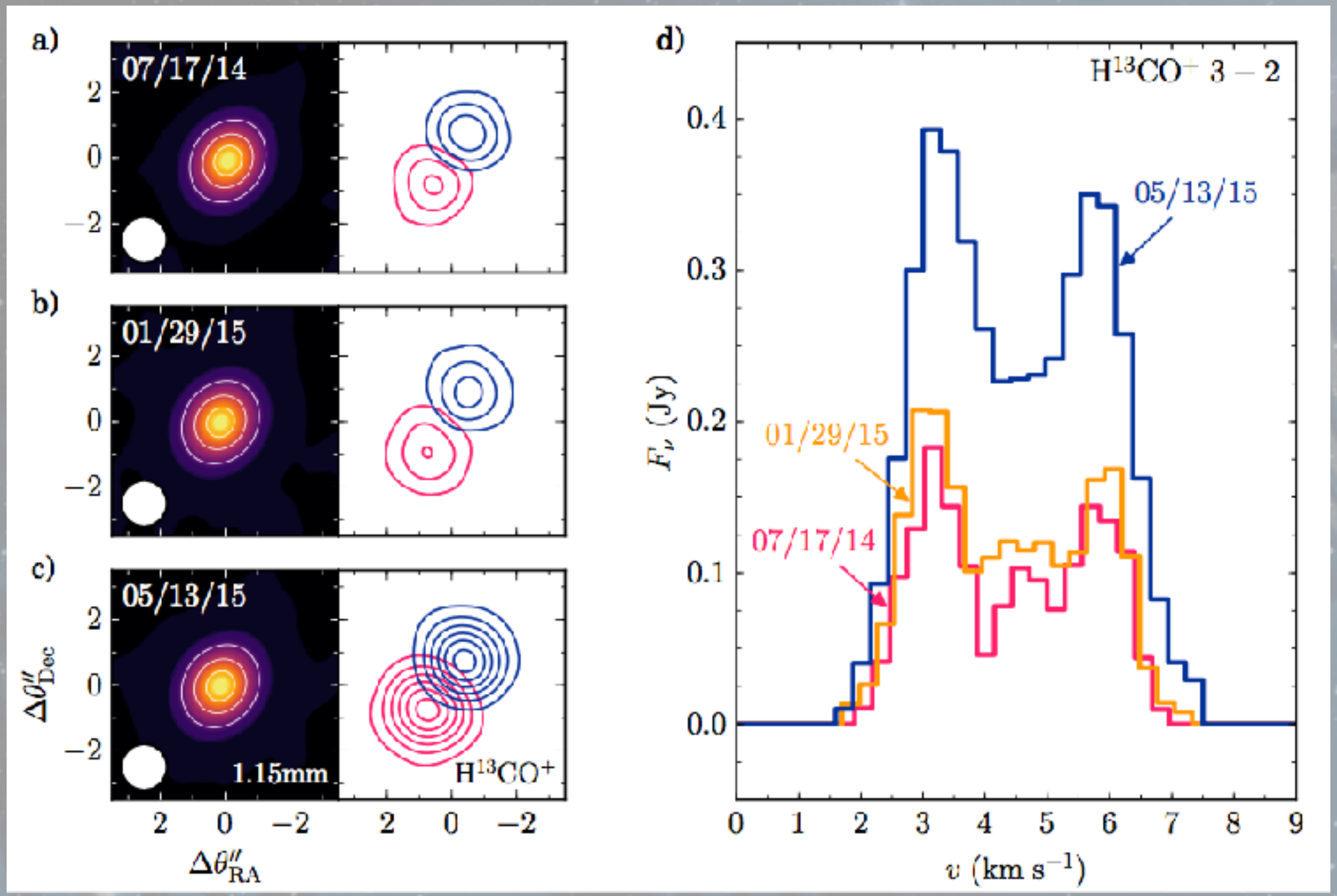
We can do these weak lines with ALMA

Suggests 3-4 times more gas mass than previous analyses

Booth, A., Walsh, C., et al. 2019, in prep

HCO^+ tracing real-time ionisation

Multi-epoch observations of $H^{13}CO^+$ in IM Lup

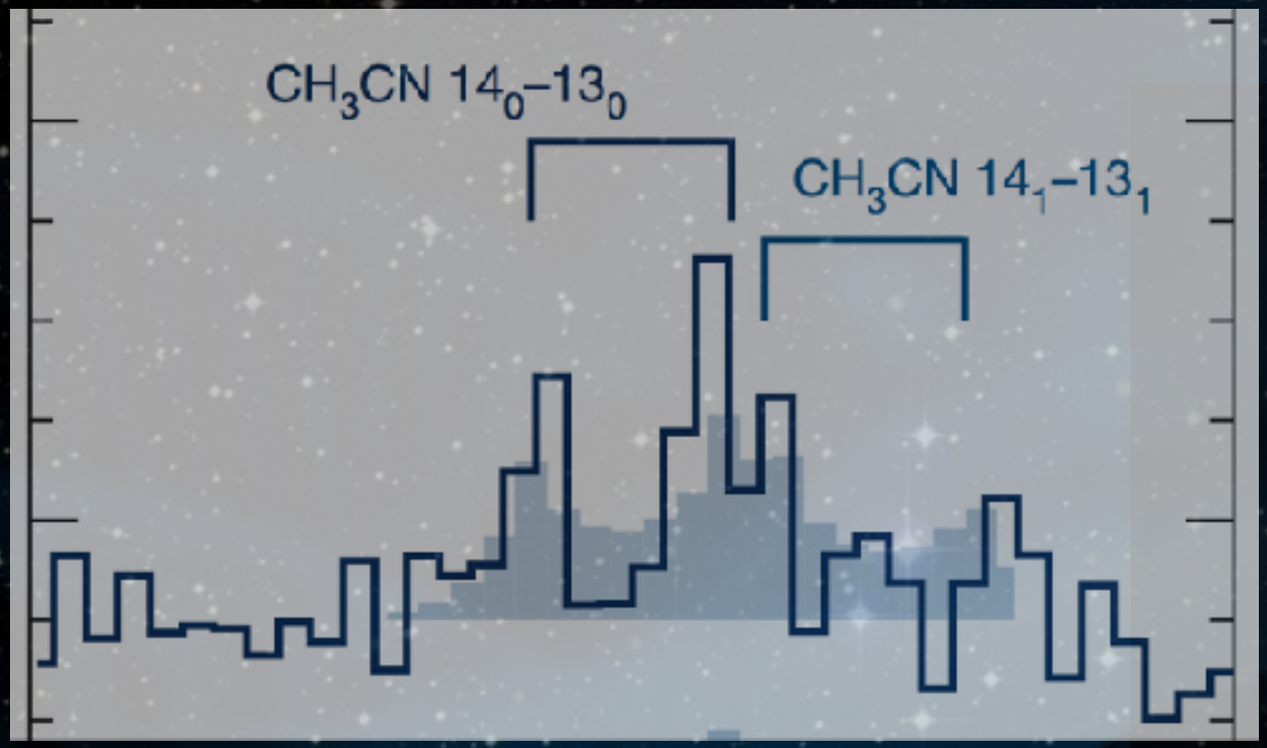


Confirmation of real-time stellar variability in ionisation in the disk atmosphere

Cleeves, L. I., et al. 2017, ApJL, 843, L3

What is ALMA revealing about the chemical complexity of protoplanetary disks?

Searching for complex molecules



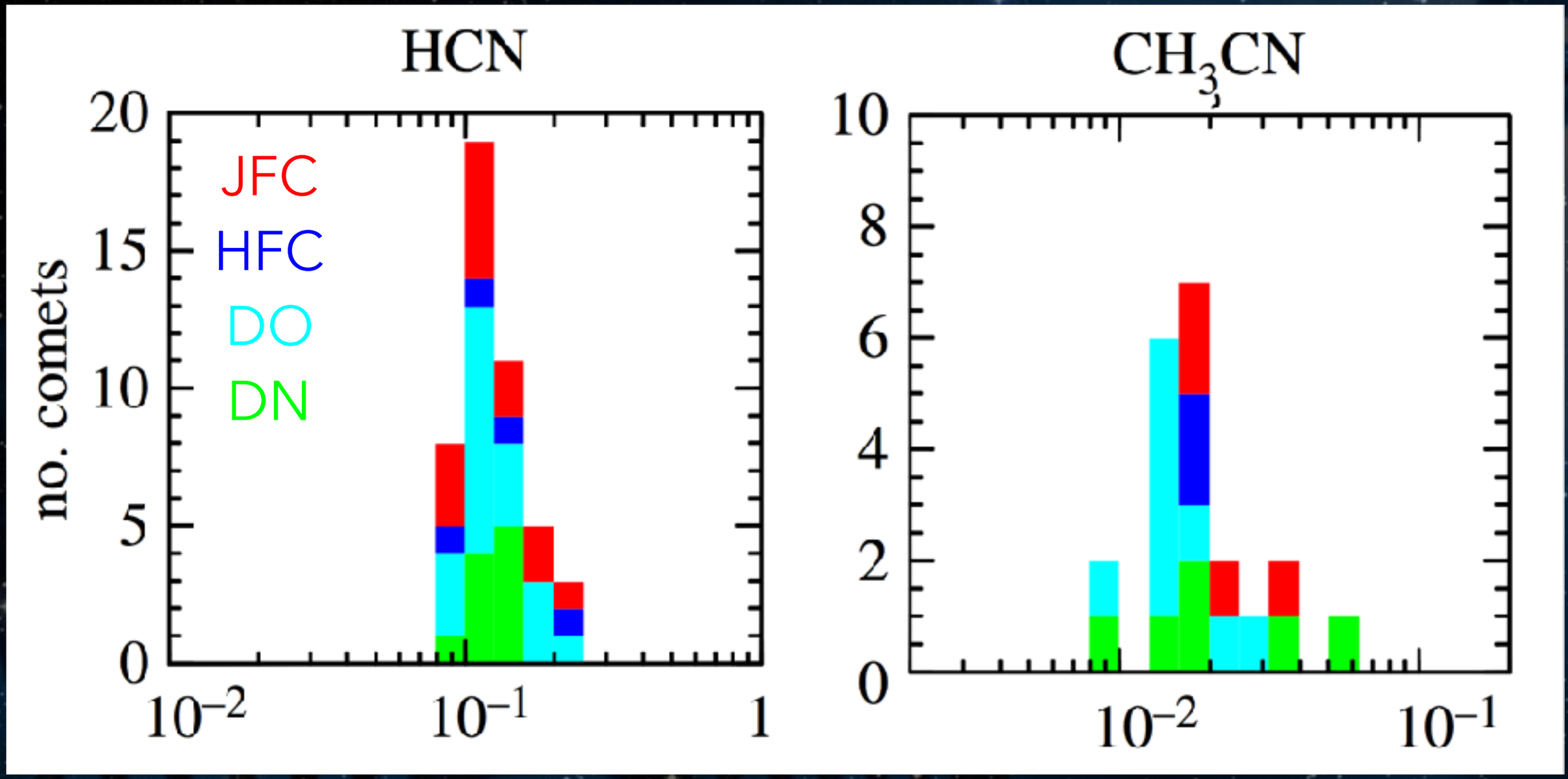
Cyanides (-CN) play a role in the synthesis of amino acids

CH_3CN/HCN
~ 5 - 20%

MWC 480
T_{eff} ~ 8000 K

Credit: B. Saxton (NRAO/AUI/NSF)
Öberg et al. 2015, Nature, 520, 198; Loomis et al. 2018, ApJ, 859, 131

How does this compare with comets?



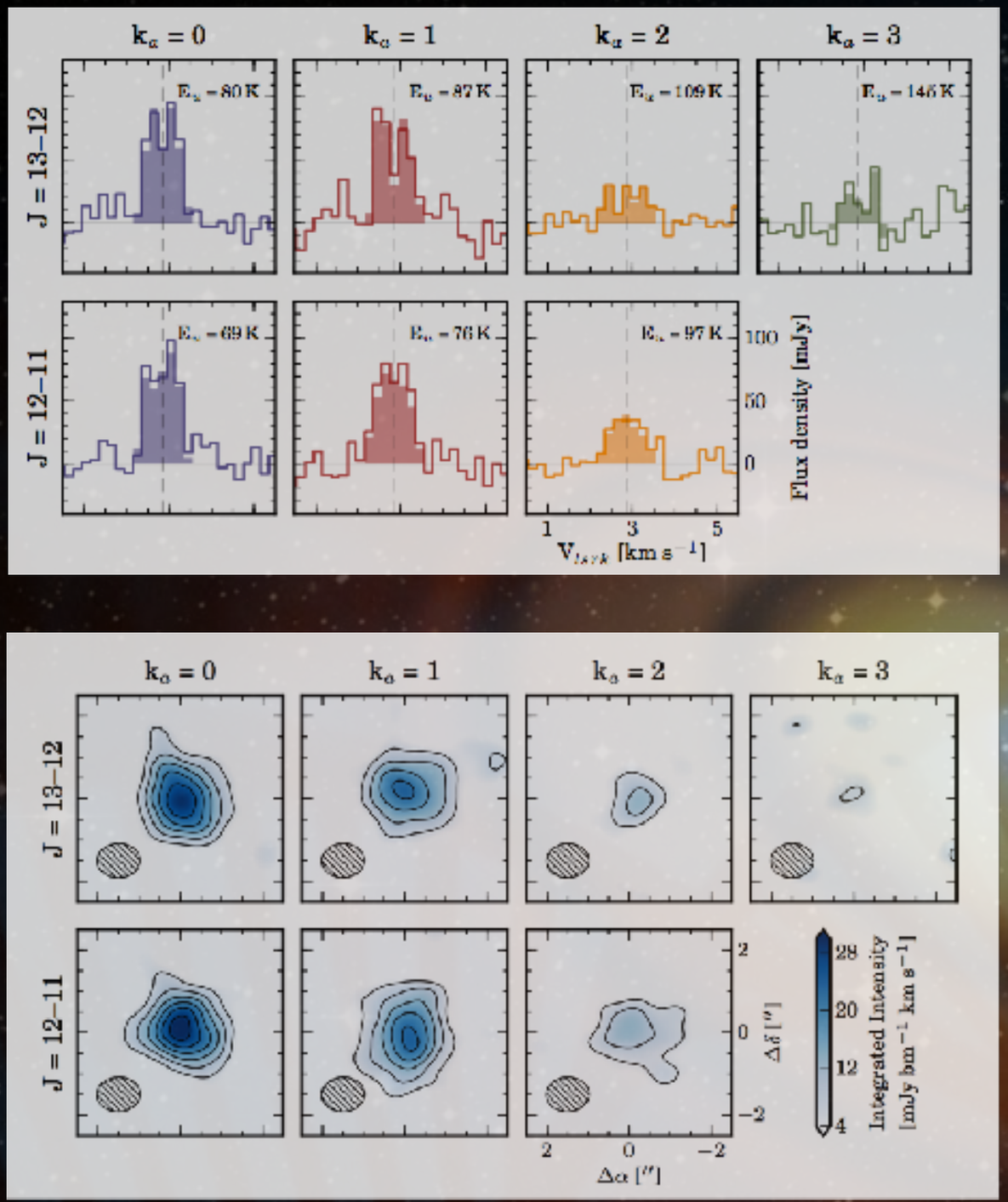
% abundance relative to H_2O
Based on radio observations

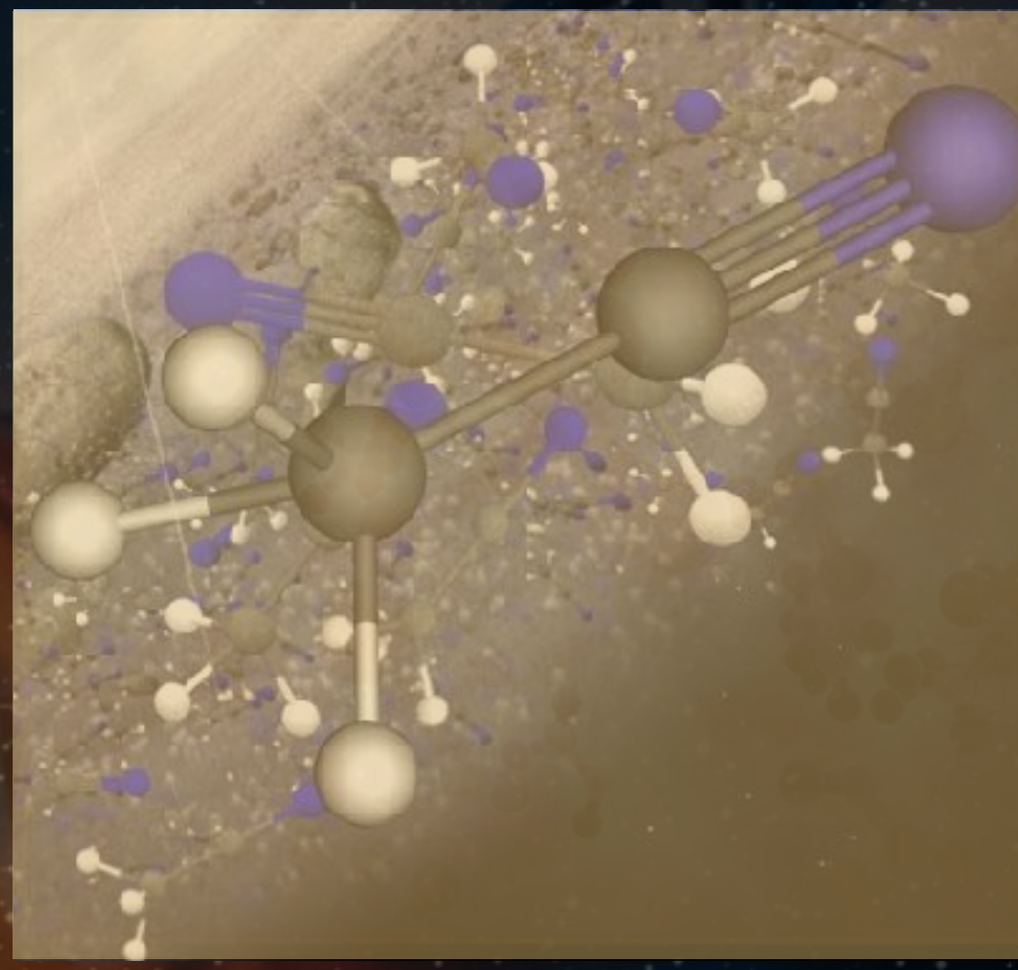
Bockelee-Morvan & Biver 2017

Searching for complex molecules

TW Hya

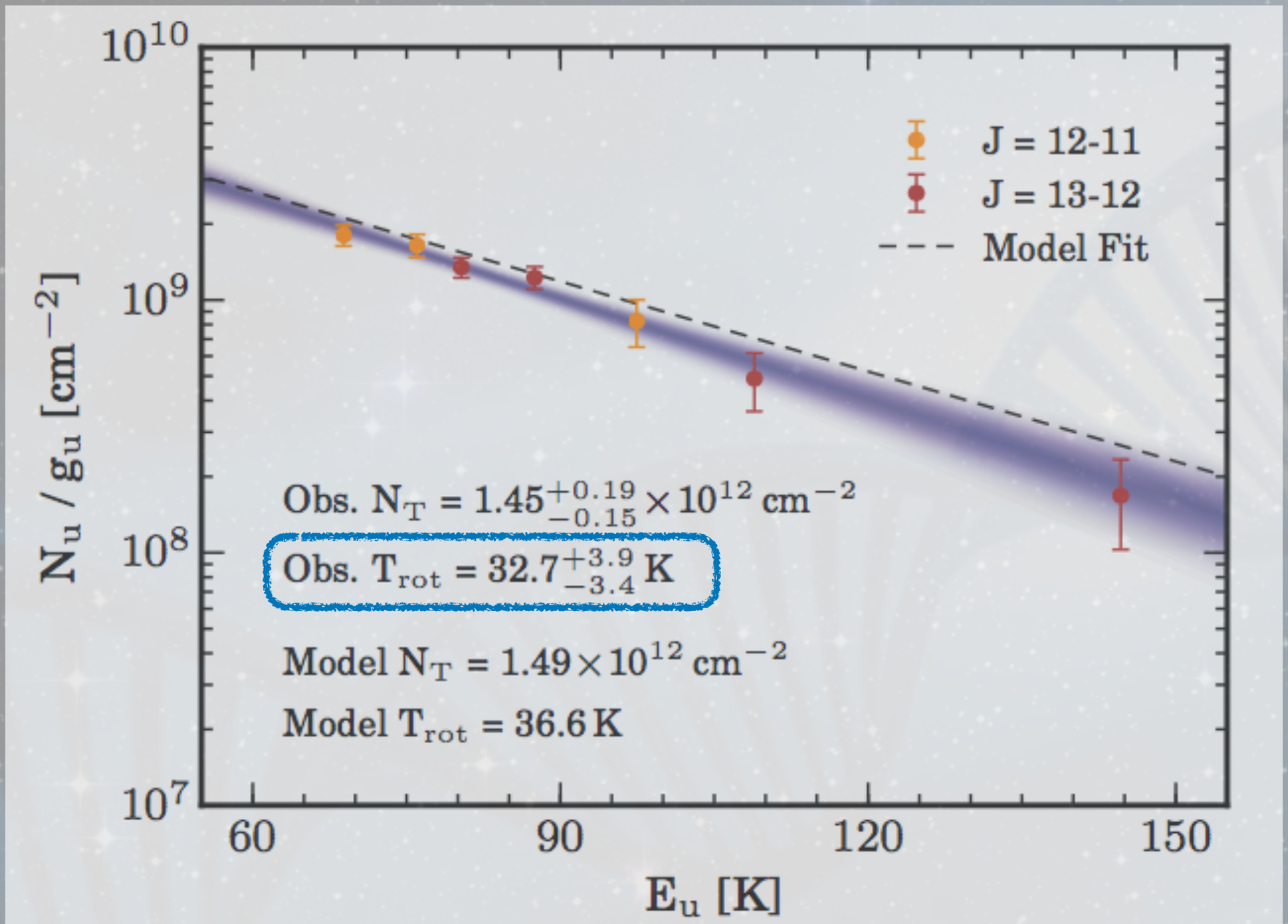
T_{eff} ~ 4000 K





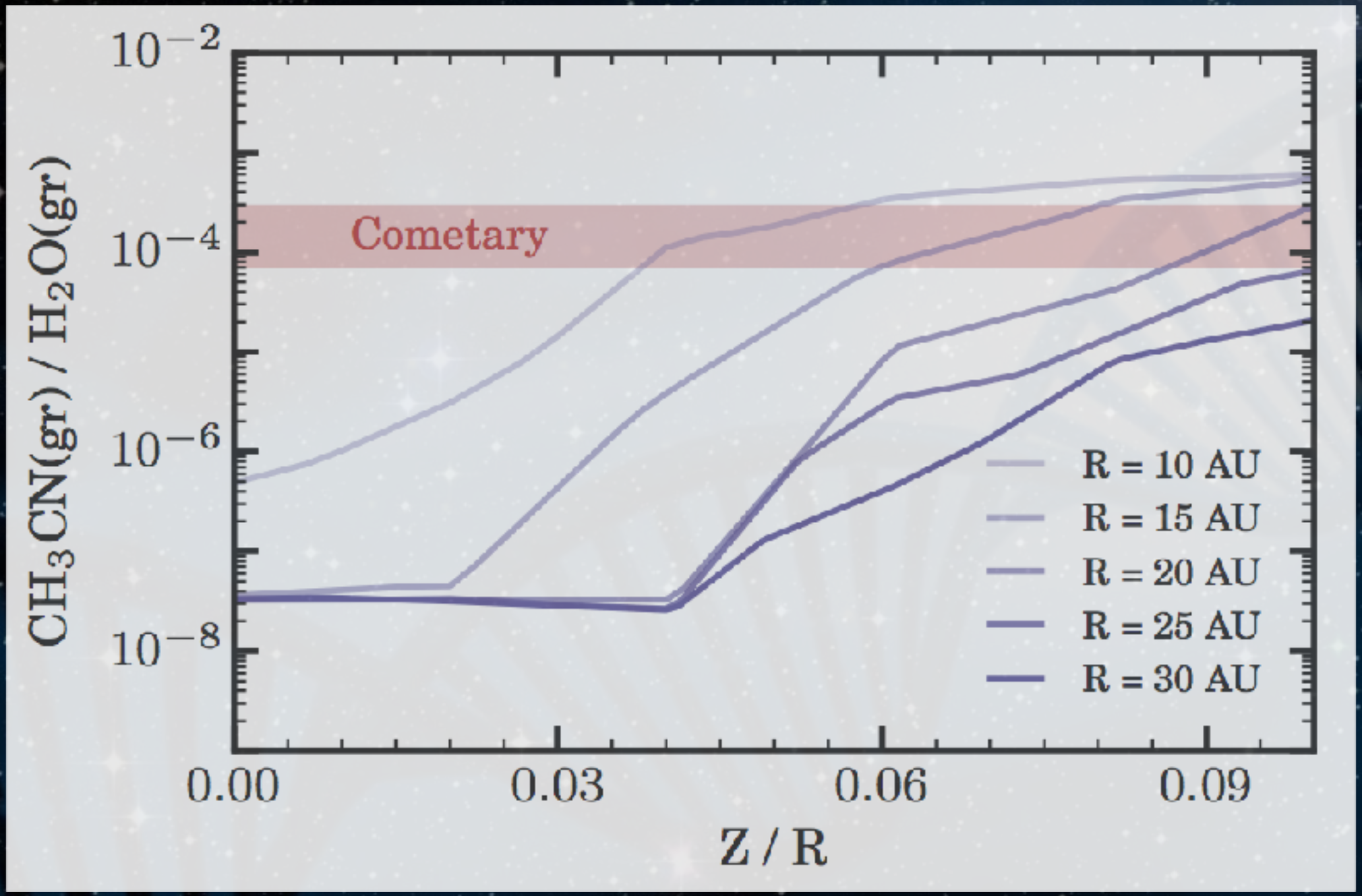
Credit: ESO/M. Kornmesser; Loomis, R.. et al. 2018, ApJ, 859, 131

CH_3CN in TW Hya



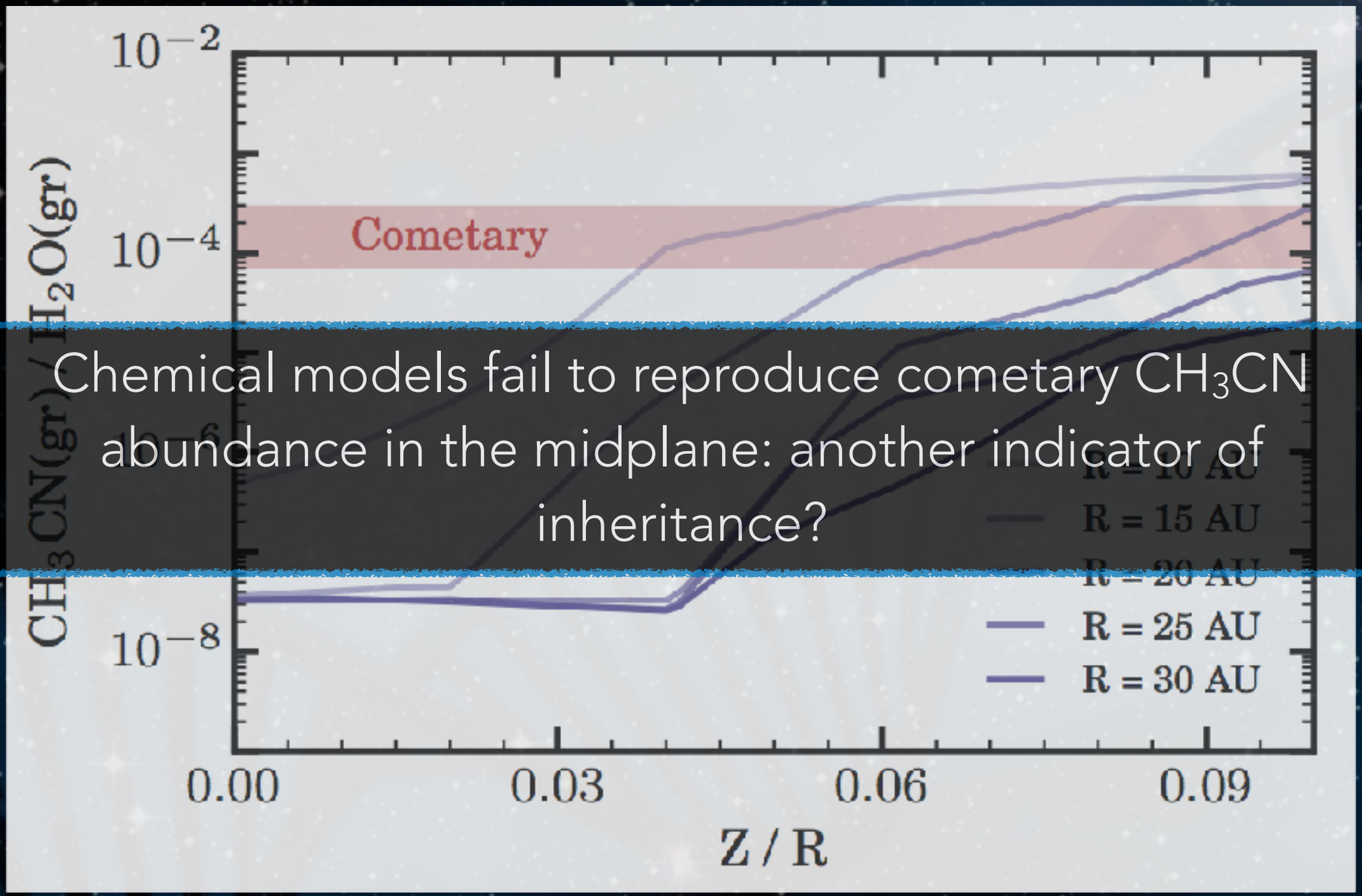
Loomis, R., et al. 2018, ApJ, 859, 131

CH_3CN in TW Hya



Loomis, R. et al. 2018, ApJ, 859, 131

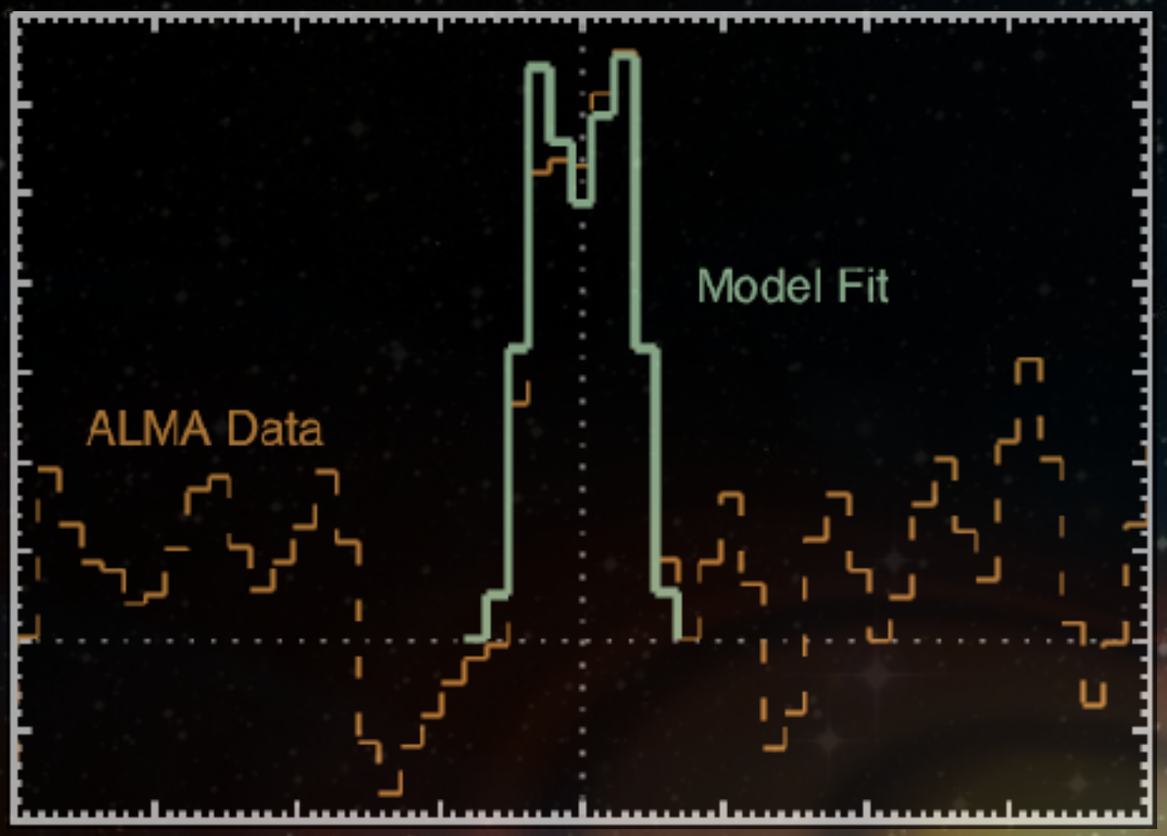
CH_3CN in TW Hya



Chemical models fail to reproduce cometary CH_3CN abundance in the midplane: another indicator of inheritance?

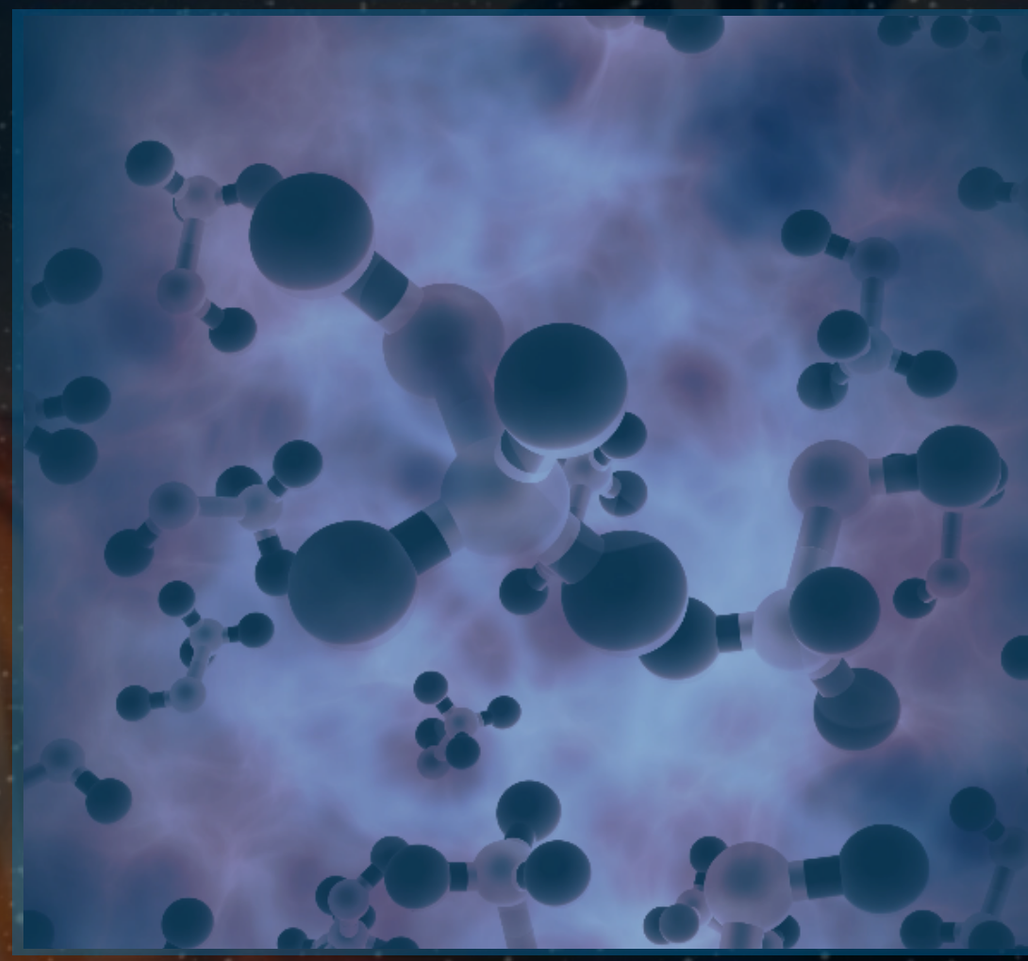
Loomis, R. et al. 2018, ApJ, 859, 131

Searching for complex molecules



TW Hya

T_{eff} ~ 4000 K



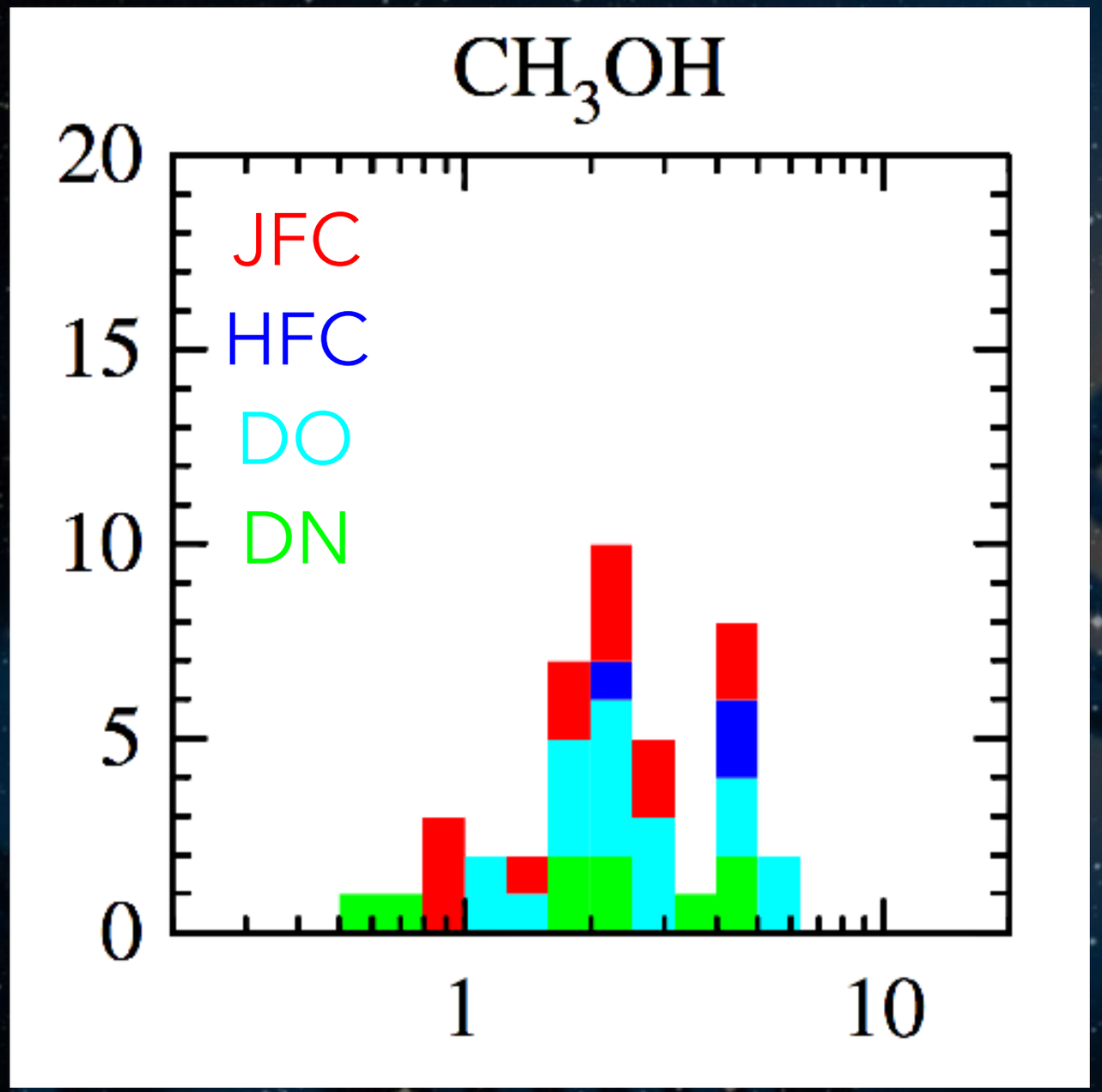
Methanol is an interstellar ice molecule and a feedstock for more complex molecules

CH_3OH/H_2O

~ 1 - 5%

Credit: ESO/M. Kornmesser; Walsh, C. et al. 2016, ApJL, 823, L10

How does this compare with comets?

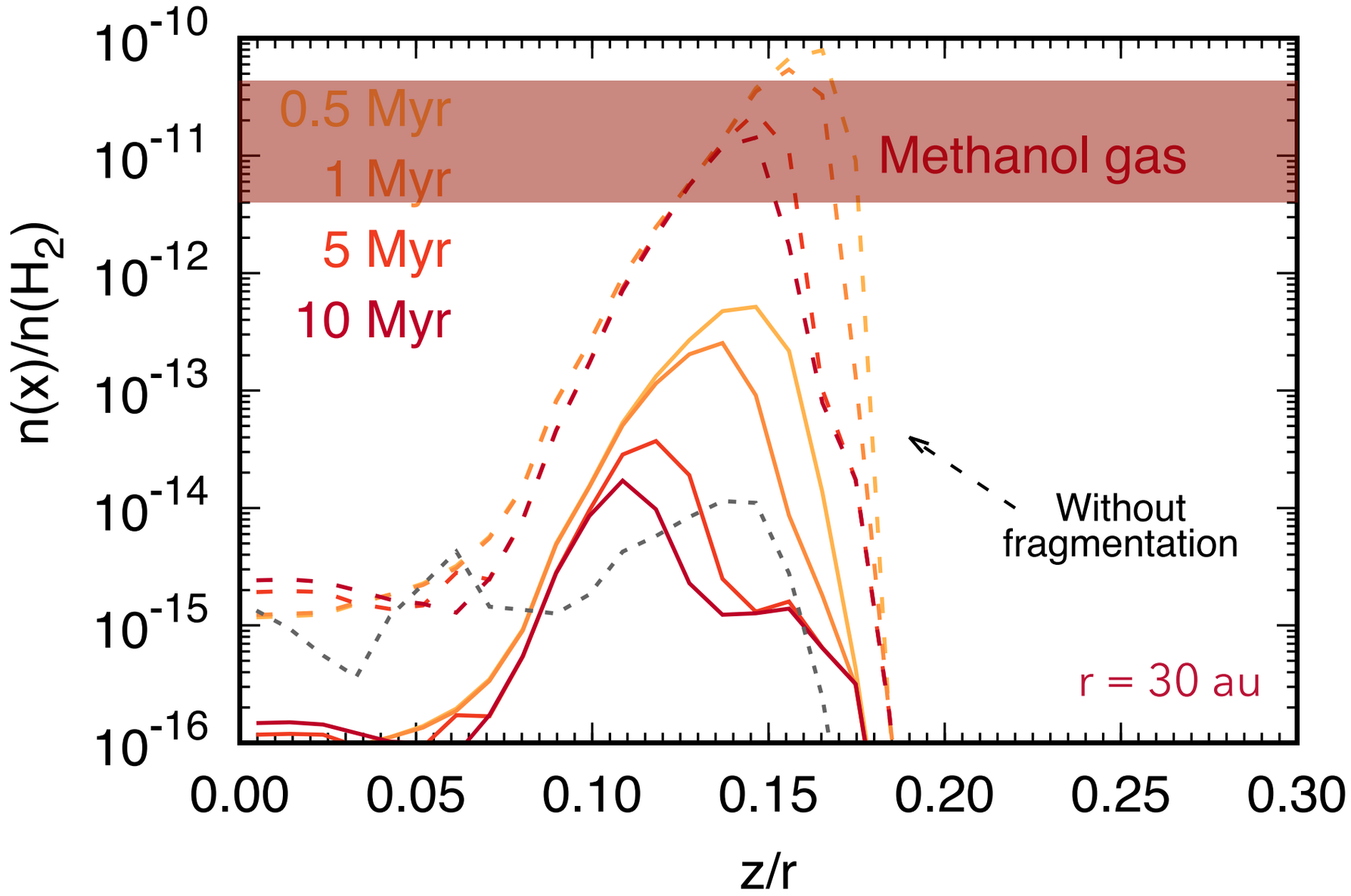


% abundance relative to H_2O
Based on radio observations

Bockelee-Morvan & Biver 2017

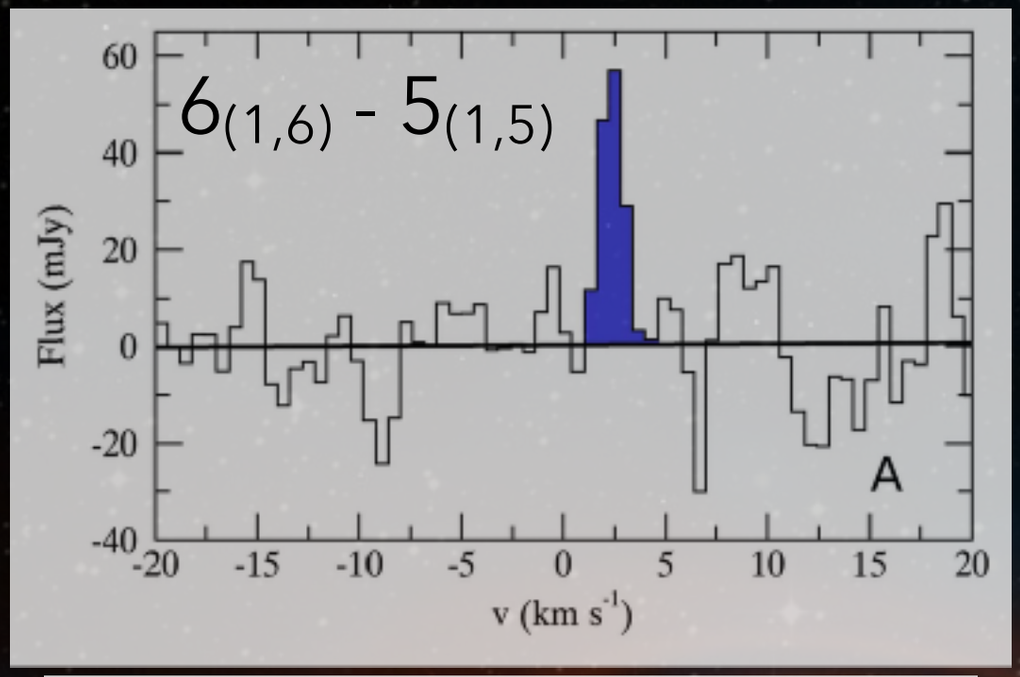
CH_3OH in TW Hya

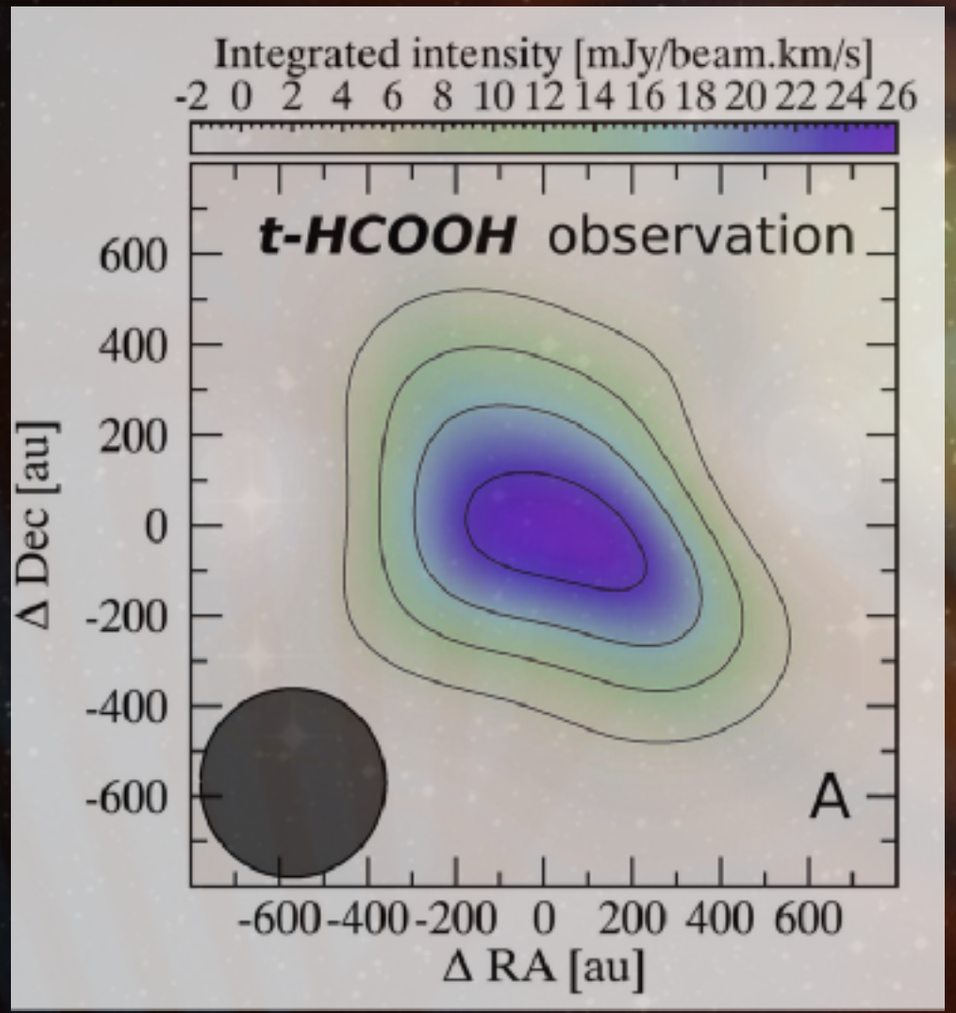
Problem: CH_3OH ice fragments when photodesorbing



Bertin, M., et al. 2016, ApJL, 817, L12; Cruz Diaz, G., et al. 2016, A&A,592, A68; Ligterink, N., et al. 2018, A&A, 612, A88

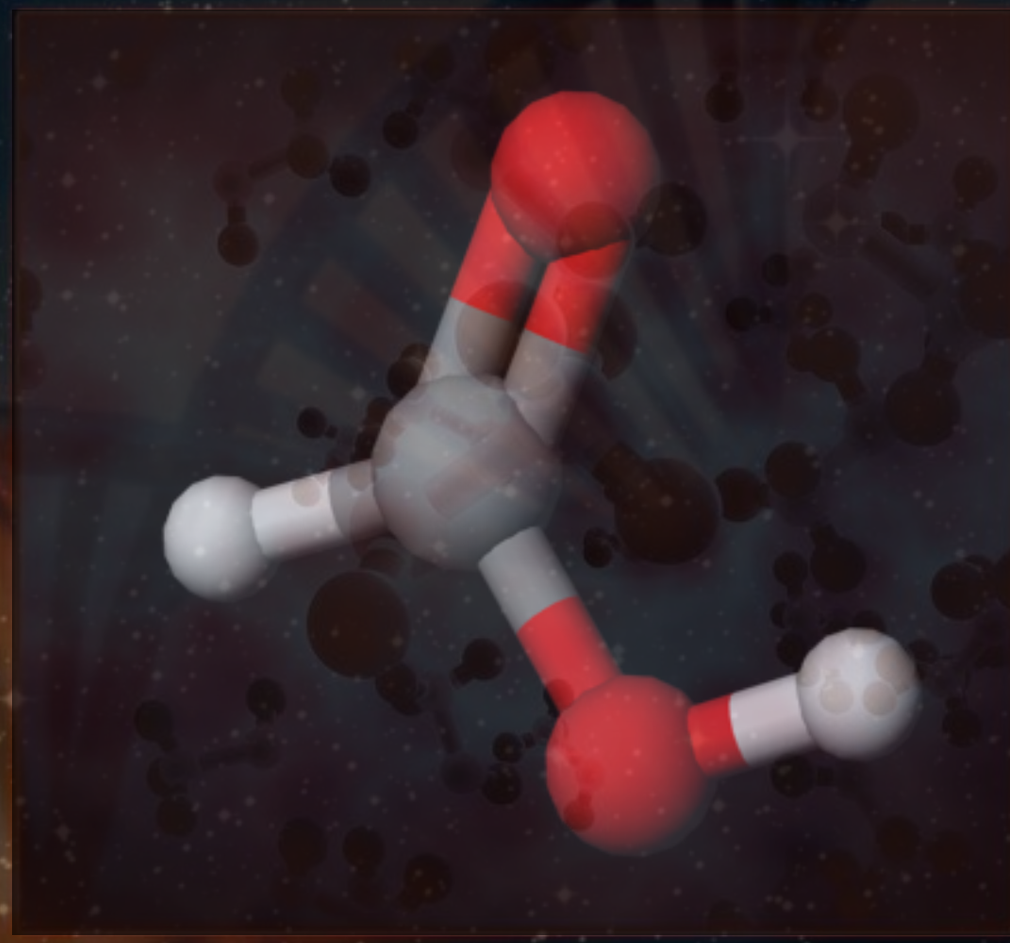
HCOOH in TW Hya





HCOOH in TW Hya

T_{eff} ~ 4000 K



$HCOOH/CH_3OH$ ~ 1

Comets ~ 0.01 - 1

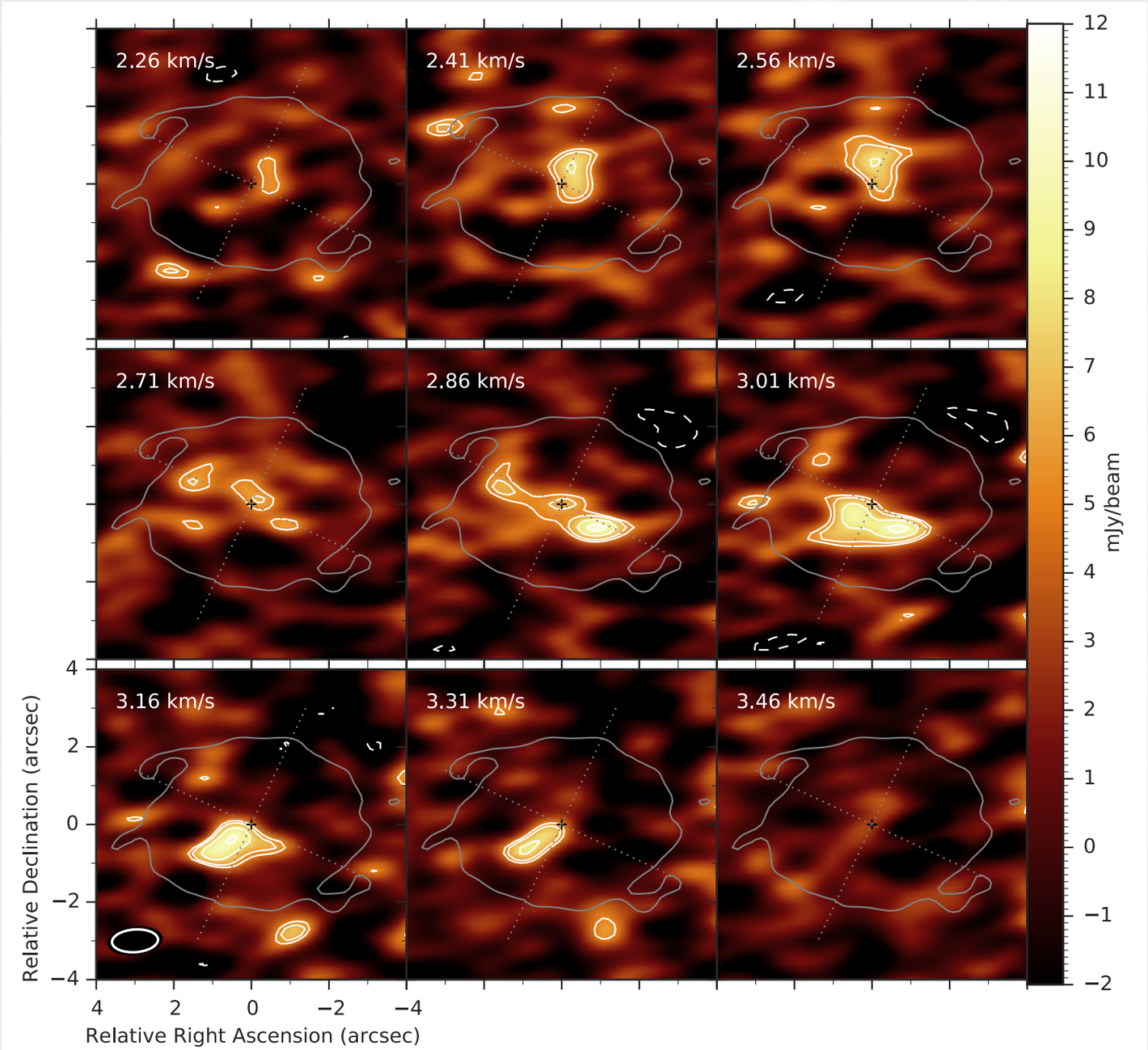
Credit: ESO/M. Kornmesser; Favre, et al. 2018, ApJ, 862, L2

Chemical complexity in protoplanetary disks

Next steps?

Next steps?

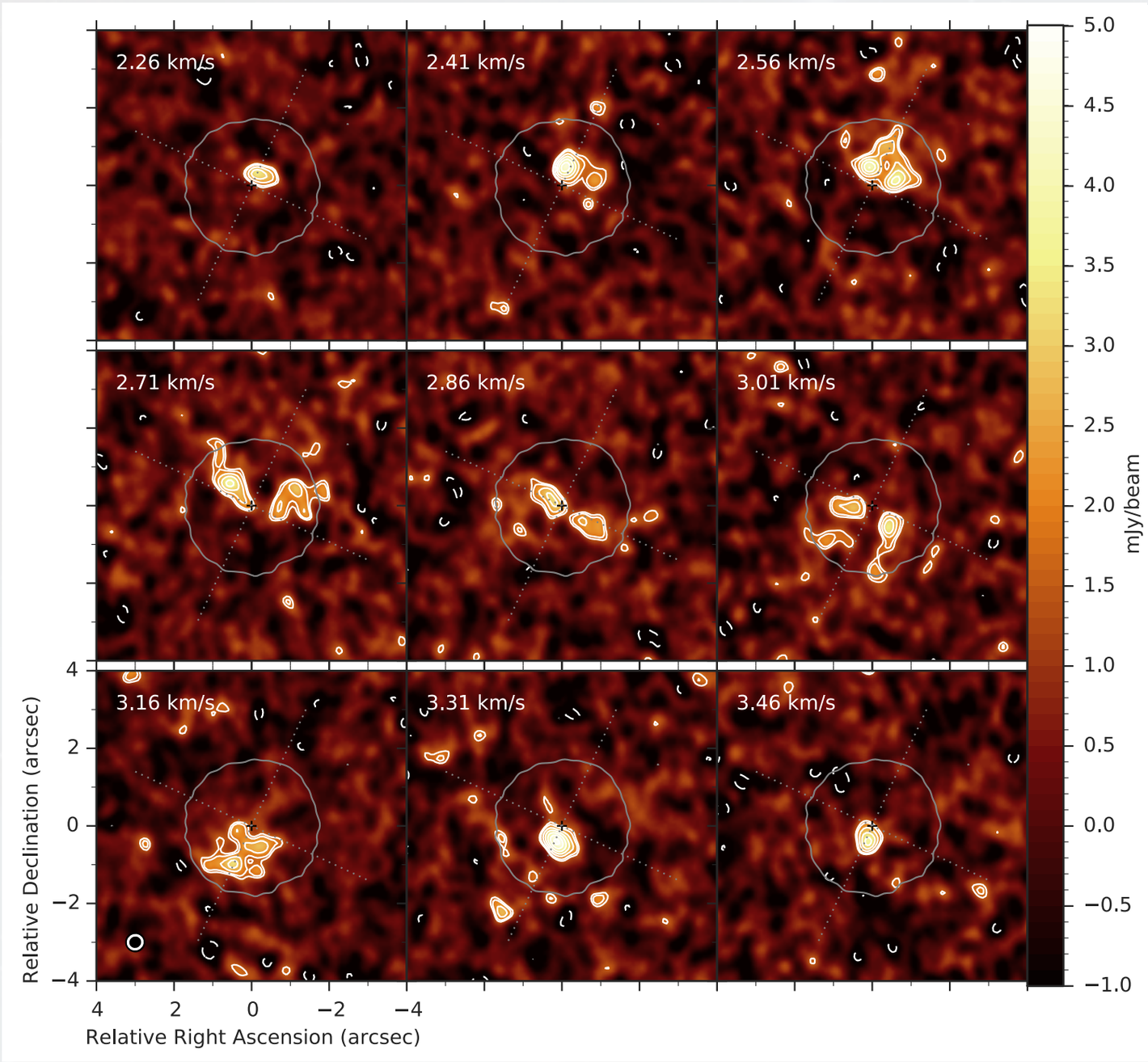
Cycle 2
Methanol
TW Hya



Ilee, J., Walsh, C., et al. 2019, in prep

Next steps?

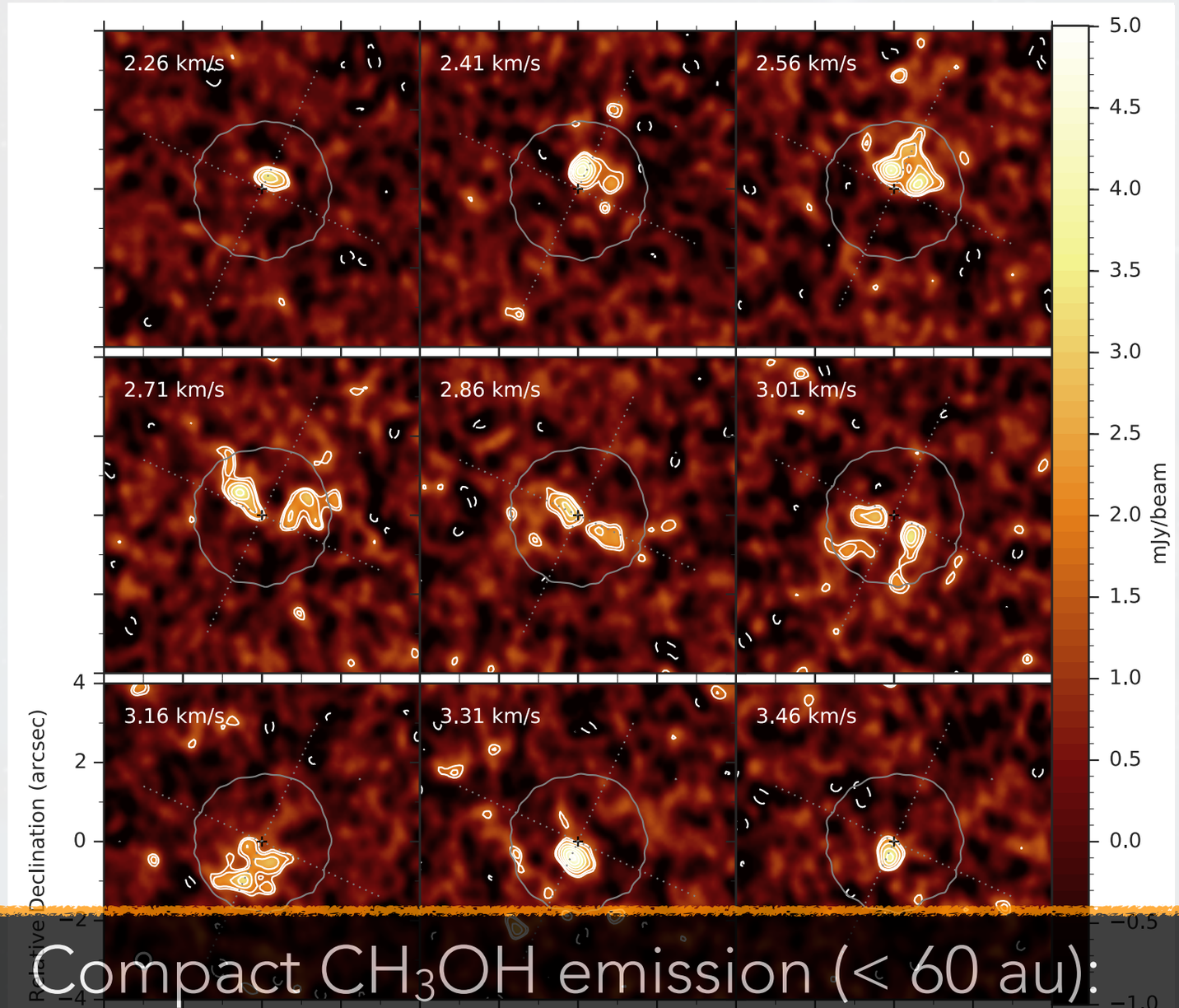
Cycle 4
Methanol
TW Hya



Ilee, J., Walsh, C., et al. 2019, in prep

Next steps?

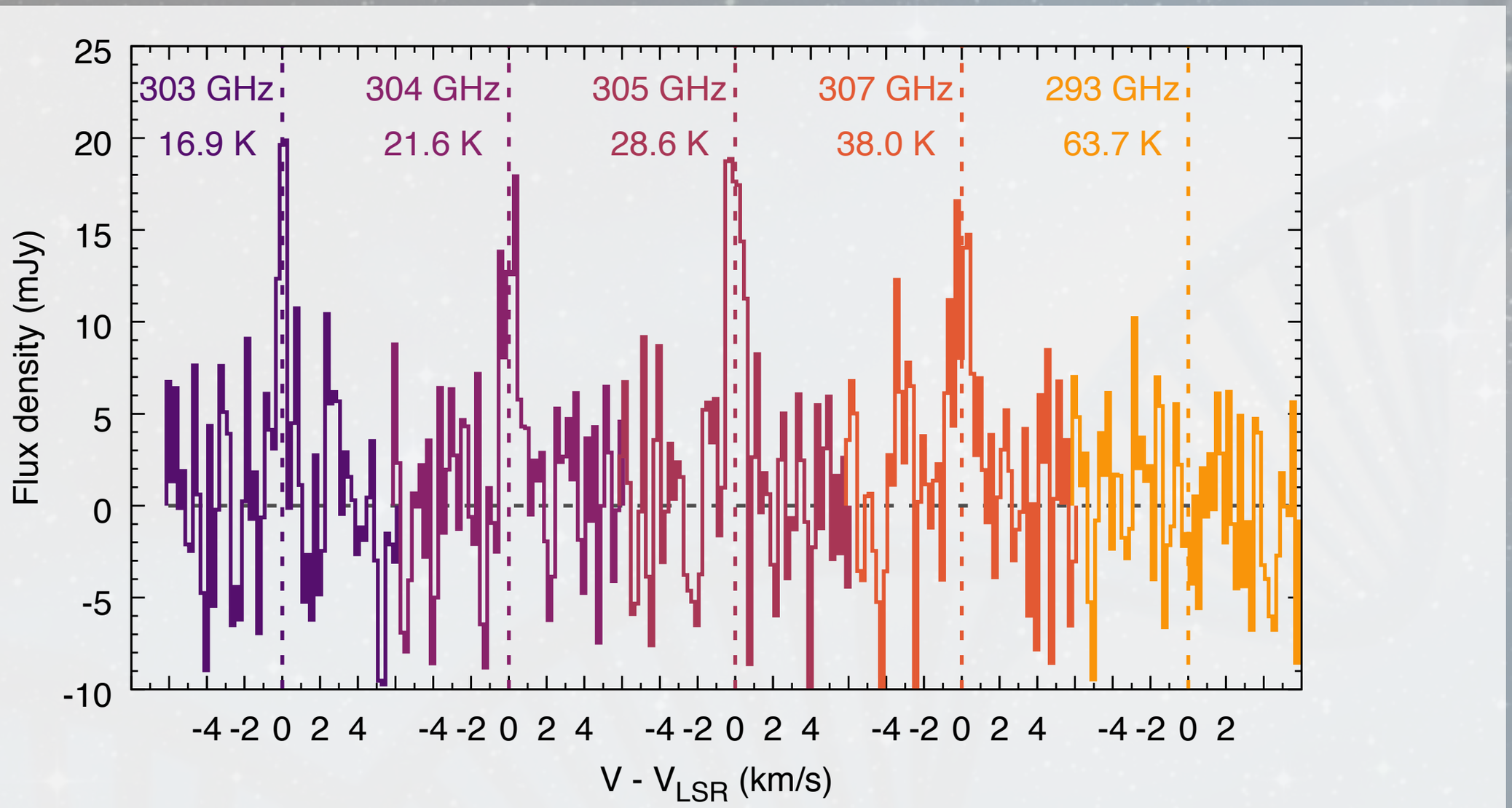
Cycle 4
Methanol
TW Hya



Compact CH_3OH emission (< 60 au):
following the large dust grains?

Ilee, J., Walsh, C., et al. 2019, in prep

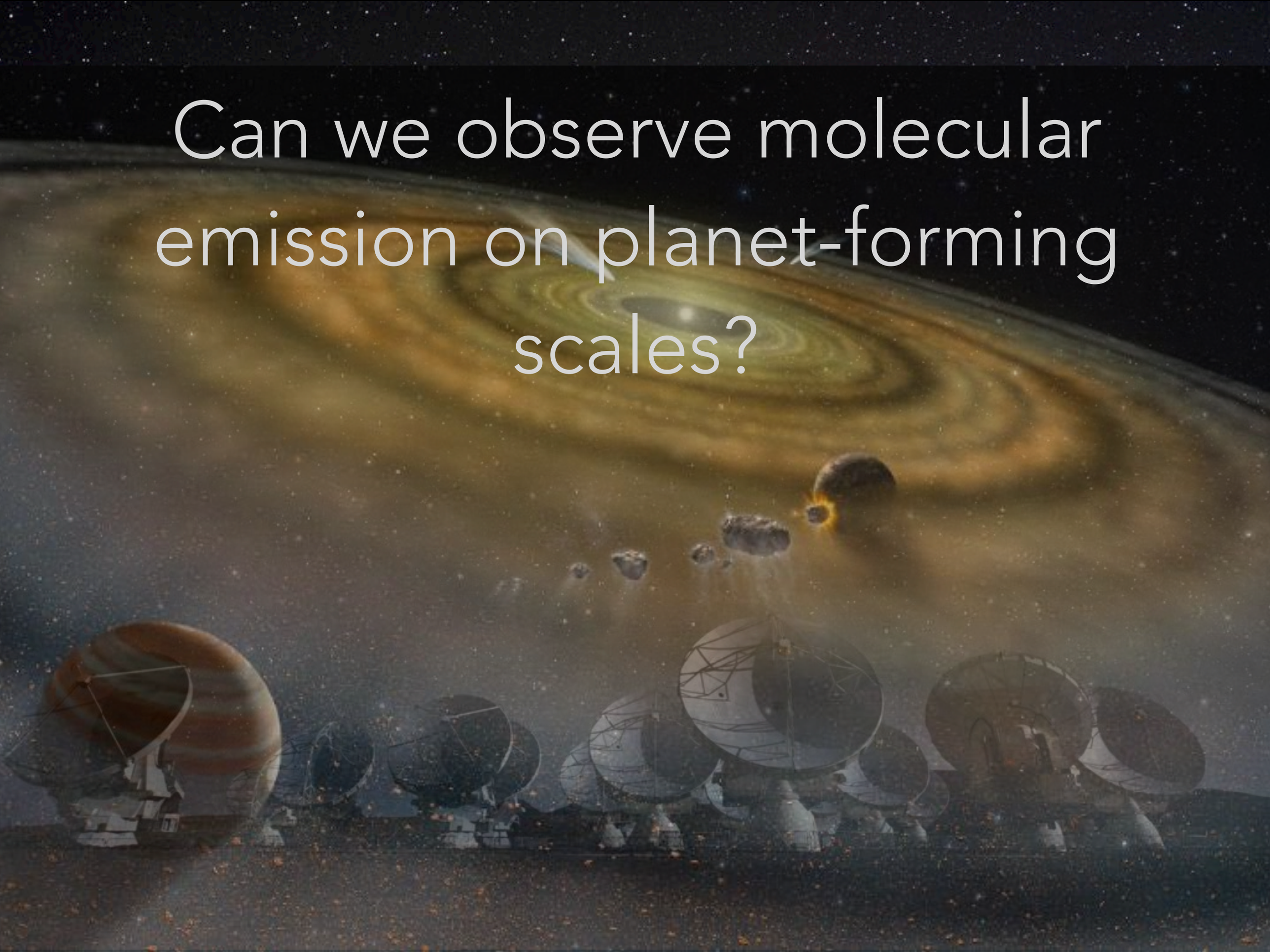
Next steps?



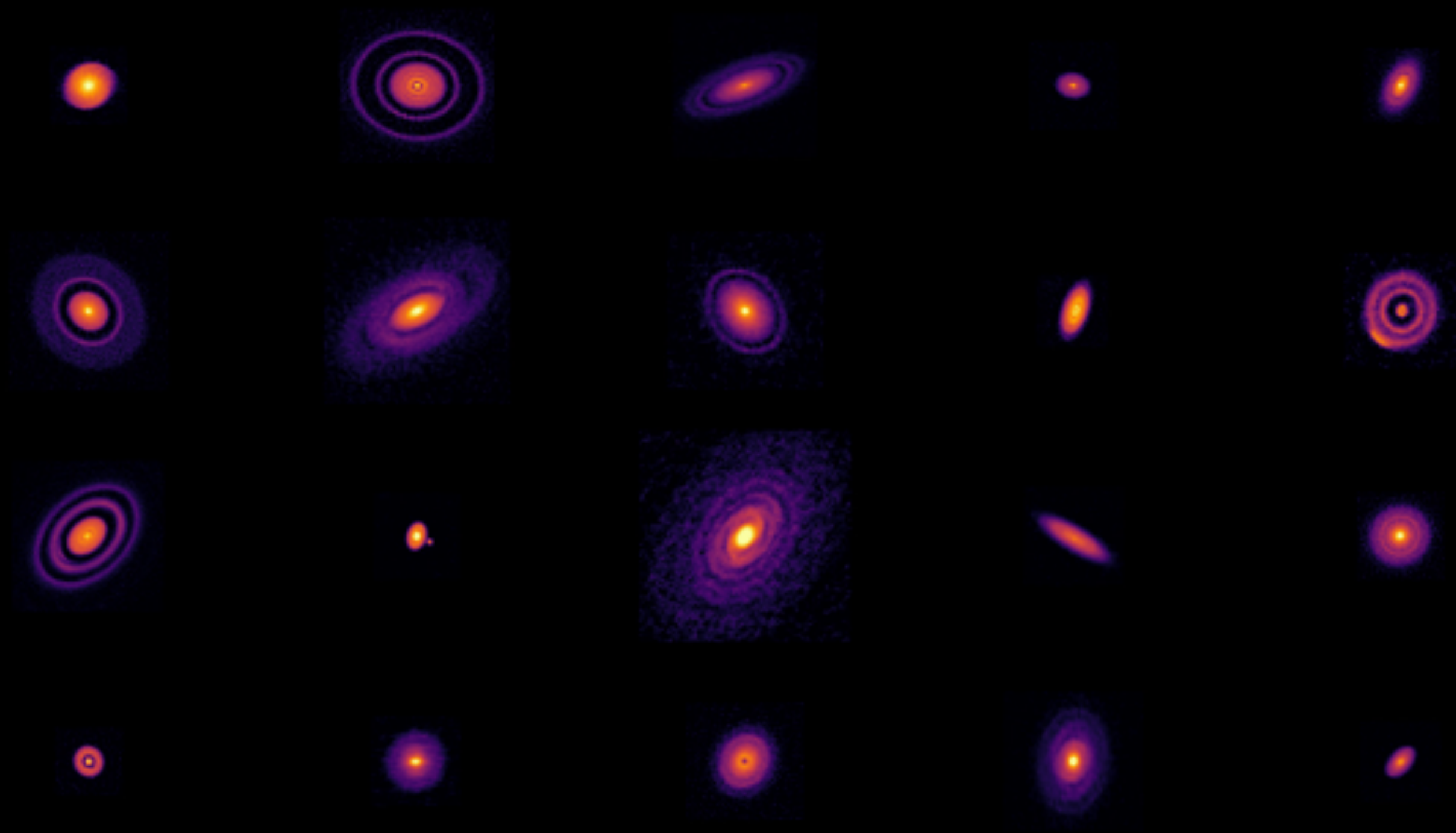
Cycle 4 data: lines with low E_{up} only detected (< 38 K)

Ilee, J., Walsh, C., et al. 2019, in prep

Can we observe molecular emission on planet-forming scales?



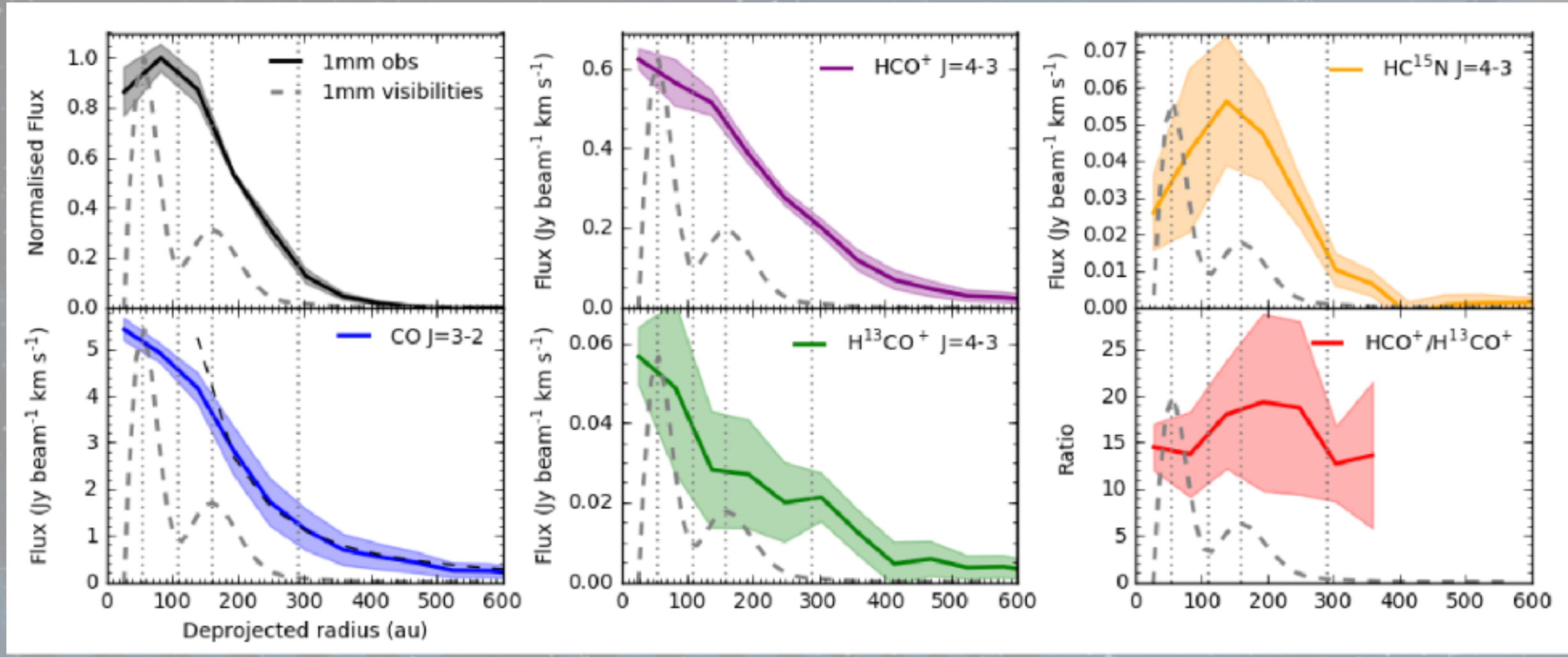
DSHARP: Disk Substructure at High Angular Resolution Project



Andrews, S. M., et al. 2018, ApJ, 869, L41; Credit: ALMA (ESO/NAOJ/NRAO), S. Andrews et al.; NRAO/AUI/NSF, S. Dagnello

Chemical evidence of dust evolution

Resolved molecular emission in the ringed disk around HD 97048

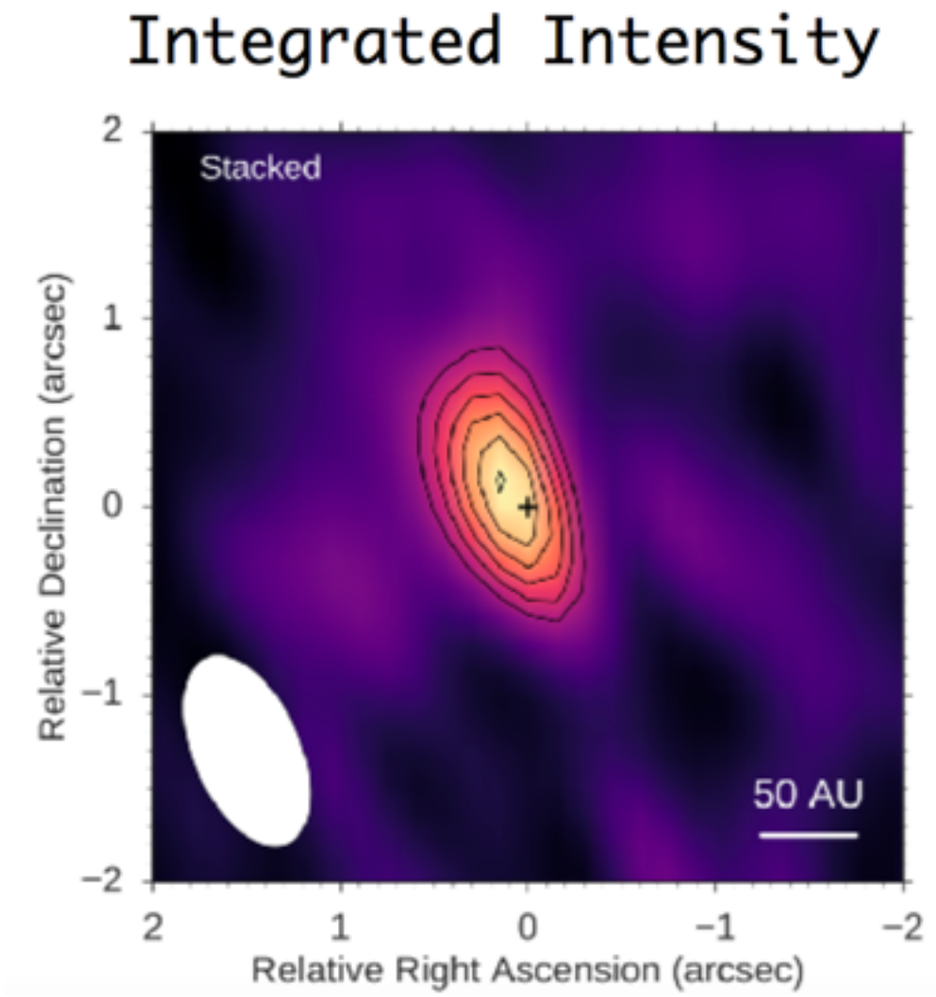


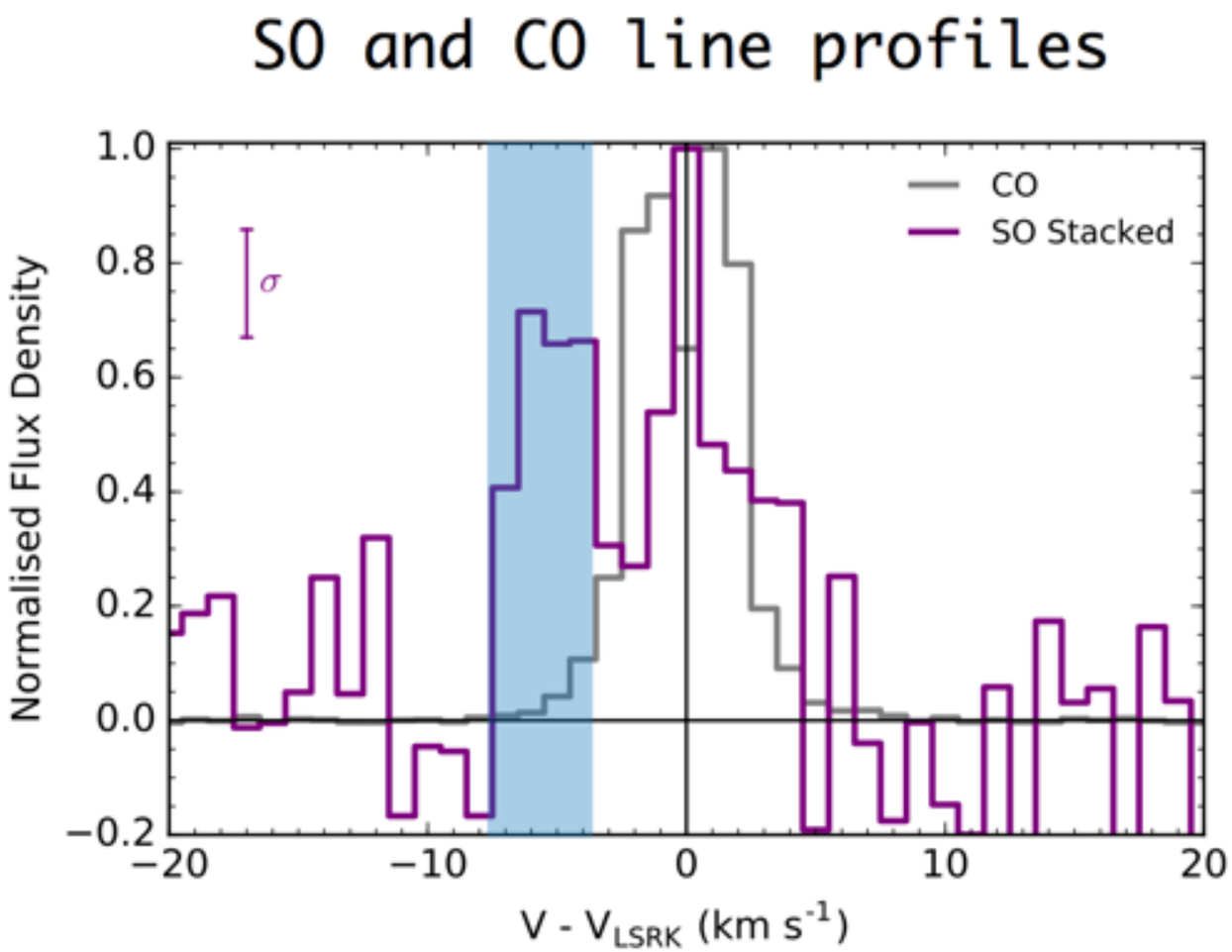
The data cannot be fit by a fixed abundance ratio between $HCO^+/H^{13}CO^+$
There is mounting evidence that gas-phase chemistry is strongly influenced by the dust evolution in the disk (see also Bergin et al. 2016).

Booth, A. & Walsh, C. 2019, A&A, under review

Chemical evidence of planets?

Detection of SO in HD 100546: SO is a known shock tracer



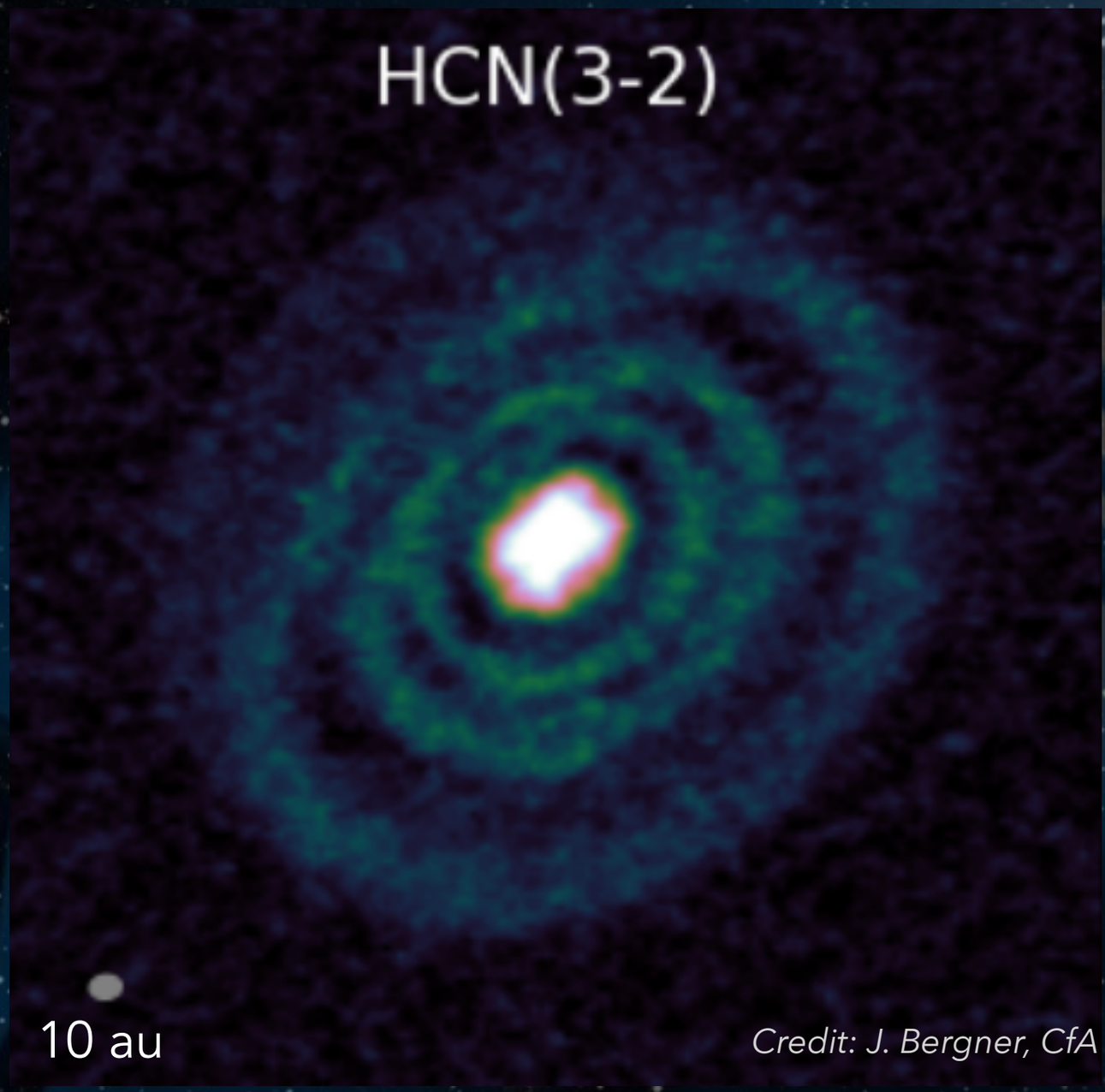


Could this be a disk wind? Or an accreting protoplanet?

Need a "high" abundance of S to match the line flux: ~10^{-6} wrt H_2

Booth, A., et al. 2018, A&A, in press

MAPS: Molecules with ALMA on Planet-forming Scales



Aikawa, Bergin, Guzmán, Öberg, Walsh

Chemistry is useful!

Not only as a tracer of composition of ice and gas ....

... also as a sensitive tracers of physics, ...

..., and other molecules are available!

Happy to share chemical codes: c.walsh1@leeds.ac.uk