Star-forming regions at sub-Solar metallicity: astrochemical modelling

Serena Viti (Leiden University/University of Bonn)

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Universiteit Leiden
The Netherlands

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UCL CDT DIS

European Research Council
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Outline

- Importance of chemical predictions (for subsolar systems)
- Metallicity, dust to gas ratio, and non solar elemental abundances
- Chemical models at subsolar metallicities
- Predictions and comparison with observations

The ingredients of cosmic chemistry: Gas and Dust

Take away message

Solar elemental abundances relative to the *total number of hydrogen nuclei*.

H 1
He 9(-2)
O 5(-4)
C 3(-4)
N 7(-5)
Si 3(-5)
Mg 4(-5)
Fe 3(-5)
S 1(-5)
Na, Ca 2(-6)

1. Metallicity may vary from galaxy to galaxy → depends on the star formation rates and efficiencies
2. Also, supernovae of different masses may lead to different relative abundances

It is important to understand the molecular chemistry obtained from different metallicities and different relative abundances

Elemental abundances, H_2 formation, Metallicity and dust to gas ratio

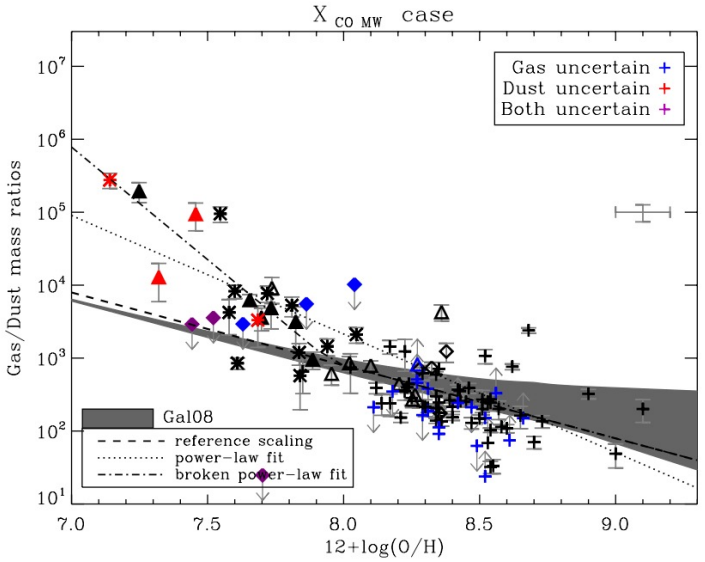
TABLE 3

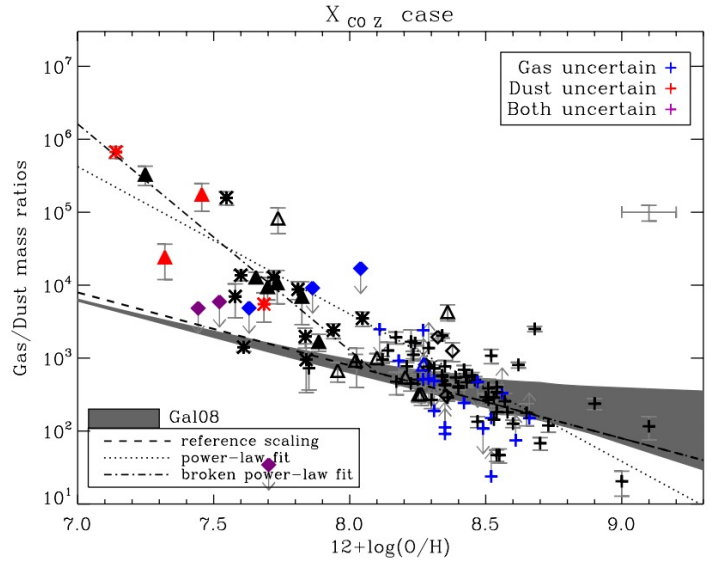
INITIAL ABUNDANCE RATIO VALUES USED IN TABLE 2

	ST	CL02	HW02	UN02
C/H	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}	1.4×10^{-4}
O/H	3.2×10^{-4}	4.54×10^{-4}	1.53×10^{-3}	1.18×10^{-3}
N/H	6.5×10^{-5}	5.99×10^{-11}	1.58×10^{-9}	3.24×10^{-7}
He/H	7.5×10^{-2}	7.5×10^{-2}	7.5×10^{-2}	7.5×10^{-2}
Mg/H	5.1×10^{-6}	1.83×10^{-5}	1.2×10^{-4}	6.18×10^{-5}

NOTE.—The abbreviations CL02, HW02, and UN02 refer to Chieffi & Limongi (2002); Heger & Woosley (2002); and Umeda & Nomoto (2002), respectively (see § 3). The standard initial abundance ratios values are from Sembach & Savage (1996); Sofia et al. (1997); Meyer et al. (1998); Snow et al. (2002); and Knauth et al. (2003). We did not include in this table the values of the initial elemental abundance S/H ratio since they have already been listed in Table 2.

$$\left.\frac{d}{dt} n(H_2)\right|_{form^n} \propto n(H) n_g \bar{v}_H \pi a^2 P$$



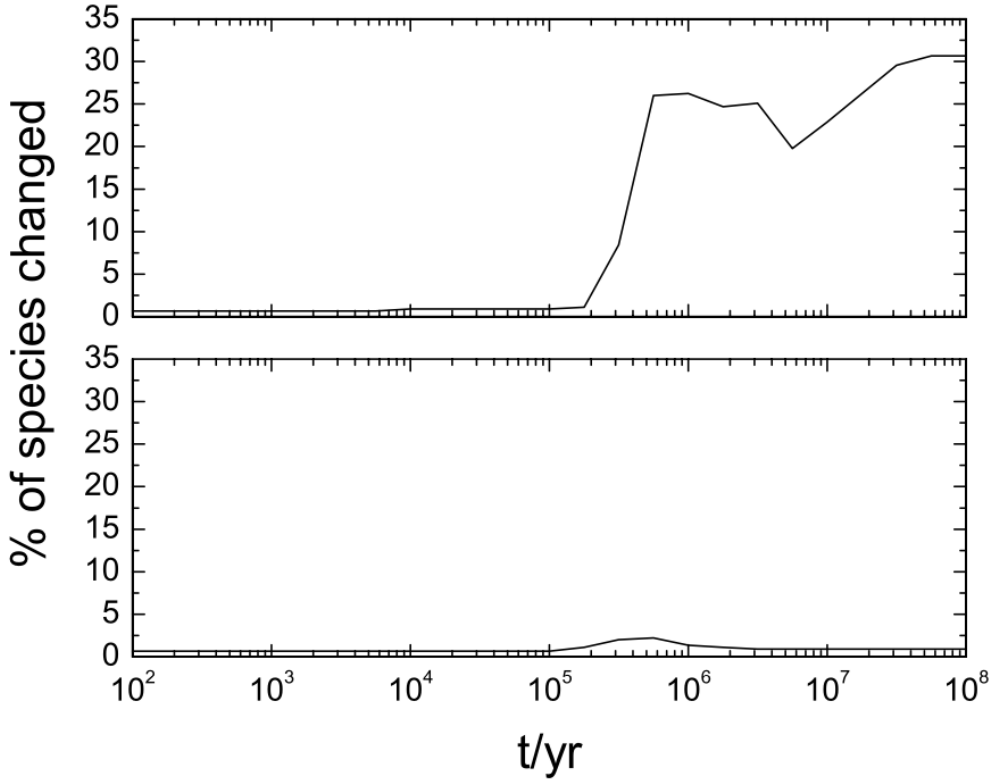


Selection of initial abundances for atomic species is crucial e.g.

H	1
He	0.085
O	4.898(-4)
C	2.692(-4)
N	6.761(-5)
Mg	3.981(-5)
Cl	3.162(-7)
S	1.318(-5)
Si	3.236(-5)
Etc.	

Solar: Asplund et al. (2009, ARA&A)

H	1
He	0.060
O	1.76(-4)
C	7.3(-5)
N	2.14(-5)
Mg	7(-9)
Cl	4(-9)
S	8(-8)
Si	8(-9)
Etc.	



Low metallicity "L134N" (e.g. Quan et al. 2008)

Metallicity vs varied initial elemental ratio chemical effects

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Model	Metallicity[a] ($Z_\odot$)	Ga
0.....	1	ST
1.....	1/10	ST/10
2.....	1/100	ST/100
3.....	1/1000	ST/1000

METALLICITY

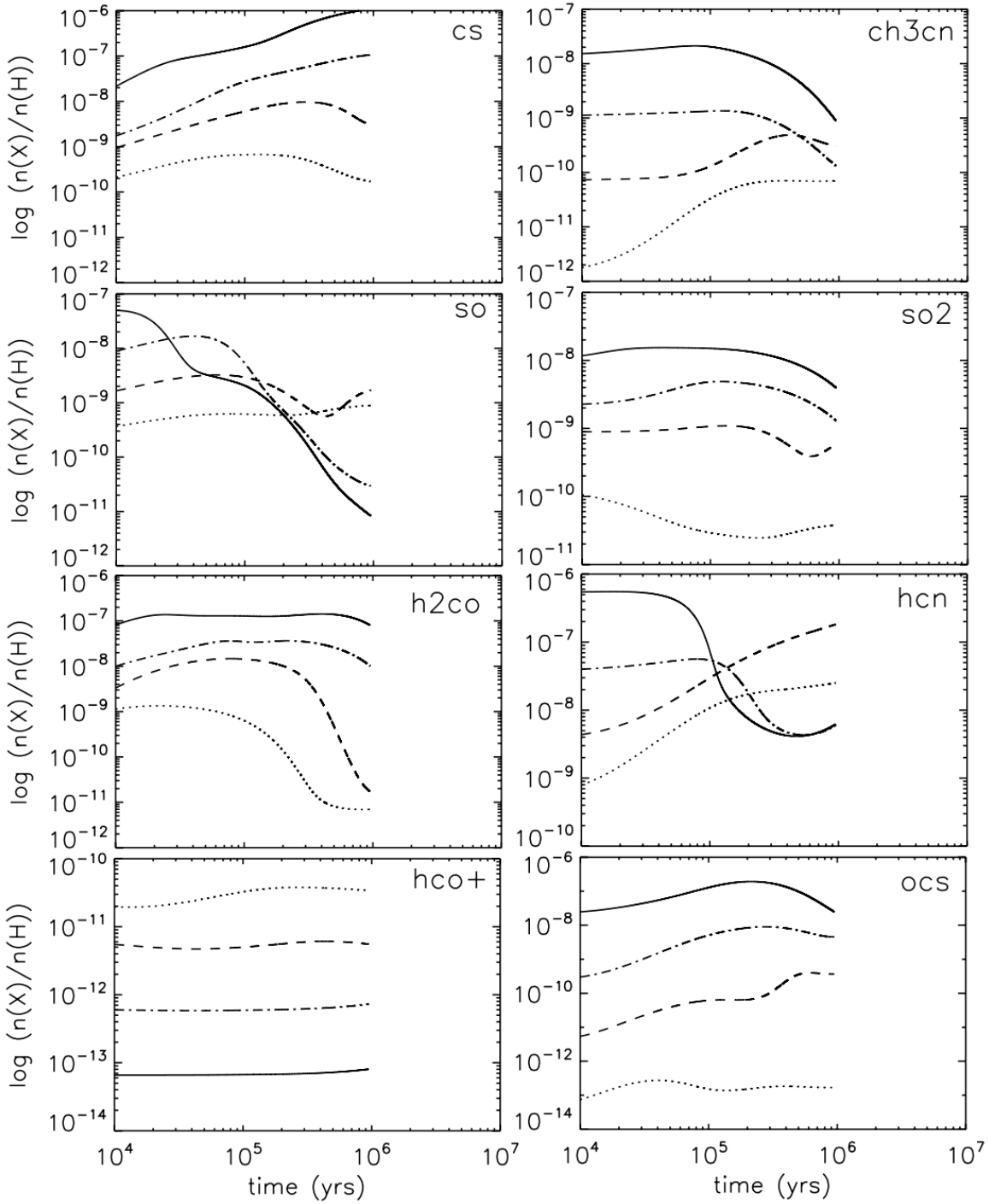
High Density ("hot cores") models

Initial elemental ratios

	ST
C/H	1.4×10^{-4}
O/H	3.2×10^{-4}
N/H	6.5×10^{-5}
He/H	7.5×10^{-2}
Mg/H	5.1×10^{-6}

Model 0 (solid lines),
Model 1 (dash-dot lines)
Models 2 ((dashed lines)
Model 3 (dotted lines)

But see Rob Garrod's talk



INITIAL ELEMENTAL ABUNDANCES

Model	Metallicity[a] ($Z_\odot$)	Ga
0.....	1	ST (solid line)
4.....	1	CL02 (dotted)
5.....	1	HW02 (dash)
6.....	1	UN02 (dash-dotted)

High Density (“hot cores”) models

TABLE 3

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	ST	CL02	HW02	UN02
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Note.—The abbreviations CL02, HW02, and UN02 refer to Chieffi & Limongi (2002); Heger & Woosley (2002); and Umeda & Nomoto (2002), respectively (see § 3). The standard initial abundance ratios values are from Sembach & Savage (1996); Sofia et al. (1997); Meyer et al. (1998); Snow et al. (2002); and Knauth et al. (2003). We did not include in this table the values of the initial elemental abundance S/H ratio since they have already been listed in Table 2.

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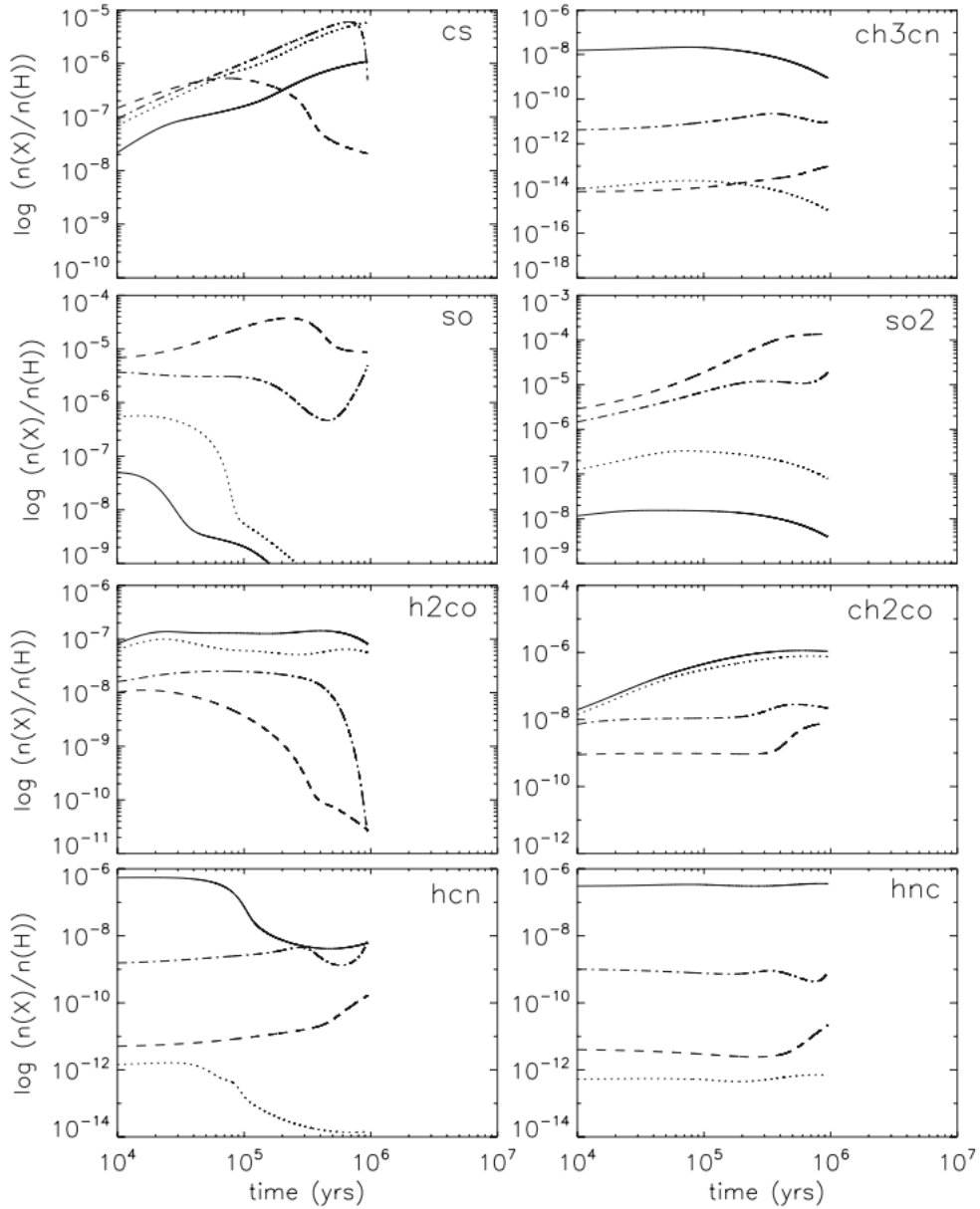
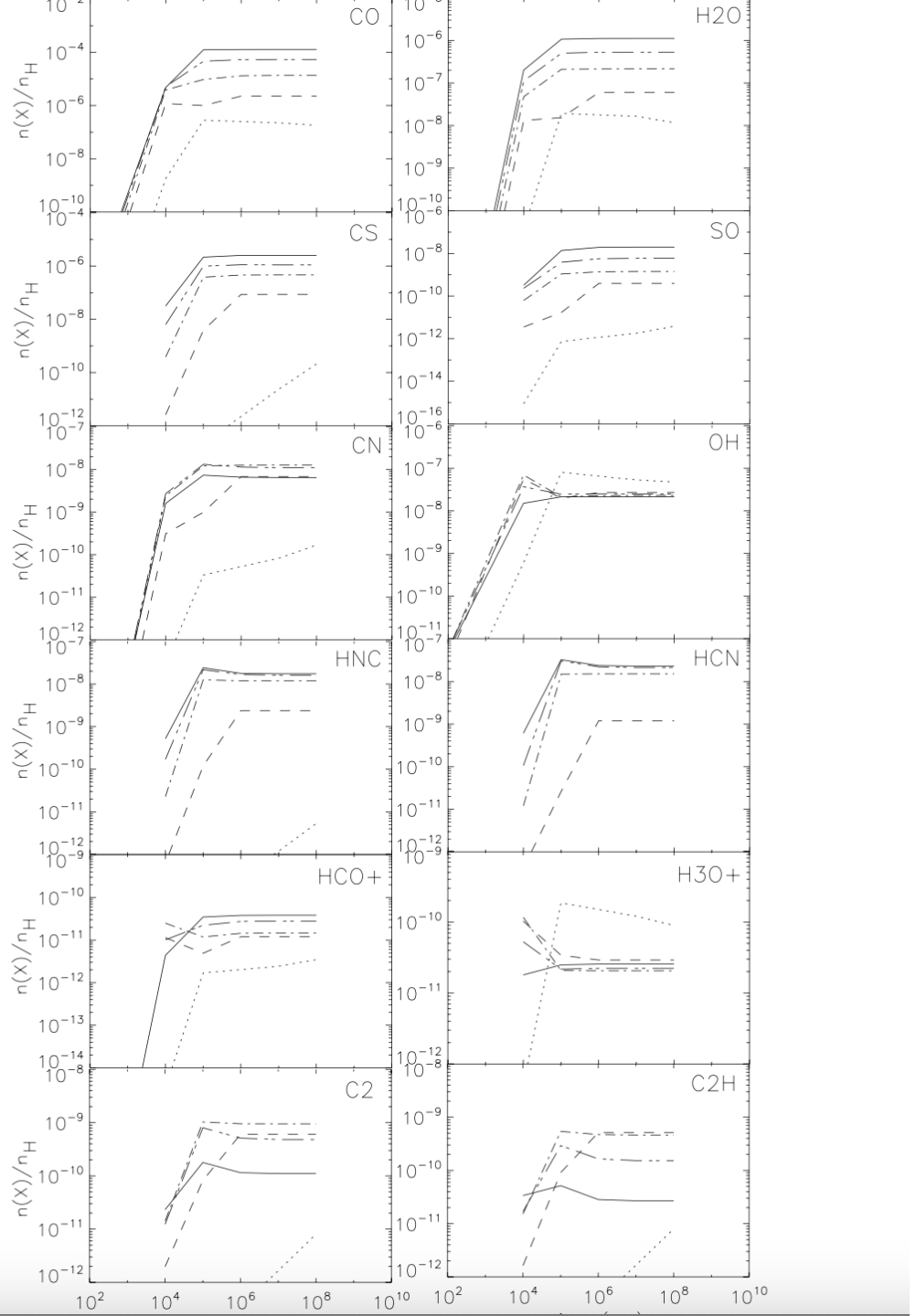


METALLICITY

Model	Metallicity ($z_\odot$)	Gas-to-Dust Mass Ratio ($d_\odot$)	H_2 Form. Rate Coeff. ($R_\odot$)	A_v	Ini. Elem. Abund. Ratios	FUV Rad. Field ($I_\odot$)
0	1	1	1	8	ST	10^3
1	1/2	1/2	1/2	8	ST/2	10^3
2	1/4	1/4	1/4	8	ST/4	10^3
3	1/10	1/10	1/10	8	ST/10	10^3
4	1/100	1/100	1/100	8	ST/100	10^3

Model 0 black lines,
Model 1 dash–two-dots lines,
Models 2 dash–one-dot lines,
Model 3 dashed lines,
Model 4 dotted lines

PDR gas



INITIAL ABUNDANCES

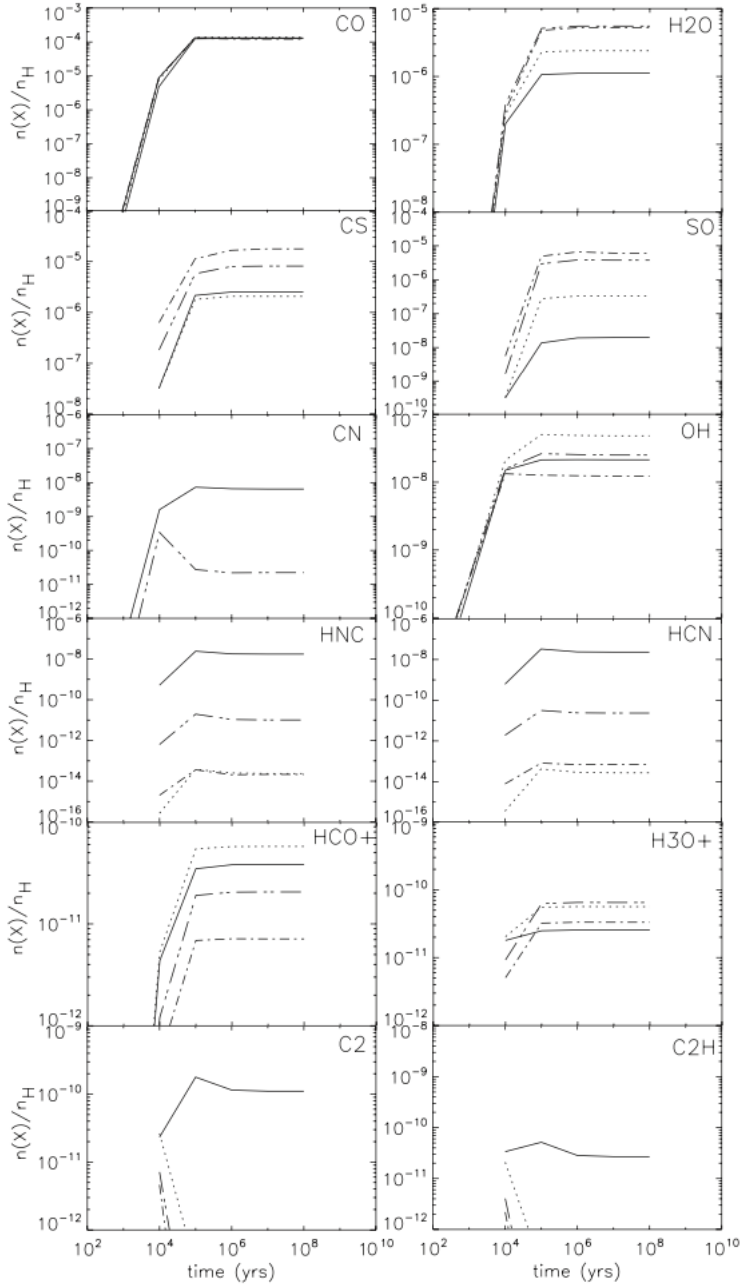
Table 2
Input Parameters of the UCL_PDR Models Used to Perform this Study (see Sections 3 and 4)[a]

Model	Metallicity ($z_\odot$)	Gas-to-Dust Mass Ratio ($d_\odot$)	H_2 Form. Rate Coeff. ($R_\odot$)	A_v	Ini. Elem. Abund. Ratios	FUV Rad. Field ($I_\odot$)	ζ ($\zeta_\odot$)	Gas Density (cm^{-3})
0	1	1	1	8	ST	10^3	1	10^4
9	1	1	1	8	CL02	10^3	1	10^4
10	1	1	1	8	HW02	10^3	1	10^4
11	1	1	1	8	UN02	10^3	1	10^4
12	1/10	1/10	1/10	8	ST/10	10^5	100	10^4

Note. [a]The abbreviation "ST" represents the standard values while the abbreviations "CL02," "HW02," and "UN02" are the initial elemental abundance ratio references detailed in Table 3. This table does not present all the input parameters of the UCL_PDR code for each model but only lists the parameters set to values different from the standard ones.

PDR gas

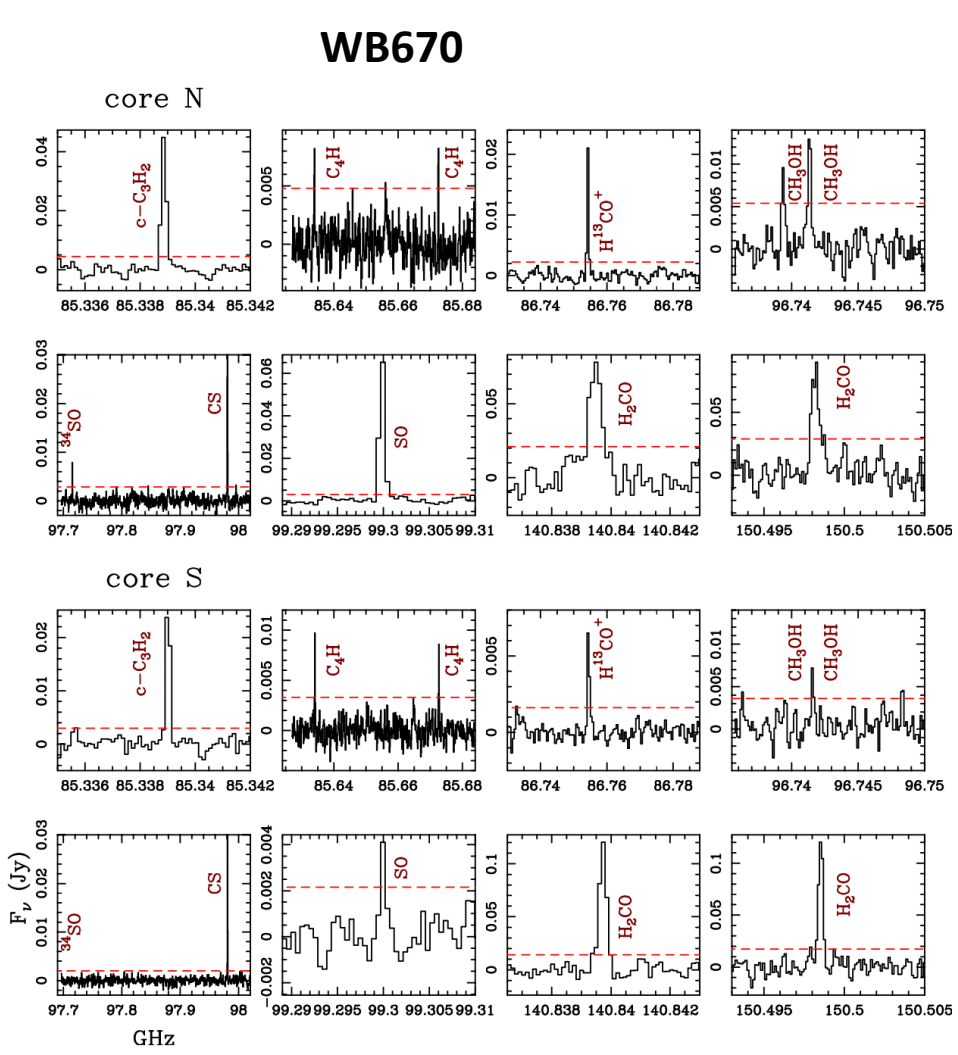
Model 0 black lines,
Model 9 dotted lines,
Models 10 dash–one-dot lines,
Model 11 dash two dot lines lines

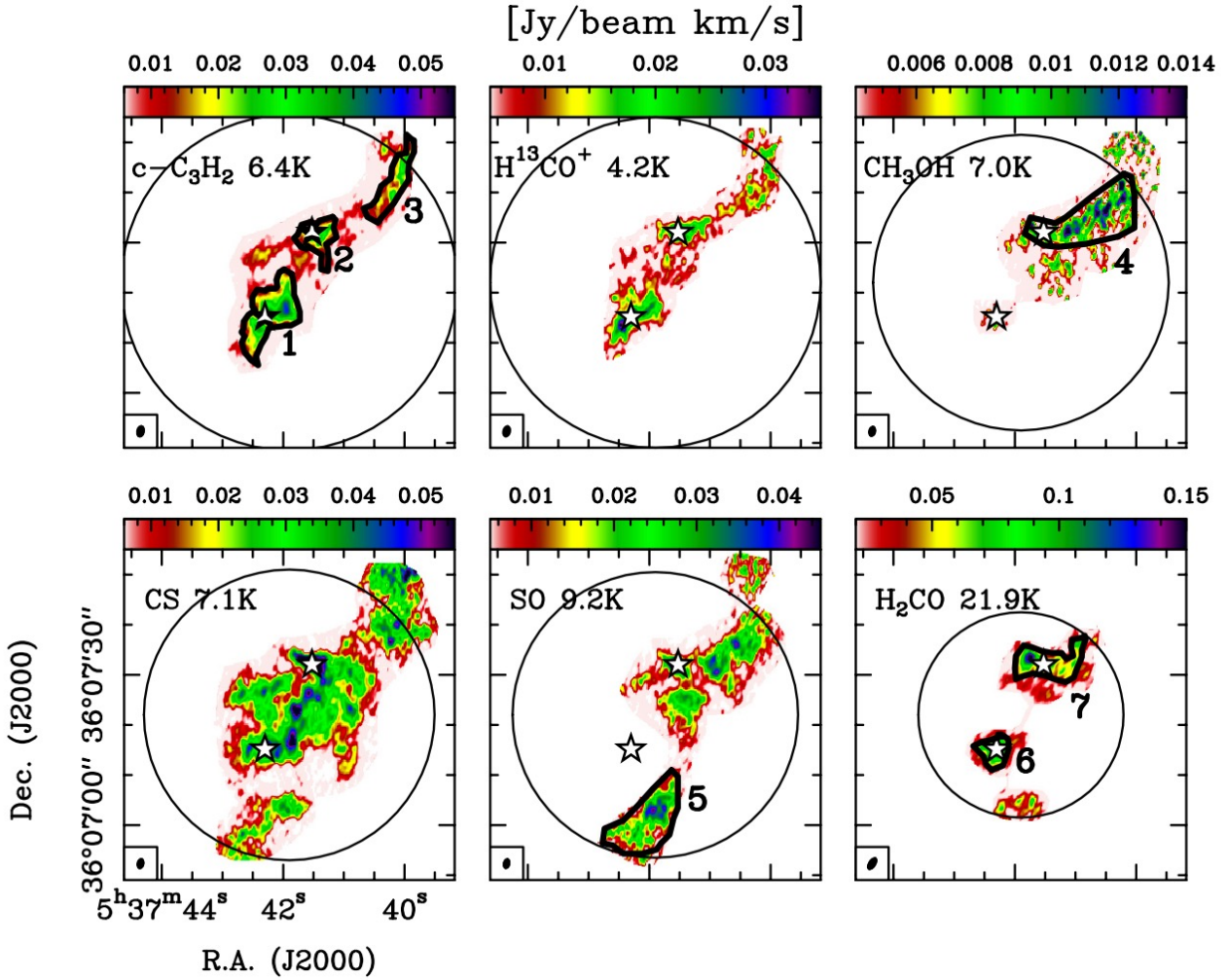


CHEMOUT: CHEMical complexity in star-forming regions of the OUTer Galaxy

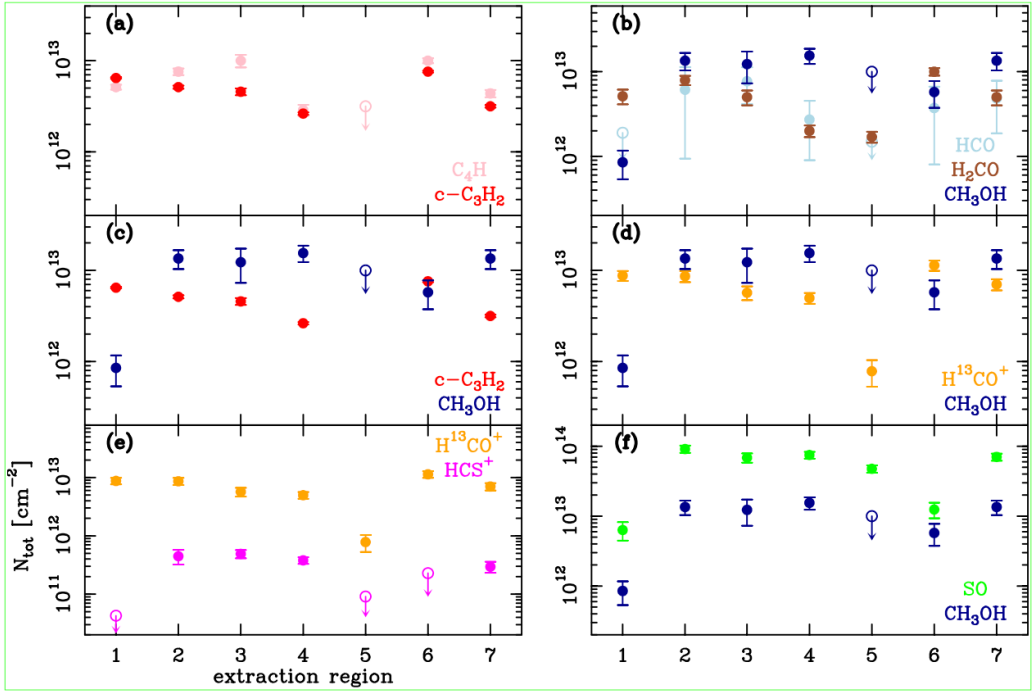
IV. ALMA observations of organic species at Galactocentric radius ~ 23 kpc

F. Fontani[1,2,3], G. Vermariën[4], S. Viti[4], D. Gigli[1,5], L. Colzi[6], M.T. Beltrán[1], P. Caselli[2], V.M. Rivilla[6], and A. Sánchez-Monge[7,8]





- The molecular emission comes from an extended filamentary structure + multiple cores are detected
- Each tracer has a different morphology → spatial anti-correlation between hydrocarbons, molecular ions, HCO, and H_2CO vs CH_3OH and SO → different formation mechanisms?
- Low excitation temperature 5-15 K
- Methanol abundance consistent with metal poor environments.

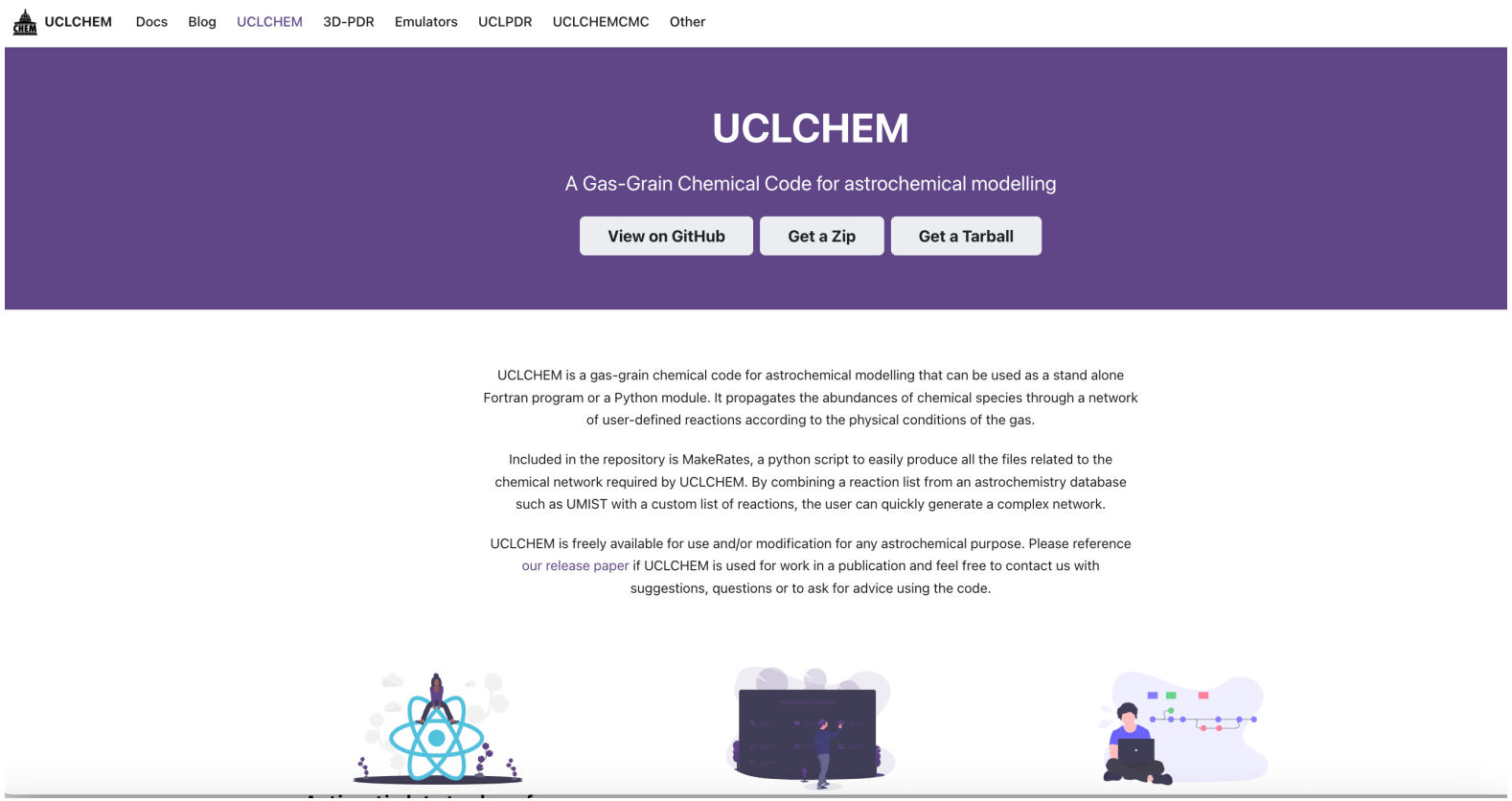


molecule	V km s^{-1}	FWHM km s^{-1}	T_{ex} K	N_{tot} $\times10^{12}$cm^{-2}	[X]^a $\times10^{-9}$
		N			
c-C_3H_2	–17.40(0.01)	0.74(0.02)		7.9(0.2)	1.4
HCS^+	–	–		≤ 0.4	≤ 0.07
C_4H	–17.32(0.05)	0.9(0.1)		19(2)	3.3
HCO	–	–		≤ 3.2	≤ 0.6
$HN^{13}C$	–	–		≤ 0.3	≤ 0.05
$H^{13}CO^+$	–17.37(0.07)	2.01(0.08)		1.5(0.1)	0.3
CH_3OH	–17.4(0.1)	0.92(0.08)	9(2)	2.2(0.3)	0.4
CS	–17.46(0.03)	2.00(0.04)		17(2)	3.0
SO	–17.44(0.02)	2.01(0.05)		43(1)	7.5
H_2CO	–17.37(0.04)	1.25(0.09)		8.5(0.5)	1.5
		S			
c-C_3H_2	–18.0(0.1)	0.7(0.1)		7.6(0.8)	3.6
HCS^+	–	–		≤ 0.6	≤ 0.3
C_4H	–17.93(0.03)	0.69(0.06)		44(4)	21
HCO	–	–		≤ 2.1	≤ 1
$HN^{13}C$	–	–		≤ 0.4	≤ 0.2
$H^{13}CO^+$	–18.0(0.6)	1.6(1)		1.0(0.3)	0.5
CH_3OH	–18.0(0.7)	1.1(0.5)	15(3)	23(3)	11
CS	–17.92(0.02)	1.87(0.03)		11.7(1)	5.6
SO	–17.8(0.2)	2.1(0.4)		3.4(0.8)	1.6
H_2CO	–17.96(0.01)	0.63(0.03)		8.5(0.8)	4.0

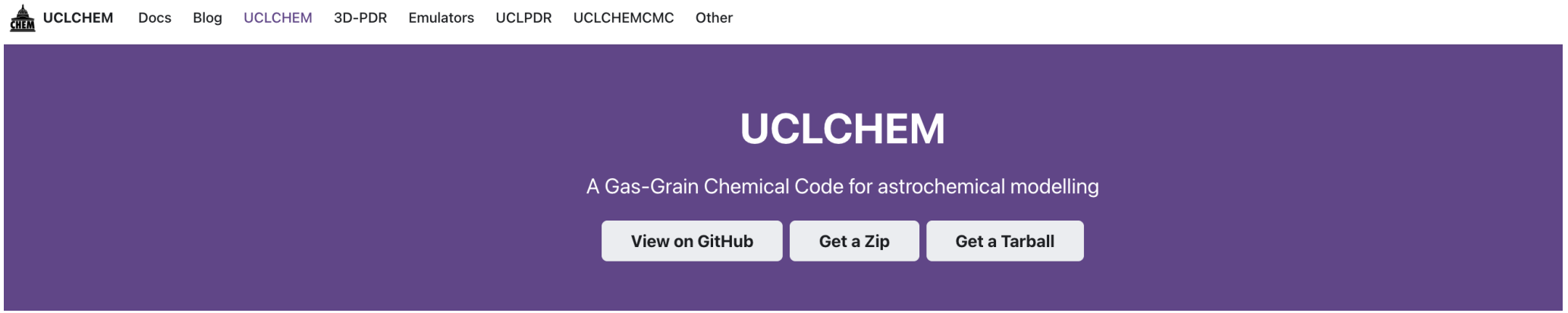
Fontani et al. (2024)

Can the measured column density ratios constrain the initial elemental abundances?

Astrochemical Modelling



UCLCHEM: a public gas-grain chemical code – Holdship et al. (2017)



A variety of physical models

Model dark clouds, hot cores/corinos, C- and J-type shocks and protostellar cores

Easy network construction

You list species and two body grain surface reactions, UCLCHEM does the rest (inc. determination of thermal/non thermal desorption by all mechanisms). UCLCHEM includes two or three phase chemistry (gas, ice surface, and ice bulk).

Python wrapped, Fortran powered

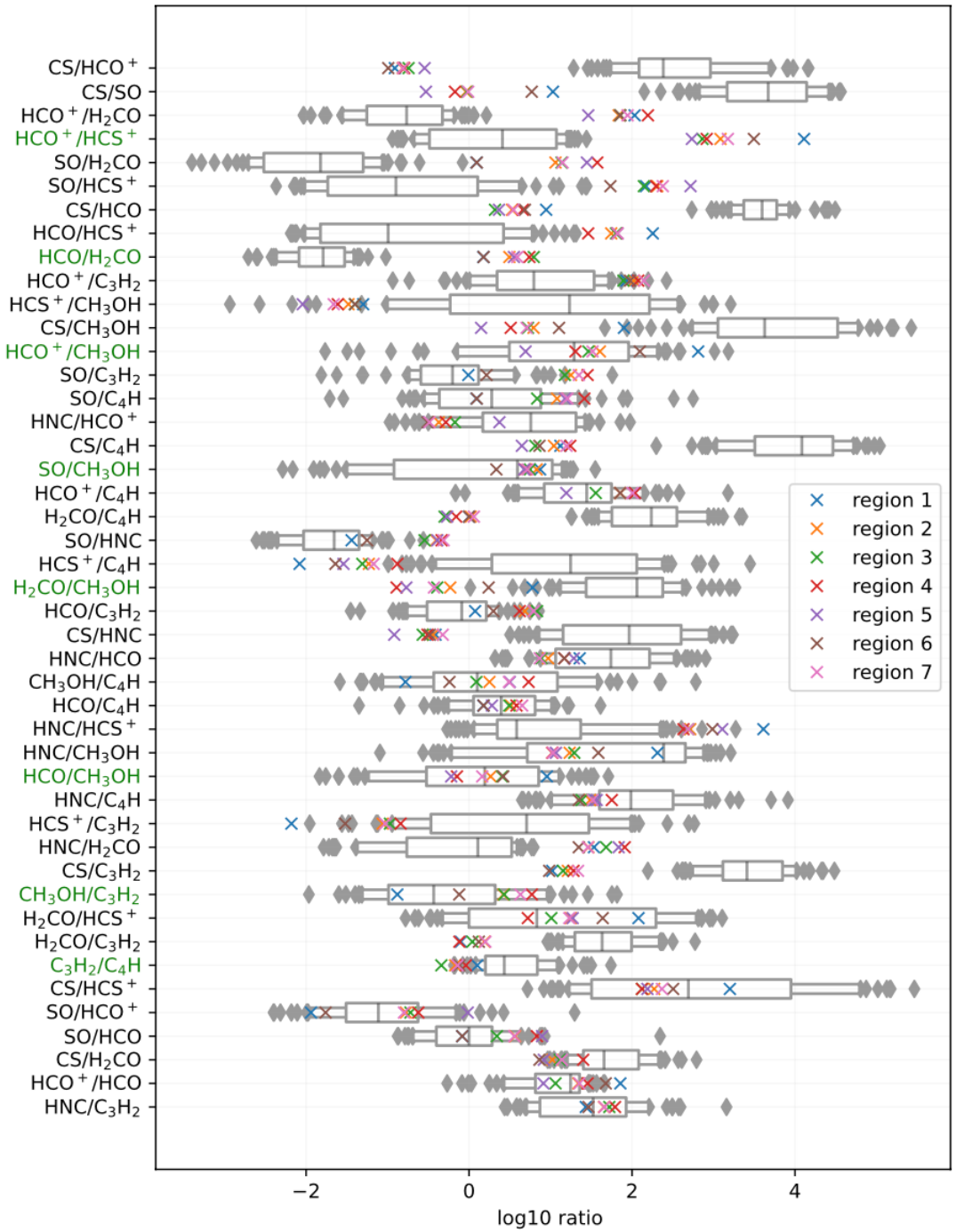
The code is written in Fortran to make integration fast but compiles to a python library that is well documented.

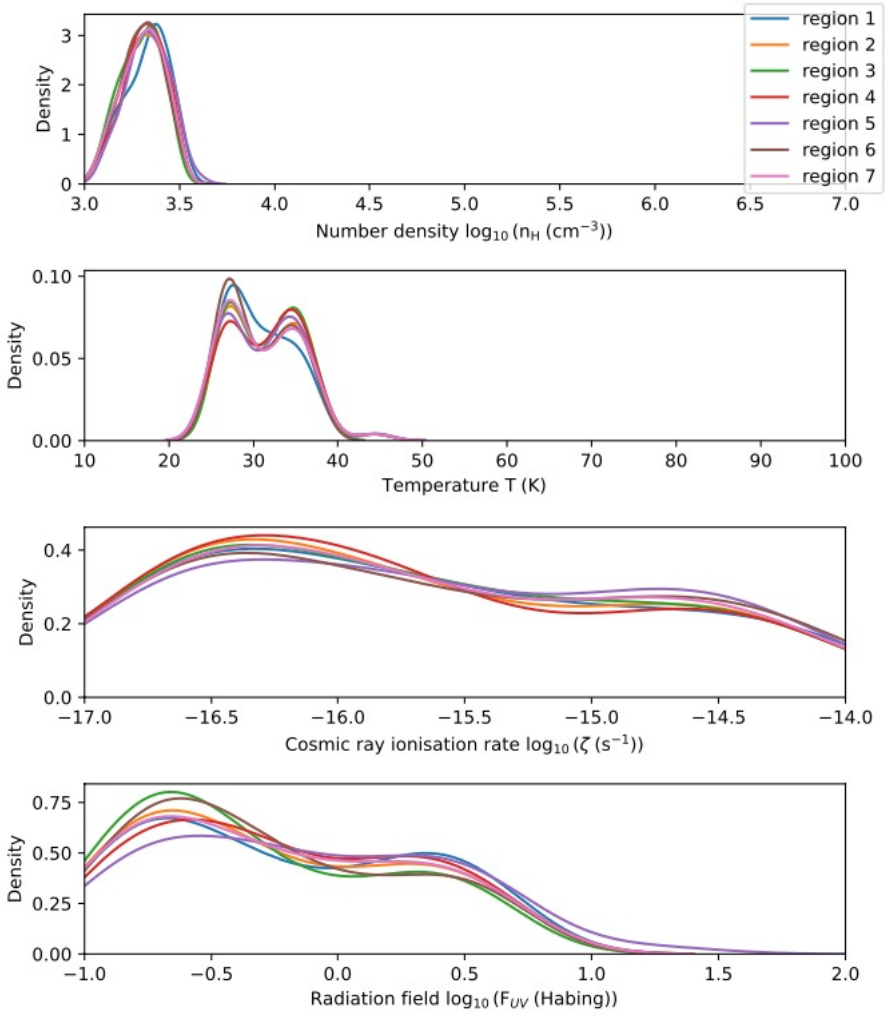
Constantly updated and released to the community. New release paper coming early 2025 (Vermarien et al. in prep)

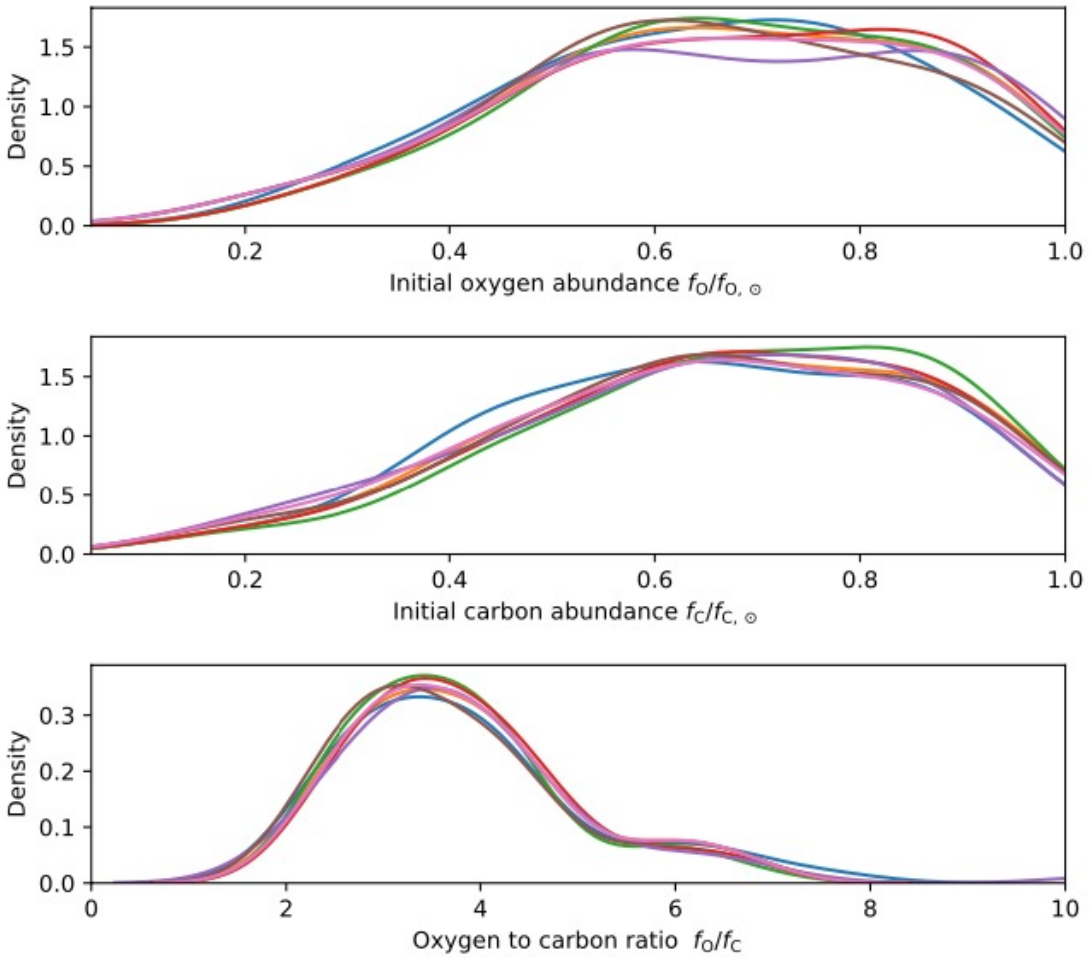
https://uclchem.github.io/

Isothermal static cloud
R = 0.5 pc
nH, T, ζ, FUV, O, C **vary**

Parameter	Min	Max	Sample space
Density $n_{\rm H}$ (cm^{-3})	1×10^{3}	1×10^{7}	log
Temperature T (K)	10	100	linear
Cosmic-ray ionisation rate ζ (s^{-1})	1×10^{-17}	1×10^{-14}	log
Radiation field $F_{\rm UV}$ (Habing)	0.1	100	log
Initial elemental abundance of oxygen $f_{\rm O}/f_{\rm O,\odot}$	$0.05 \times 3.34 \times 10^{-4}$	$1.0 \times 3.34 \times 10^{-4}$	linear
Initial elemental abundance of carbon $f_{\rm C}/f_{\rm C,\odot}$	$0.05 \times 1.77 \times 10^{-4}$	$1.0 \times 1.77 \times 10^{-4}$	linear







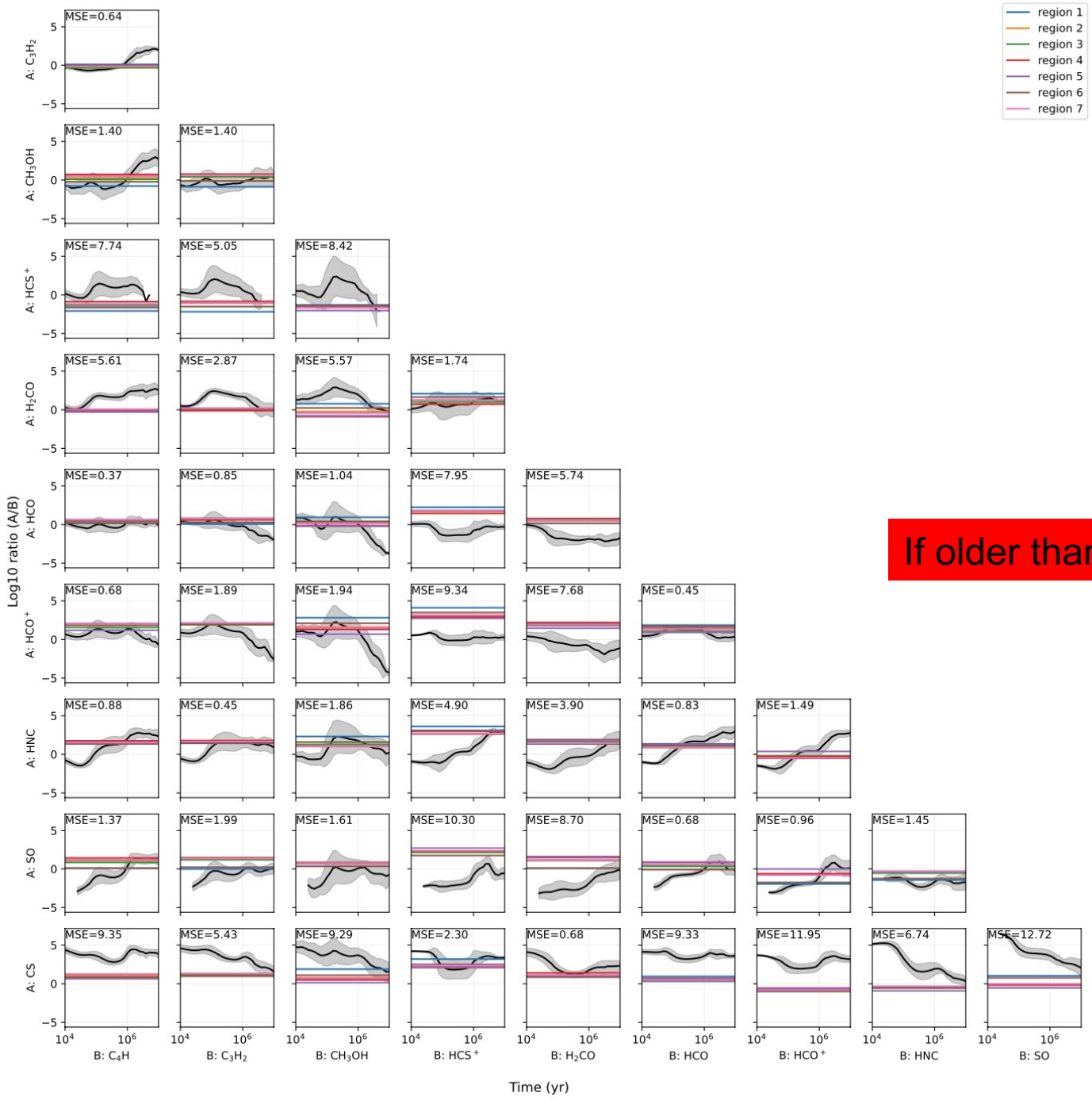
Molecules best fit:

In order: c-C3H2, HNC, HCO, C4H, CH3OH, HCO+ , SO, H2 CO, HCS+ , and finally CS.

Physical parameters best fits:

Densities: 10^3 to $10^{3.6}$ cm^{-3} Temperatures: 20 to 45 K,
FUV: < 5Go
ζ: ~ 10^{-17} s^{-1} - ~ 10^{-14} s^{-1}.

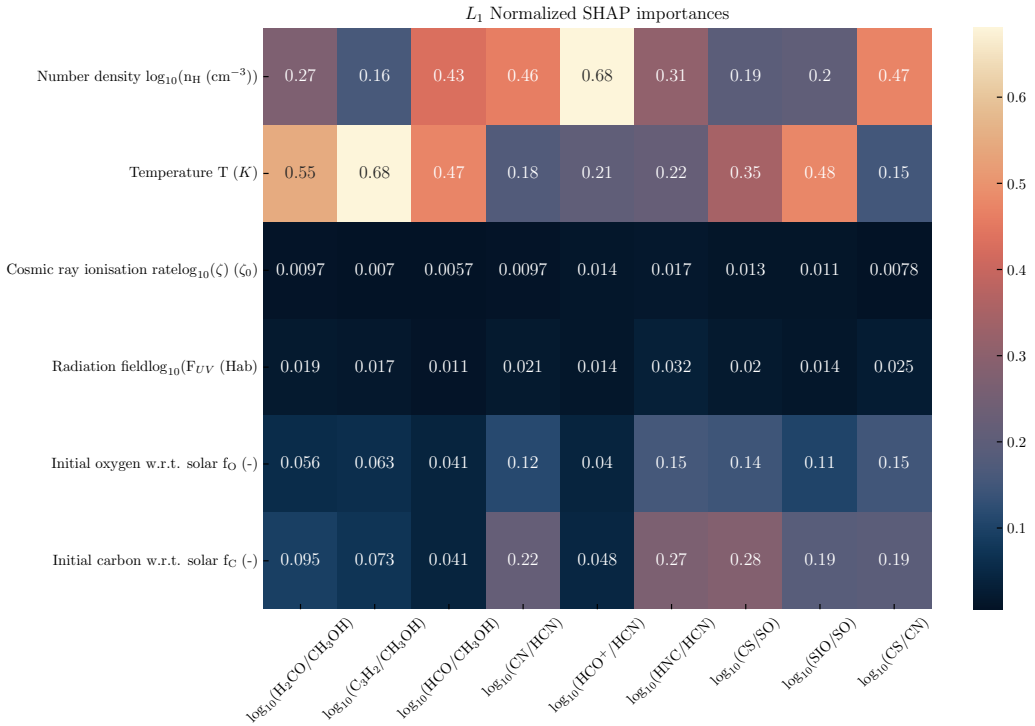
Star forming regions: young or old?



If older than 1 million years the fit is worst for most ratios

Understanding molecular ratios in the carbon and oxygen poor outer Milky Way with interpretable machine learning

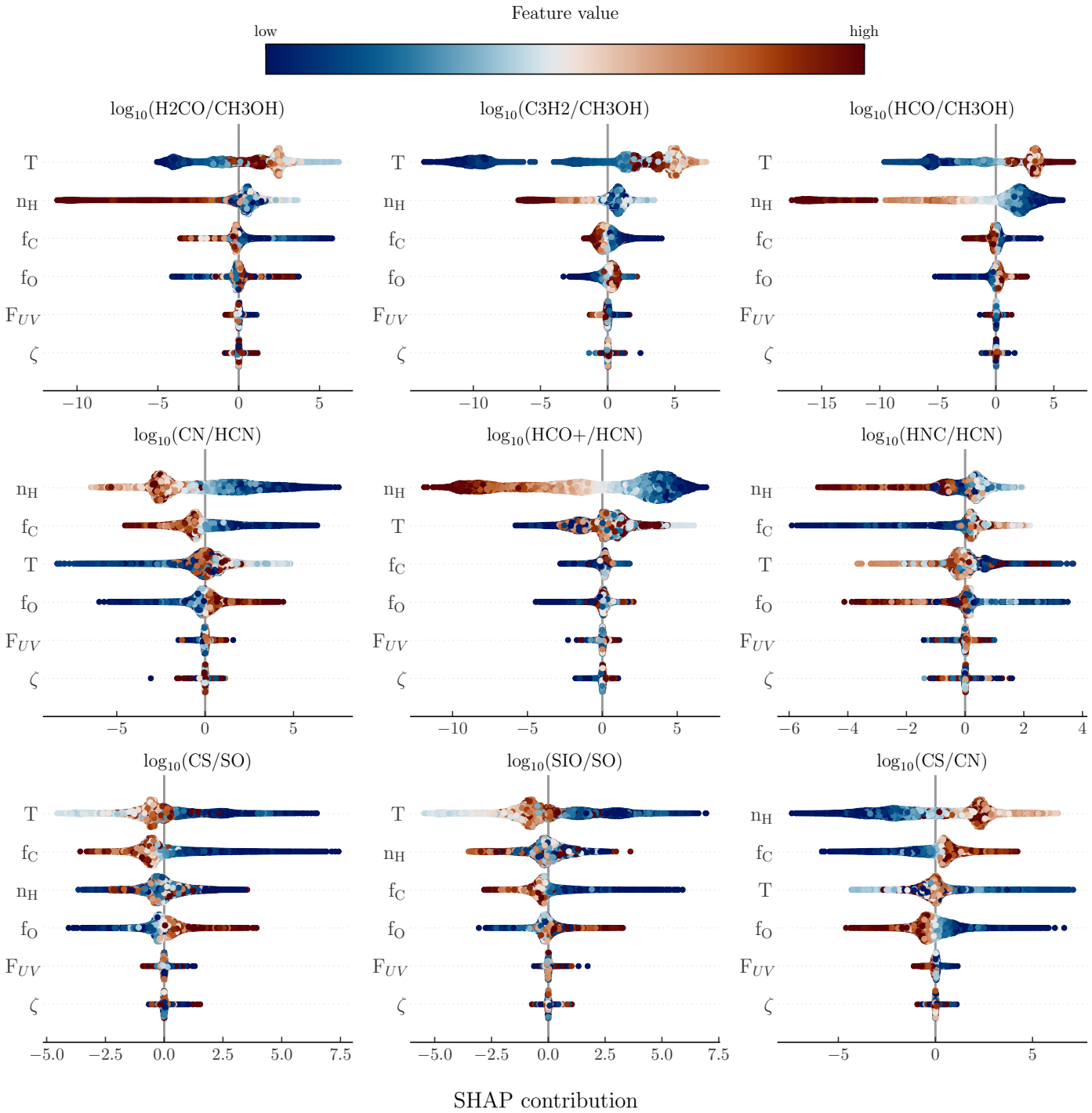
- Shapley Additive exPlainers (SHAP) → quantifies the contribution of each of the input parameter to the output prediction, treating it as an additive game.
- W euse train boosted regression forests and the TreeSHAP algorithm to extract explainers for each of the ratios.



Heatmap with the relative importance for each ratio as calculated by SHAP

Vermariën, Viti, Heyl, Fontani in prep.

Beeswarm plots



Some concluding remarks

- The effects of (i) Metallicity, (ii) dust to gas ratio, and (iii) ratio of elemental abundances need to be assessed individually
- Adding varying initial elemental abundances as free parameters increases the degree of freedom of chemical models
- Statistical/Machine Learning techniques may be necessary in order to quantify as well as interpret chemical models
- Chemical and chemical evolution models should be integrated
- Outer galaxy observations are still limited in spatial resolution → obstacle for chemical modelling of molecular ratios