COSMIC RAYS 2

The salt of the star formation recipe

Florence, 8-10 November 2022

The effect of cosmic rays on carbon isotopic fractionation

Laura Colzi

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9th November 2022

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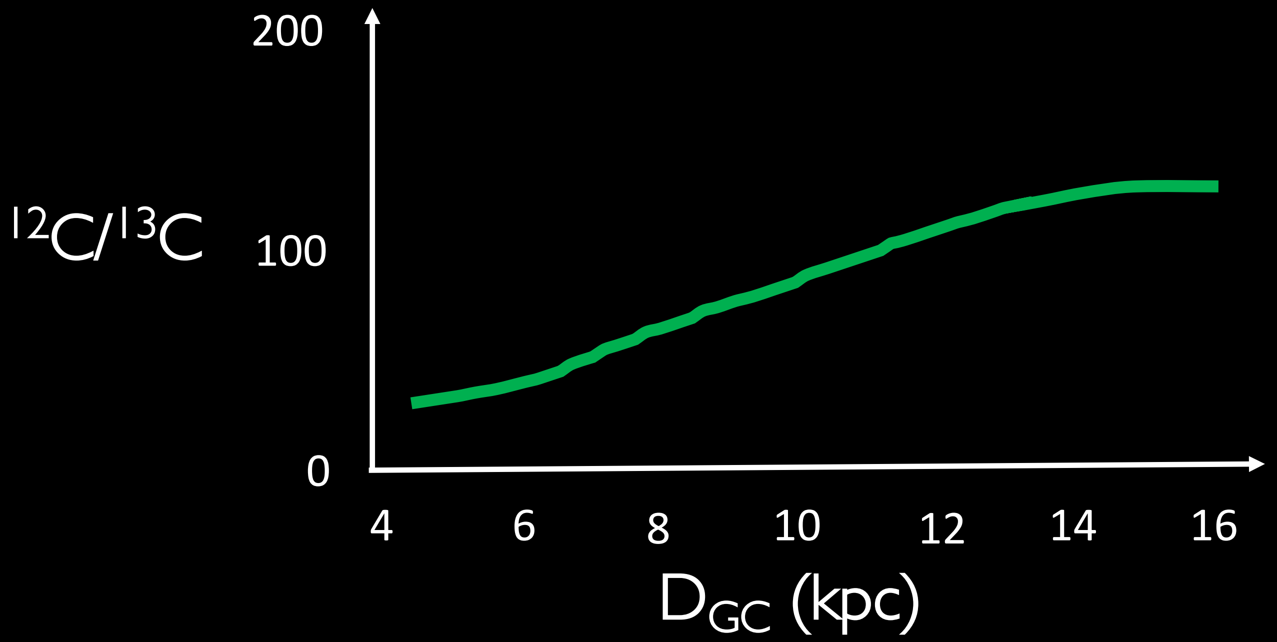
CENTRO DE ASTROBIOLOGÍA · CAB

ASOCIADO AL NASA ASTROBIOLOGY PROGRAM

CSIC INTA

AEI Retos project
PID2019-105552RB-C41

Isotopic ratios as stellar nucleosynthesis tracers



LINEAR
POSITIVE
TREND

Adapted from Colzi et al. (2022b)

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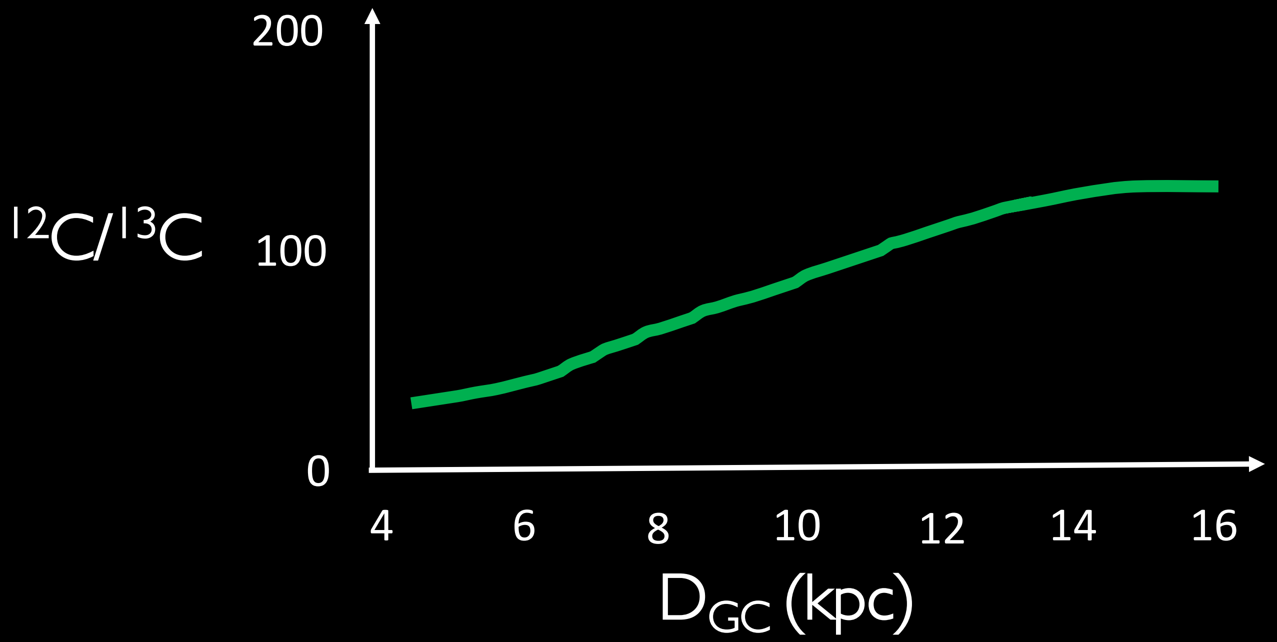


LINEAR
POSITIVE
TREND

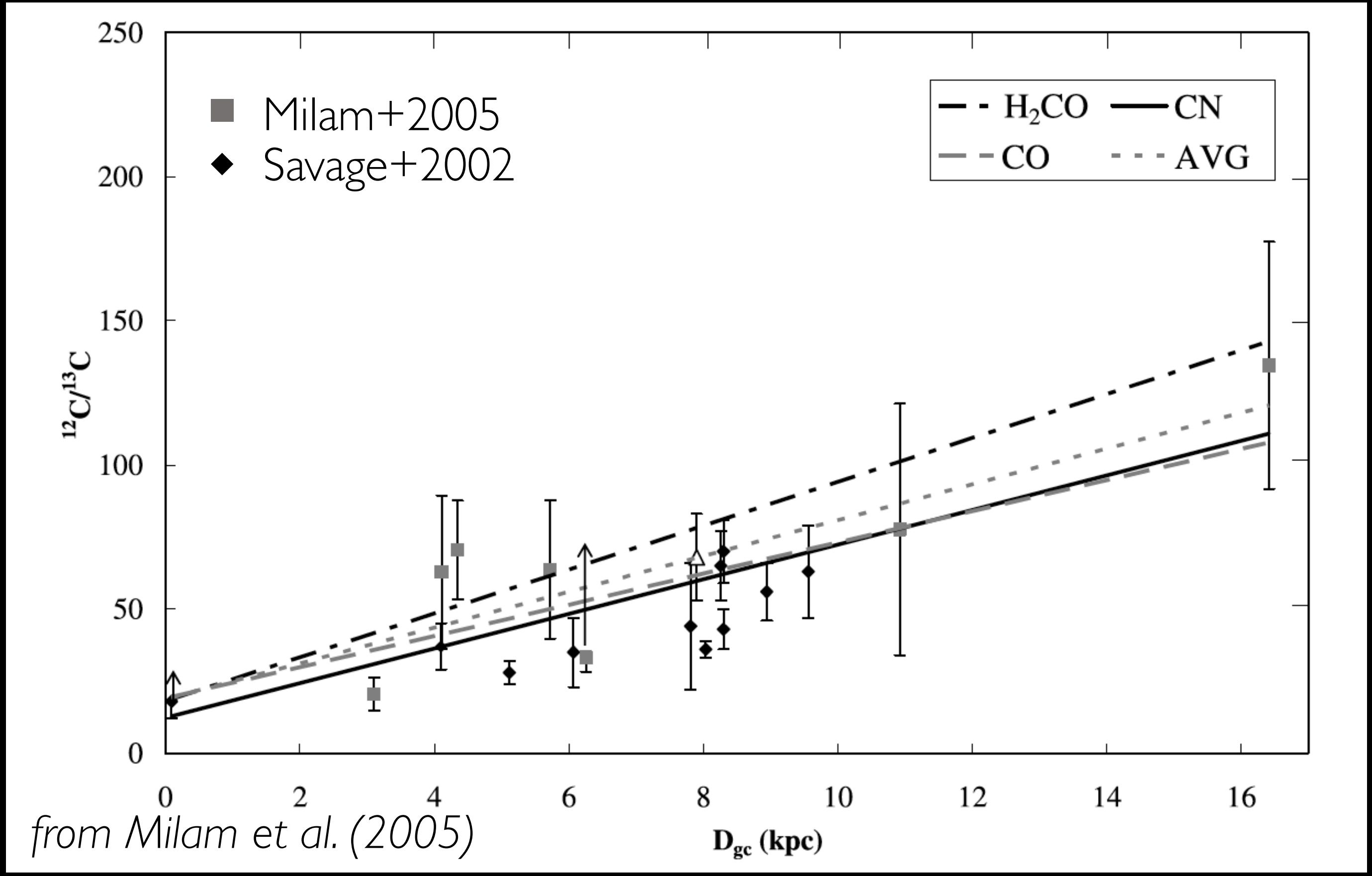
Adapted from Colzi et al. (2022b)

Galactic chemical evolution models *(e.g. Romano et al. 2017, 2019, Colzi et al. 2022b)*

^{12}C → Primary production in all stars.

^{13}C → Primary production from massive fast rotators at low metallicities,
Secondary production at high metallicity in all stars
In both cases **nova contribution on long timescales.**

$^{12}C/^{13}C$ as a function of D_{GC}



from Milam et al. (2005)

$^{12}CN/^{13}CN = (6.0 \pm 1.2)\, D_{GC}(kpc) + (12.3 \pm 9.3)$

$^{12}CO/^{13}CO = (5.4 \pm 1.1)\, D_{GC}(kpc) + (19.0 \pm 7.9)$

$H_2{}^{12}CO/H_2{}^{13}CO = (7.6 \pm 1.8)\, D_{GC}(kpc) + (18.0 \pm 10.8)$

$^{12}C/^{13}C = (6.2 \pm 1.0)\, D_{GC}(kpc) + (18.7 \pm 7.4)$

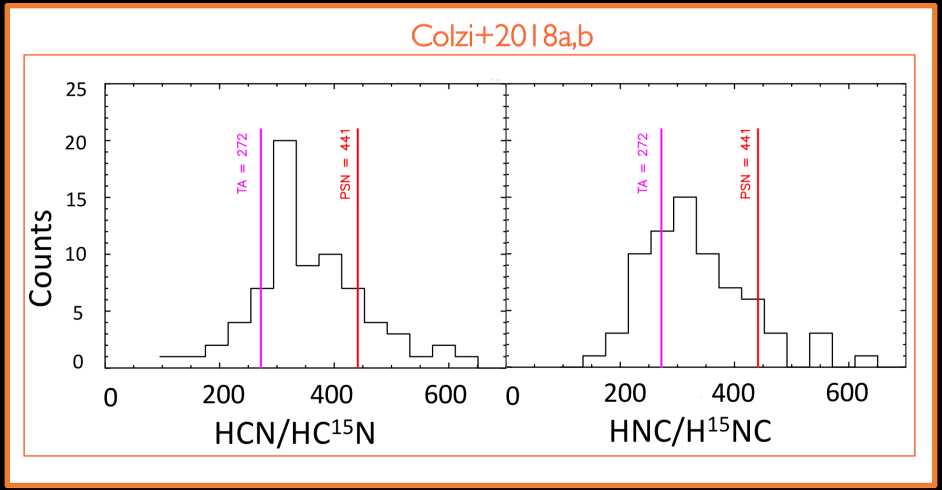
Sun distance 7.9 kpc

(Hunt et al. 2016 and Boehle et al. 2016)

→ local $^{12}C/^{13}C$=68±15

CN: Milam et al. (2005), Savage et al. (2002), CO: Langer& Penzias (1990, 1993), Keene et al. (1998), and Wouterloot & Brand (1996), H_2CO: Henkel et al. (1980, 1982, 1983, 1985), Gardner & Whiteoak (1979), and Gusten et al. (1985). See also Yan et al. (2019).

$^{14}N/^{15}N$ of nitriles derived with the double-isotope method


Colzi+2018a,b

And many more….
Adande et al. (2012)
Hily-Blant et al. (2013)
Wampfler et al. (2014)
Zeng et al. (2017)
….

$$HCN/HC^{15}N = H^{13}CN/HC^{15}N \times \boxed{^{12}C/^{13}C}$$

→ ASSUMED FROM THE GALACTOCENTRIC DEPENDENCE

$$\boxed{^{12}C/^{13}C = (6.01 \pm 1.19)\, D_{gc}(kpc) + (12.28 \pm 9.33)}$$

Milam et al. (2005)

$$\boxed{^{12}C/^{13}C = (5.08 \pm 1.10)\, D_{gc}(kpc) + (11.86 \pm 6.60)}$$

Yan et al. (2019)

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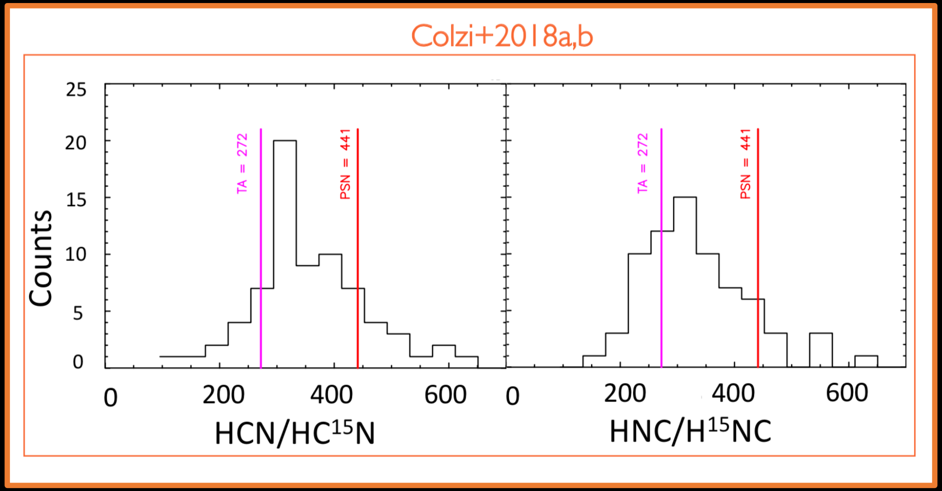

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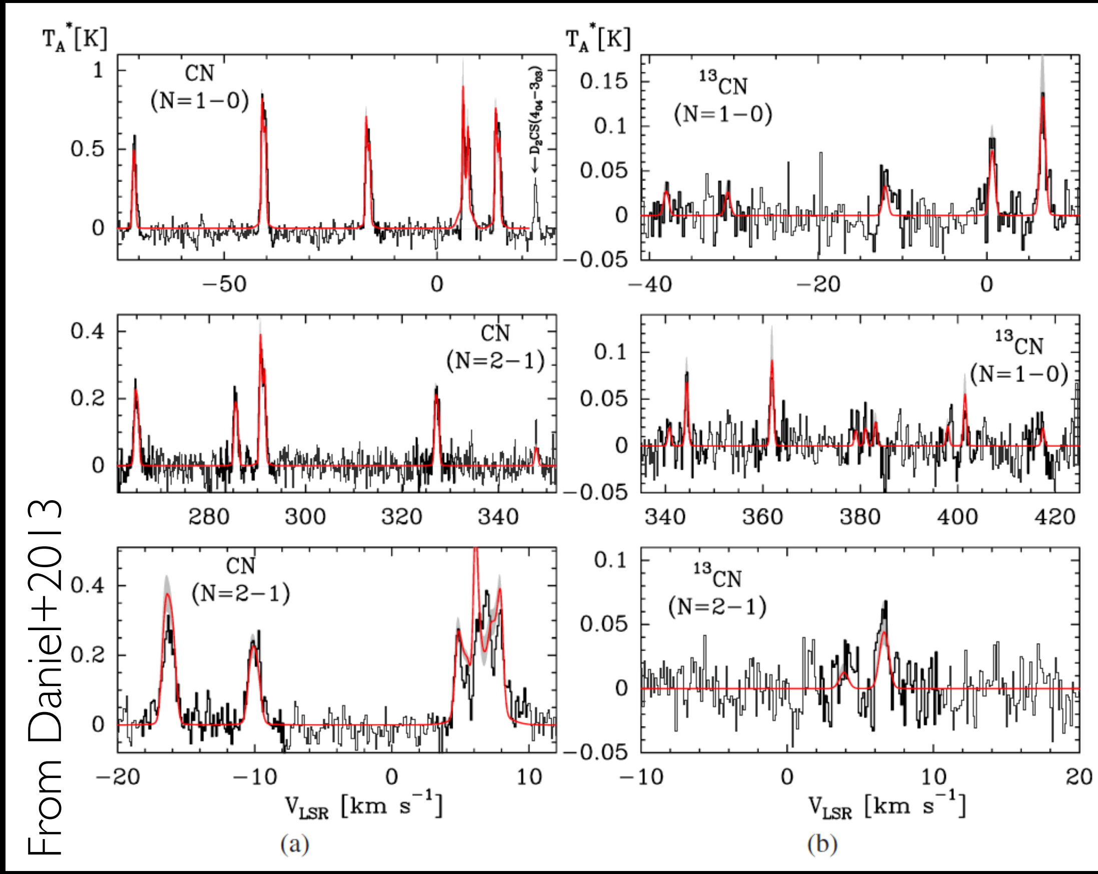
→ LOCAL CHEMICAL FRACTIONATION EFFECTS CAN ALSO BE IMPORTANT

Some observed values

Daniel et al. (2013) towards the pre-stellar core B1b found
CN/^{13}CN= 50±19
HCN/H^{13}CN= 30±7
HNC/HN^{13}C= 20±5

Magalhães et al. (2018) towards the pre-stellar core L1498 measured
HCN/H^{13}CN= 45±3



From Daniel+2013

All **values different than** the local ISM value of 68

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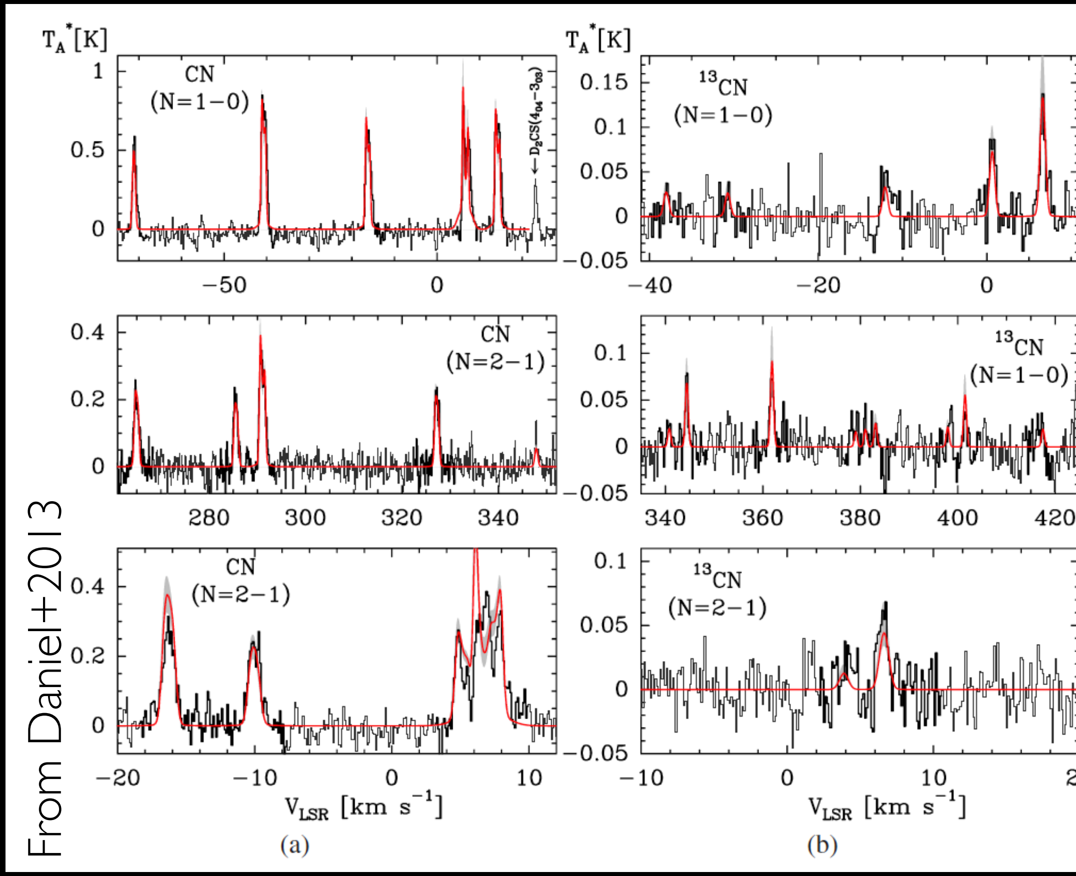


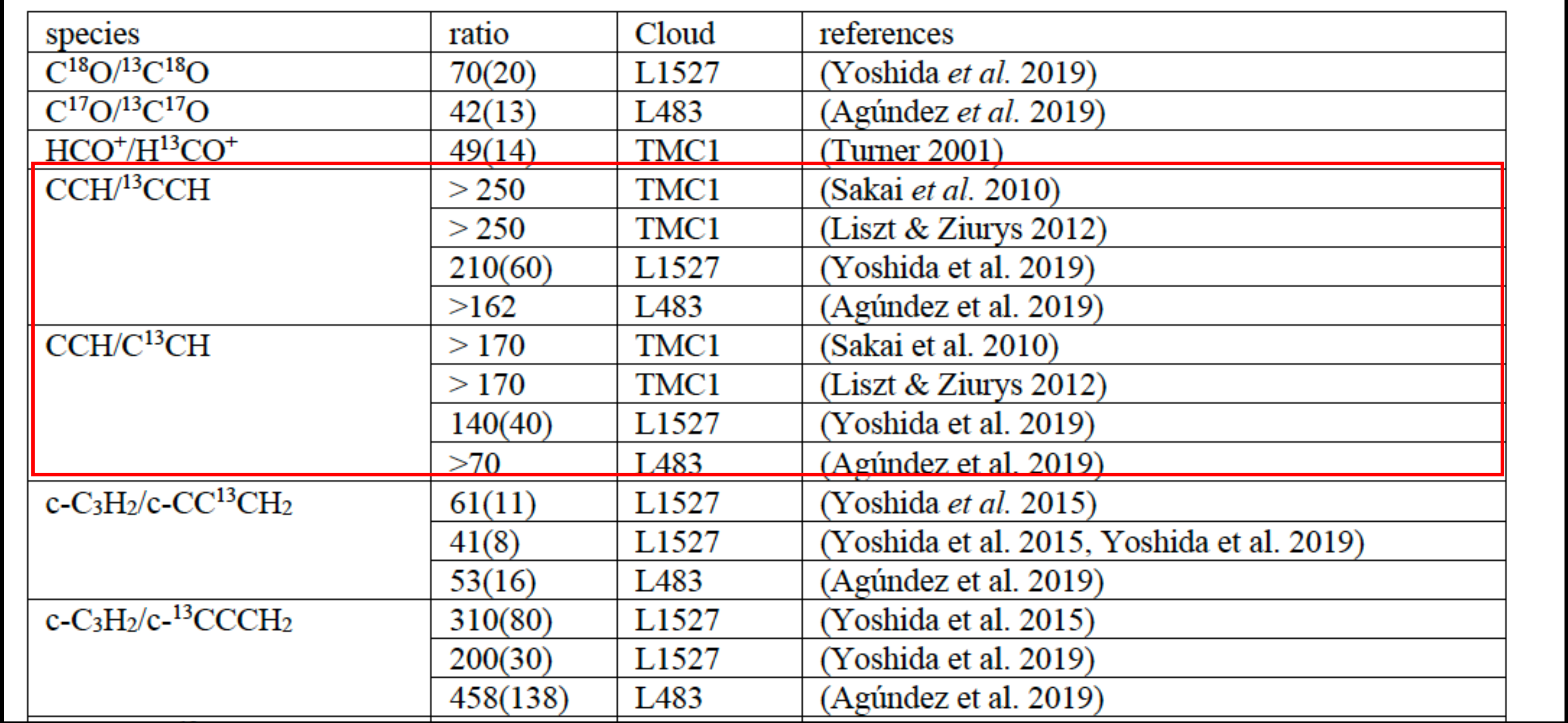
From Daniel+2013

All **values different than** the local ISM value of 68

AN INDEPENDENT DETERMINATION OF C-FRACTIONATION IS NEEDED

Some observed values

From Loison+2020

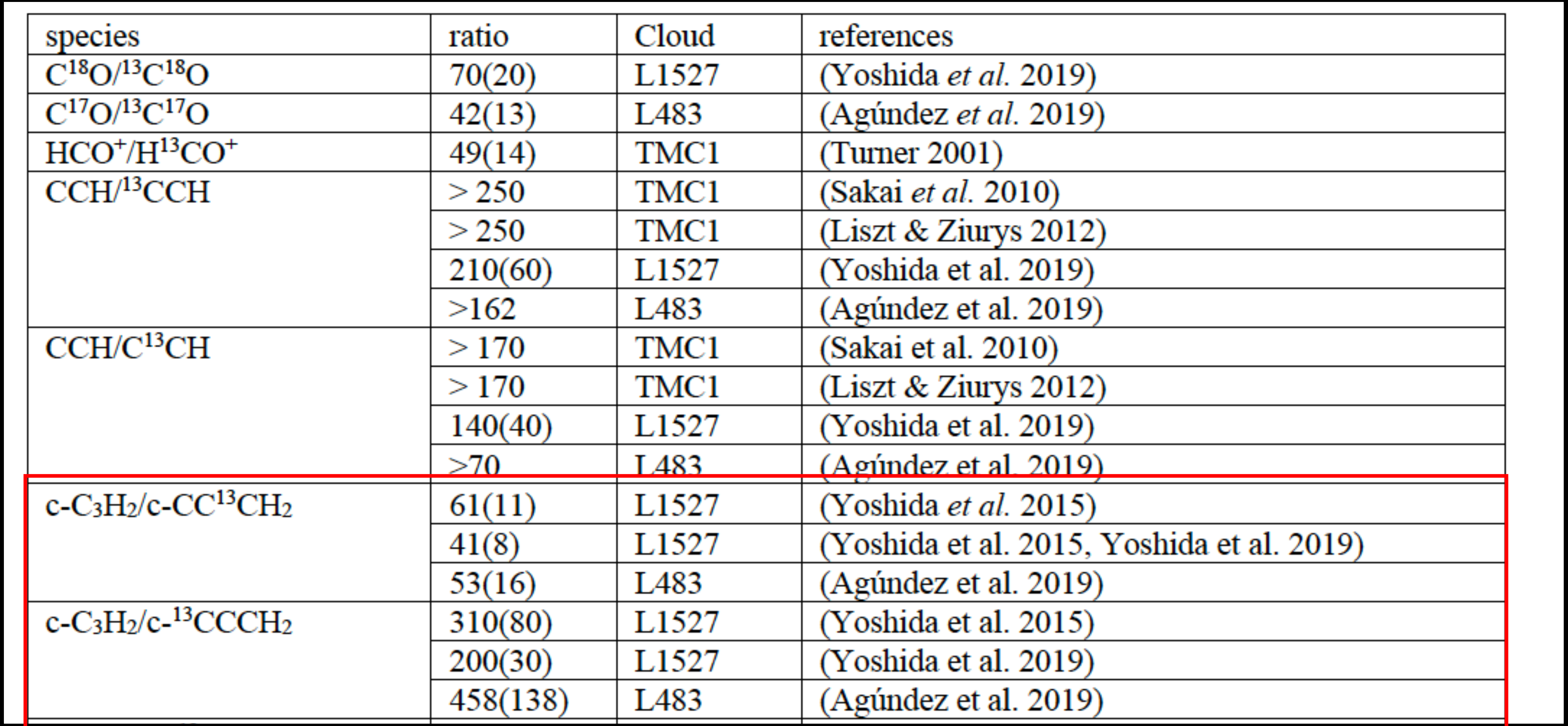


species	ratio	Cloud	references
$C^{18}O/^{13}C^{18}O$	70(20)	L1527	(Yoshida *et al.* 2019)
$C^{17}O/^{13}C^{17}O$	42(13)	L483	(Agúndez *et al.* 2019)
$HCO^+/H^{13}CO^+$	49(14)	TMC1	(Turner 2001)
$CCH/^{13}CCH$	> 250	TMC1	(Sakai *et al.* 2010)
	> 250	TMC1	(Liszt & Ziurys 2012)
	210(60)	L1527	(Yoshida et al. 2019)
	>162	L483	(Agúndez et al. 2019)
$CCH/C^{13}CH$	> 170	TMC1	(Sakai et al. 2010)
	> 170	TMC1	(Liszt & Ziurys 2012)
	140(40)	L1527	(Yoshida et al. 2019)
	>70	L483	(Agúndez et al. 2019)
$c\text{-}C_3H_2/c\text{-}CC^{13}CH_2$	61(11)	L1527	(Yoshida *et al.* 2015)
	41(8)	L1527	(Yoshida et al. 2015, Yoshida et al. 2019)
	53(16)	L483	(Agúndez et al. 2019)
$c\text{-}C_3H_2/c\text{-}^{13}CCCH_2$	310(80)	L1527	(Yoshida et al. 2015)
	200(30)	L1527	(Yoshida et al. 2019)
	458(138)	L483	(Agúndez et al. 2019)

Dependence on the molecule

Some observed values

From Loison+2020



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Dependence on the position of the ^{13}C

Chemical fractionation effects

Low-temperature isotopic exchange reactions

$^{13}C + ^{12}CO \longrightarrow ^{13}CO + ^{12}C^{+} + 34.7\ K$

Watson et al. (1976); Langer et al. (1984)

$HCO^{+} + ^{13}CO \longrightarrow H^{13}CO^{+} + ^{12}CO + 17.4\ K$

Langer et al. (1978); Smith and Adams (1980); Mladenovic and Roueff (2014)

Chemical fractionation effects

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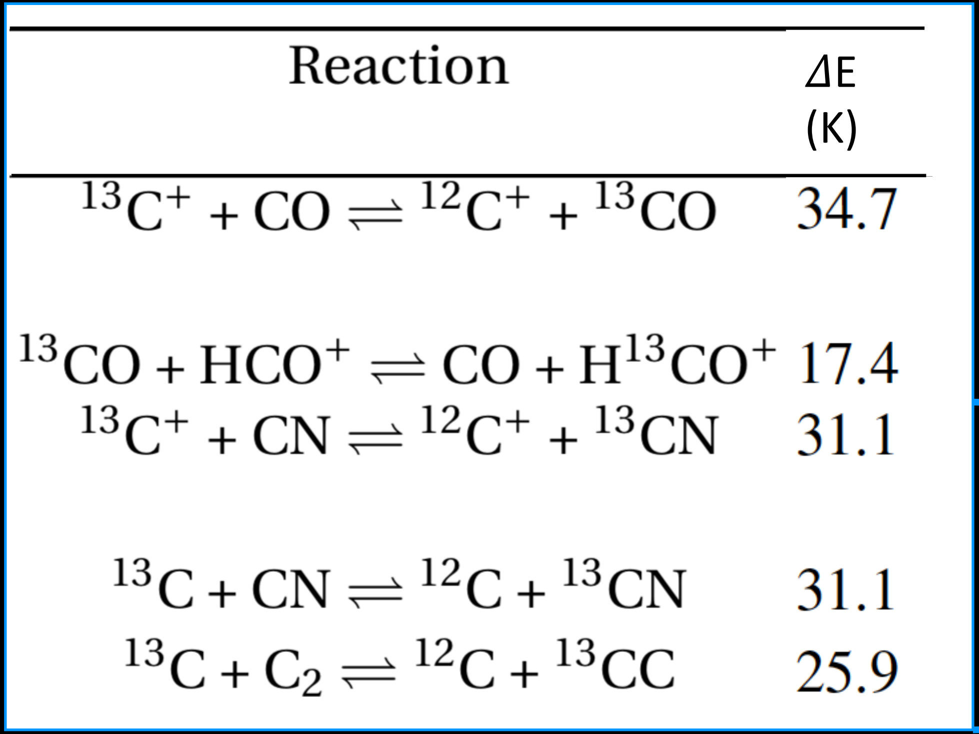
$\mathrm{HCO}^+ + {}^{13}\mathrm{CO} \rightarrow \mathrm{H}^{13}\mathrm{CO}^+ + {}^{12}\mathrm{CO} + \boxed{17.4\ \mathrm{K}}$ *Langer et al. (1978); Smith and Adams (1980); Mladenovic and Roueff (2014)*

Note: typical temperatures for low- and high-mass starless cores could be between 5 and 20 K (Crapsi+2007; Fontani+2011)

Chemical fractionation effects

Low-temperature isotopic exchange reactions

Roueff et al. (2015) – gas-phase + simulated depletion of molecules varying initial abundances



Reaction	ΔE (K)
$^{13}C^+ + CO \rightleftharpoons {}^{12}C^+ + {}^{13}CO$	34.7
$^{13}CO + HCO^+ \rightleftharpoons CO + H^{13}CO^+$	17.4
$^{13}C^+ + CN \rightleftharpoons {}^{12}C^+ + {}^{13}CN$	31.1
$^{13}C + CN \rightleftharpoons {}^{12}C + {}^{13}CN$	31.1
$^{13}C + C_2 \rightleftharpoons {}^{12}C + {}^{13}CC$	25.9

Watson et al. (1976); Langer et al. (1984)

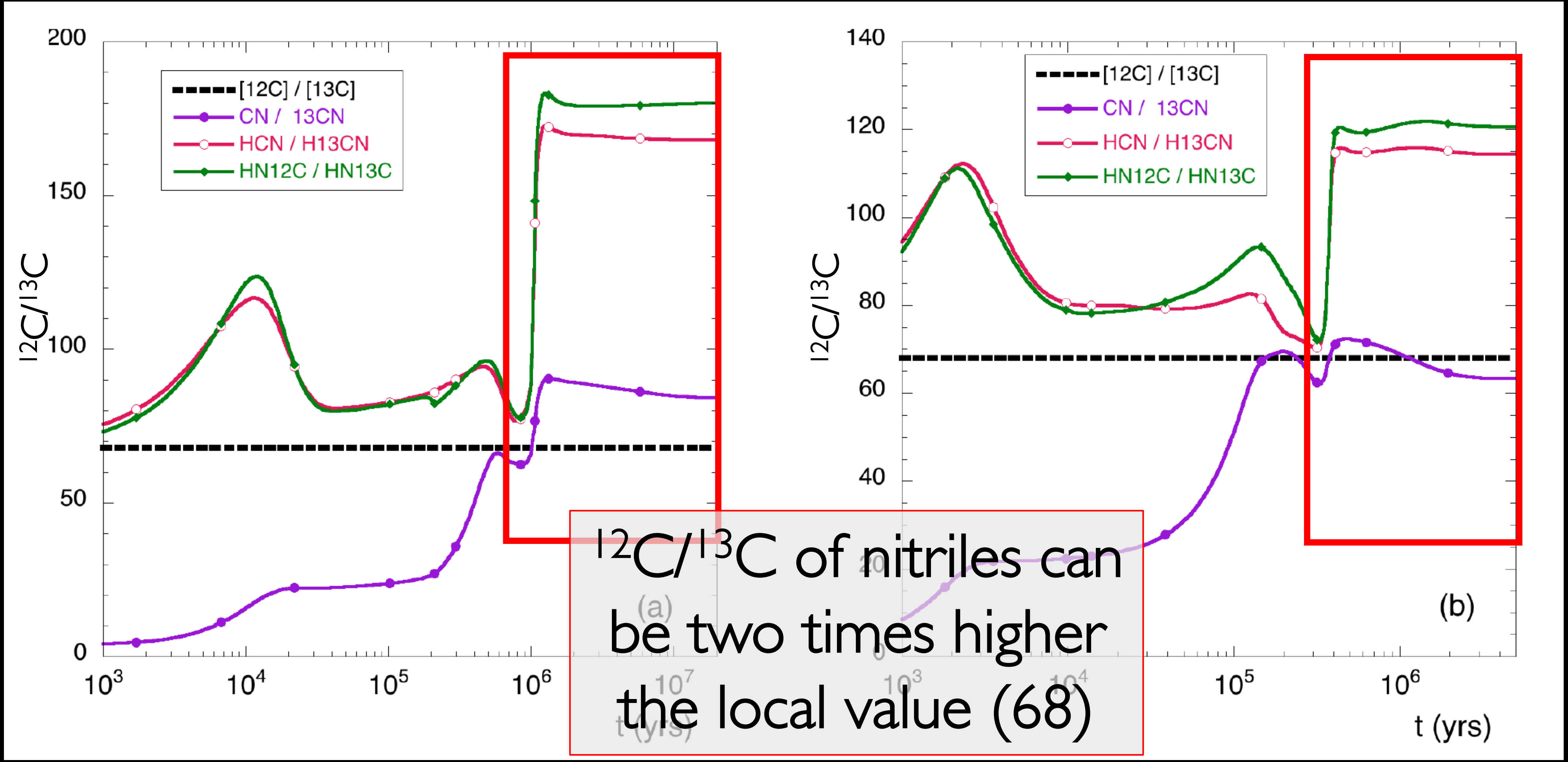
Langer et al. (1978); Smith and Adams (1980); Mladenovic and Roueff (2014)

Roueff et al. (2015)

Chemical fractionation effects

Roueff et al. (2015) – **gas-phase** + simulated depletion of molecules varying initial abundances

T=10 K   Starless core model $n_H=2\times10^4$ cm^{-3} Pre-stellar core model $n_H=2\times10^5$ cm^{-3}



$^{12}C/^{13}C$ of nitriles can be two times higher the local value (68)

Carbon isotopic fractionation in molecular clouds

Colzi et al. (2020)

gas-grain chemical model starting from KIDA network (Wakelam et al. 2015)

[For more information about the chemical code and type of reactions see Sipilä et al. (2015a, 2019b)]

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

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$H + CCN \rightarrow C + HCN$ Branching Ratio=1

$H + C^{13}CN \rightarrow C + H^{13}CN$ BR=1/2

$H + C^{13}CN \rightarrow {}^{13}C + HCN$ BR=1/2

$H + {}^{13}C^{13}CN \rightarrow {}^{13}C + H^{13}CN$ BR=1

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$H + C^{13}CN \rightarrow {}^{13}C + HCN$ BR=1/2

$H + {}^{13}C^{13}CN \rightarrow {}^{13}C + H^{13}CN$ BR=1

→ Molecules with up 5 atoms

→ Inclusion of ^{13}C in molecules with up to three carbon atoms

$H^{13}C_3N$ YES $^{13}C_3{}^{12}C$ NO

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

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$\mathbf{H + CCN \rightarrow C + HCN}$ **Branching Ratio=1**

$H + C^{13}CN \rightarrow C + H^{13}CN$ BR=1/2

$H + C^{13}CN \rightarrow {}^{13}C + HCN$ BR=1/2

$H + {}^{13}C^{13}CN \rightarrow {}^{13}C + H^{13}CN$ BR=1

→We do not take into account the different possible position of the ^{13}C

(Loison+2020; Sipilä, Colzi et al. in prep.)

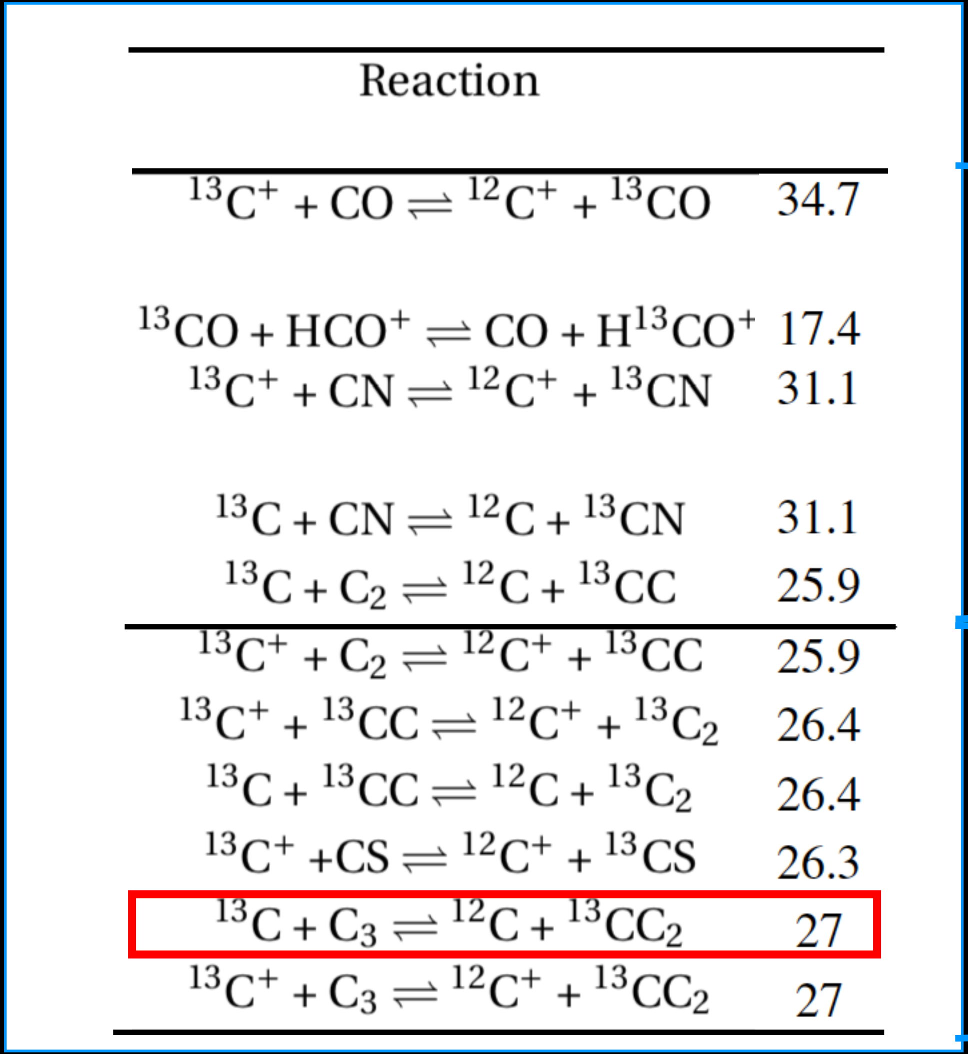
$^{13}CCN = C^{13}CN$

TOTAL of 11500 chemical reactions

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

Carbon isotopic fractionation in molecular clouds

NEW low-temperature isotopic exchange reactions



Reaction	
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$^{13}C + C_2 \rightleftharpoons {}^{12}C + {}^{13}CC$	25.9
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$^{13}C^+ + {}^{13}CC \rightleftharpoons {}^{12}C^+ + {}^{13}C_2$	26.4
$^{13}C + {}^{13}CC \rightleftharpoons {}^{12}C + {}^{13}C_2$	26.4
$^{13}C^+ + CS \rightleftharpoons {}^{12}C^+ + {}^{13}CS$	26.3
$^{13}C + C_3 \rightleftharpoons {}^{12}C + {}^{13}CC_2$	27
$^{13}C^+ + C_3 \rightleftharpoons {}^{12}C^+ + {}^{13}CC_2$	27

OLD REACTIONS FROM ROUEFF ET AL. (2015)

NEW REACTIONS FROM THIS WORK

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

Carbon isotopic fractionation in molecular clouds

The Fiducial Model

PHYSICAL PARAMETERS:

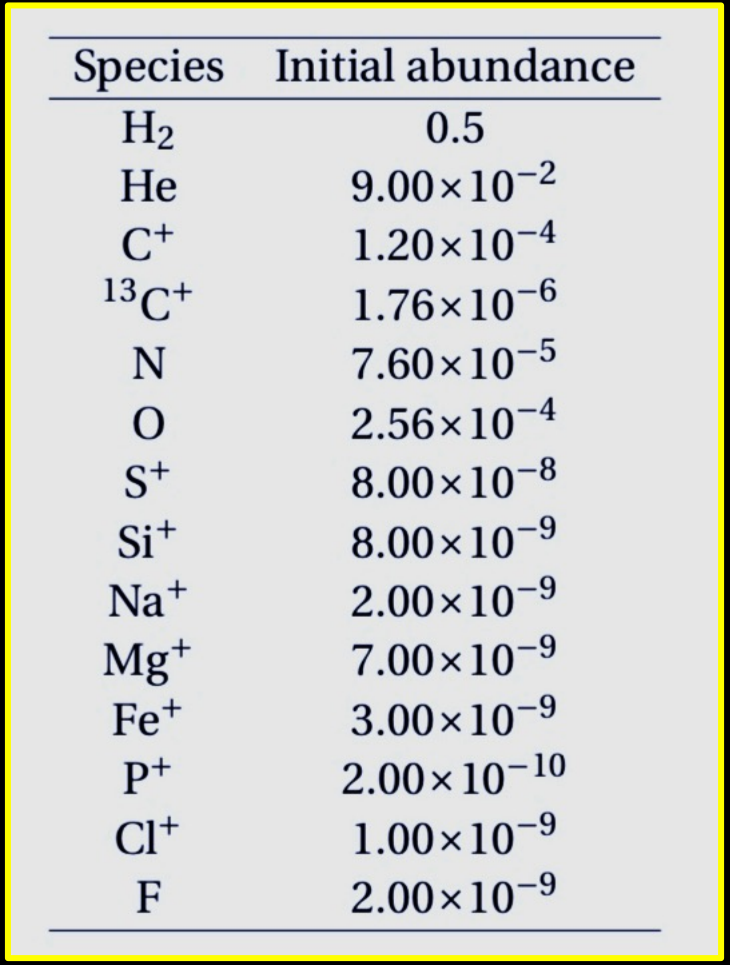
ζ = 1.3 x 10^{-17} s^{-1} cosmic-ray ionization rate

A_V = 10 mag visual extinction

T_{gas} = T_{dust} = 10 K

n_H = 2 x 10^4 cm^{-3}

Initial $^{12}C^+/^{13}C^+$=68 **(local ISM)** and gas in atomic form except H_2



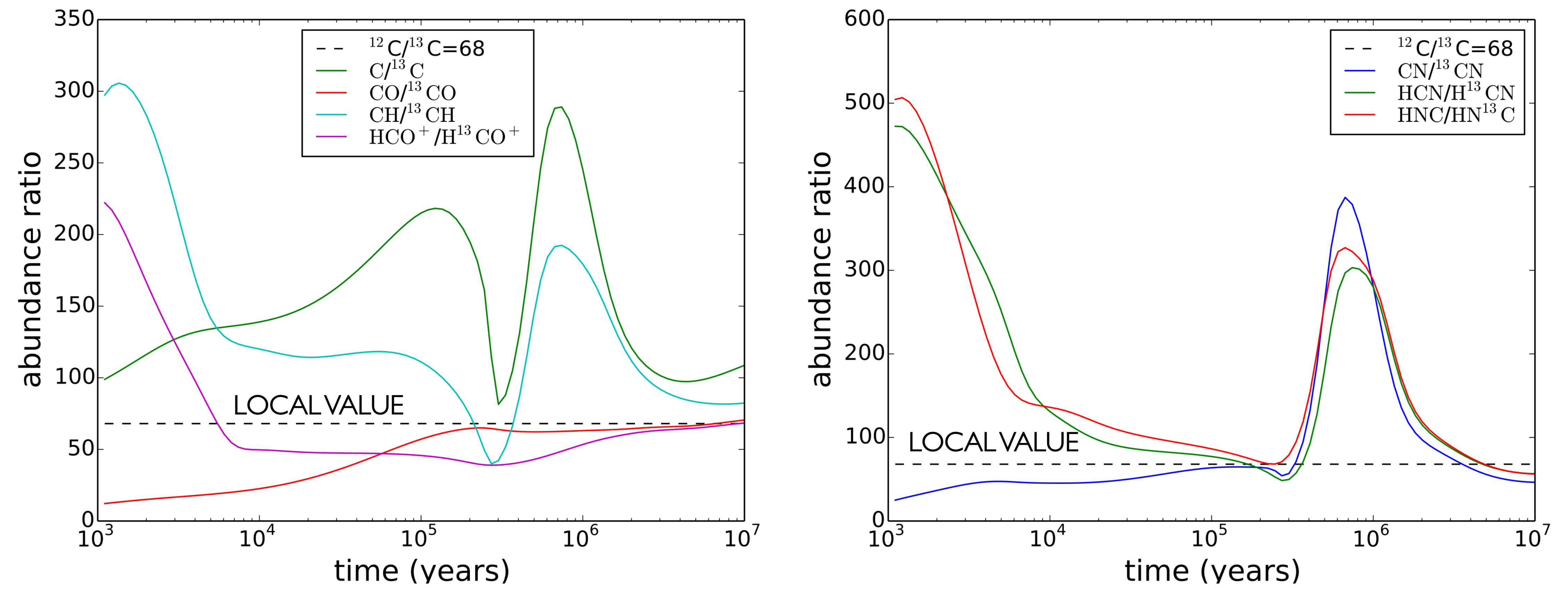
Species	Initial abundance
H_2	0.5
He	9.00×10^{-2}
C^+	1.20×10^{-4}
$^{13}C^+$	1.76×10^{-6}
N	7.60×10^{-5}
O	2.56×10^{-4}
S^+	8.00×10^{-8}
Si^+	8.00×10^{-9}
Na^+	2.00×10^{-9}
Mg^+	7.00×10^{-9}
Fe^+	3.00×10^{-9}
P^+	2.00×10^{-10}
Cl^+	1.00×10^{-9}
F	2.00×10^{-9}

Semenov et al. (2010)

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

Carbon isotopic fractionation in molecular clouds

The Fiducial Model



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Carbon isotopic fractionation in molecular clouds

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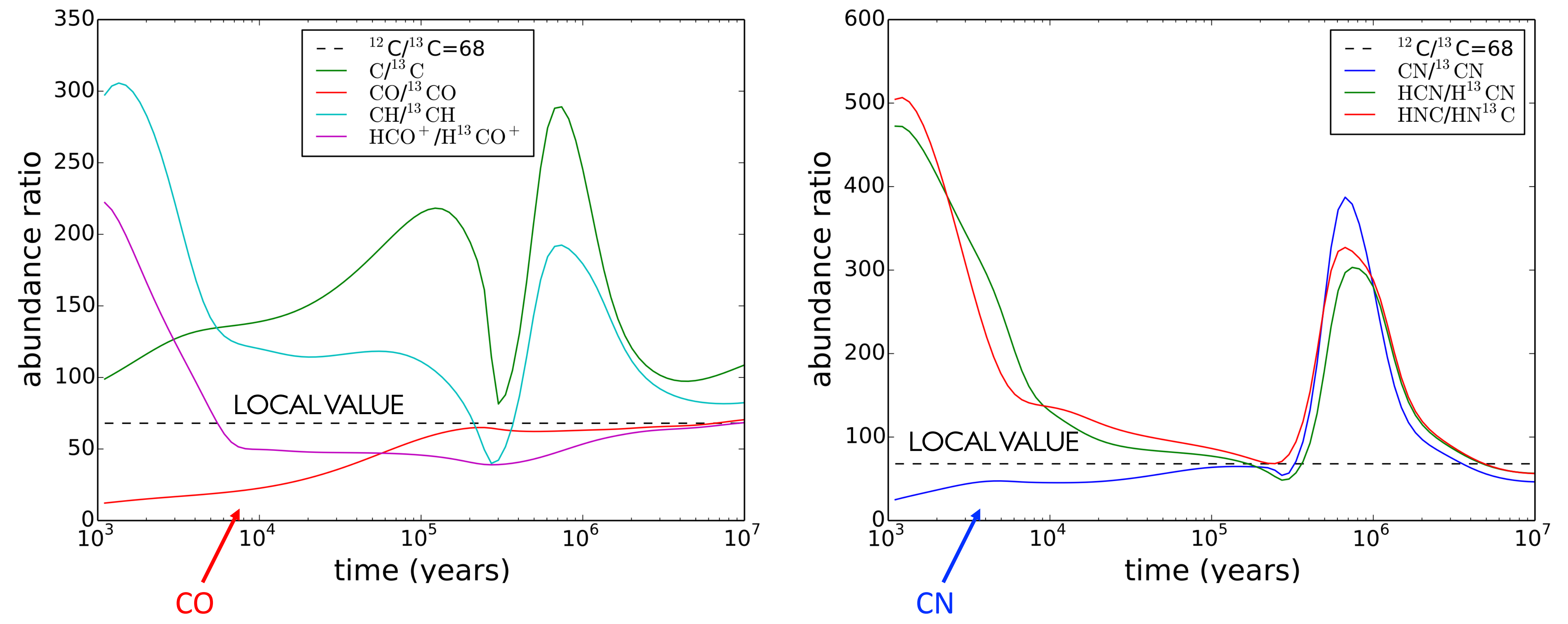


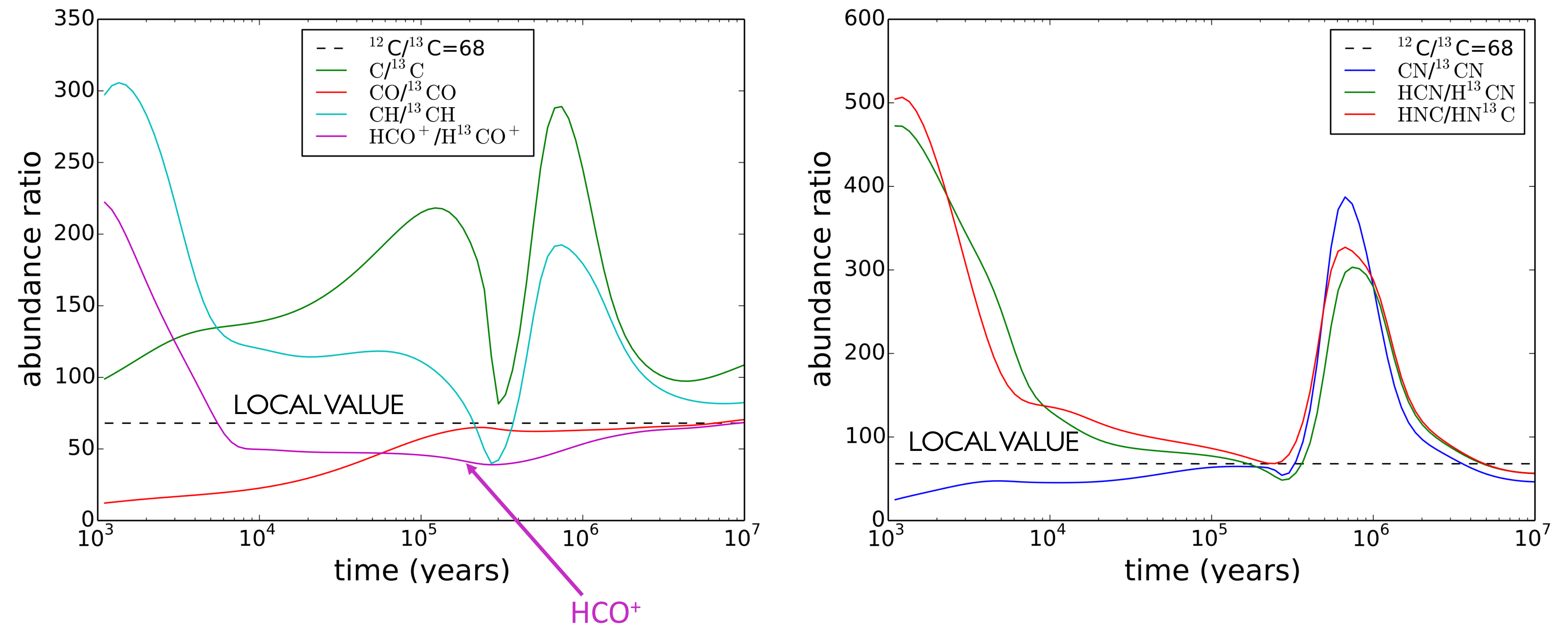
$^{13}C^+ + {}^{12}CO \rightarrow {}^{13}CO + {}^{12}C^+ + 35$ K

$^{13}C^+ + {}^{12}CN \rightarrow {}^{13}CN + {}^{12}C^+ + 31$ K

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

Carbon isotopic fractionation in molecular clouds

The Fiducial Model



$HCO^+ + {}^{13}CO \longrightarrow H^{13}CO^+ + {}^{12}CO + 17.4$ K

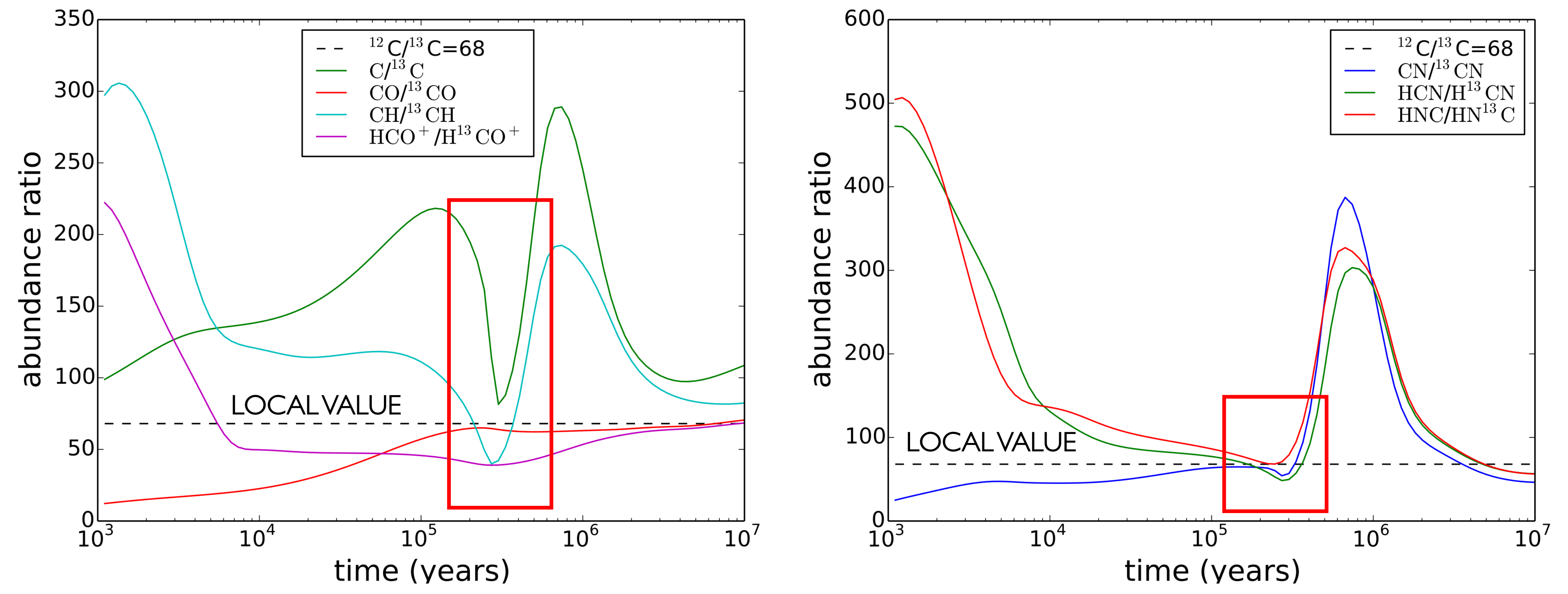
CO and HCO^+ are the main reservoirs of ^{13}C at 10 K

Laura Colzi

Reference: Colzi, L. , et al., 2020, accepted by A&A, arXiv:2006.03362

Carbon isotopic fractionation in molecular clouds

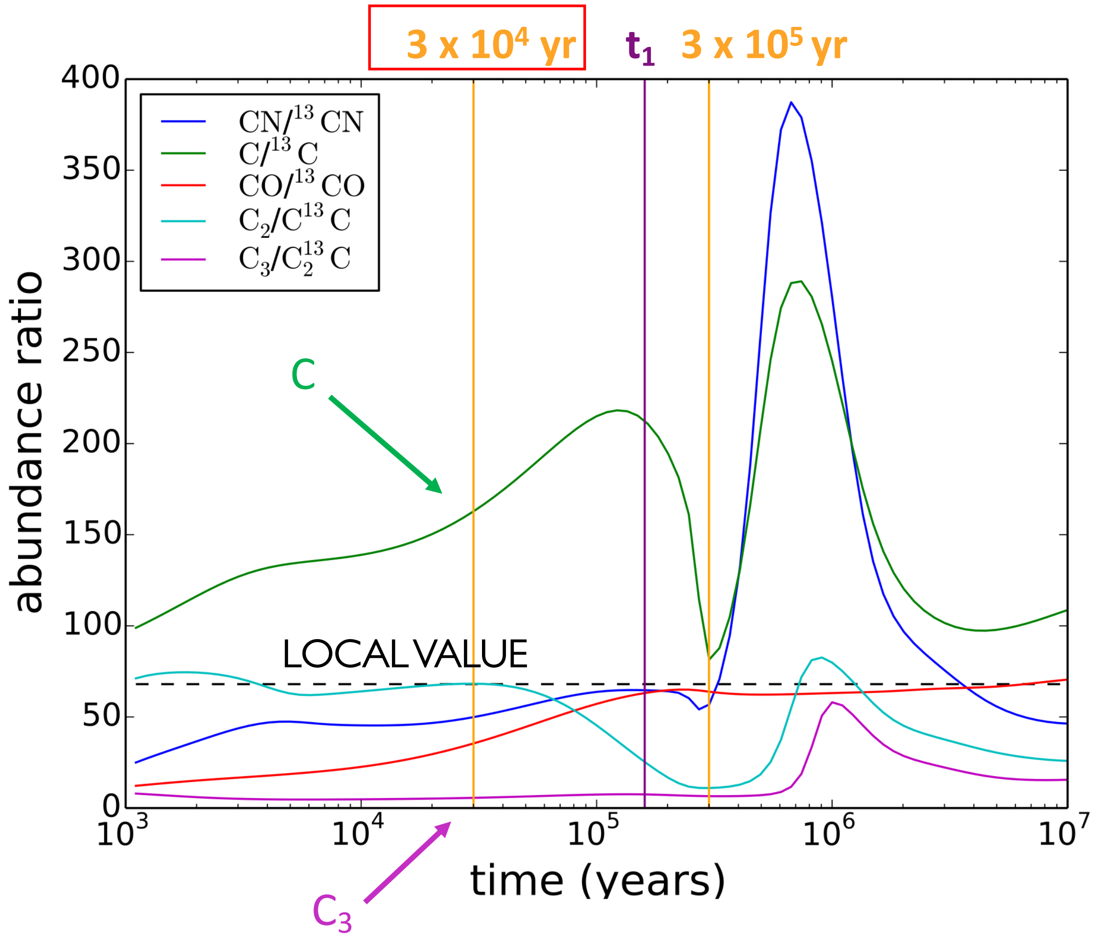
The Fiducial Model



Range of time in which ^{12}C/^{13}C ratios decrease

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The importance of C_3 isotopic exchange reaction

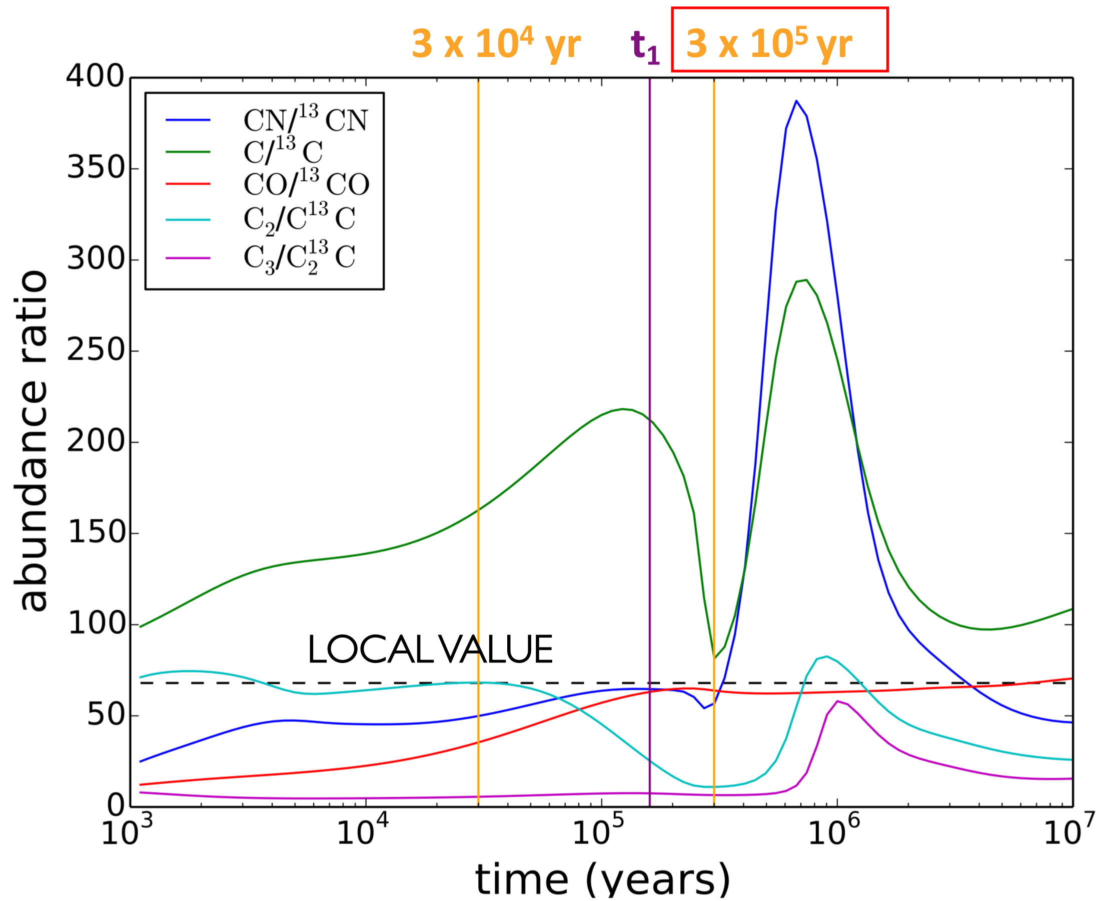


$t = 3x10^4$ yr < $t_1 = 1.6x10^5$ yr

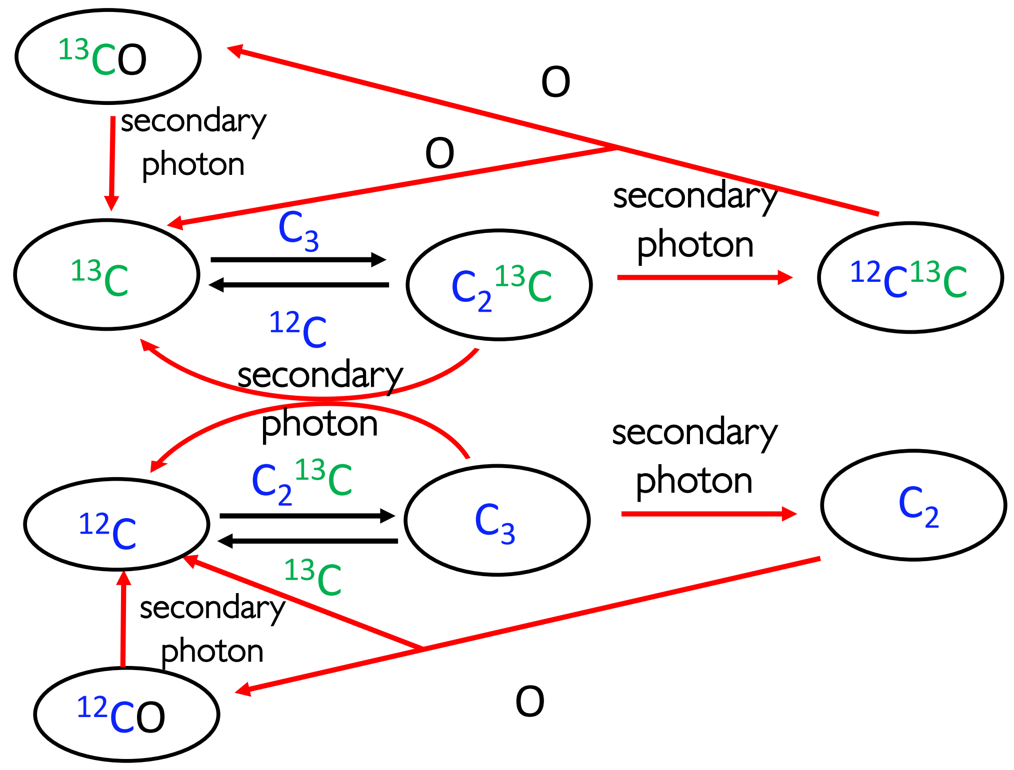
$$^{13}C + C_3 \longrightarrow {}^{12}C + {}^{13}CC_2 + 27\ K$$

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The importance of C_3 isotopic exchange reaction



$t = 3 \times 10^5$ yr > $t_1 = 1.6 \times 10^5$ yr



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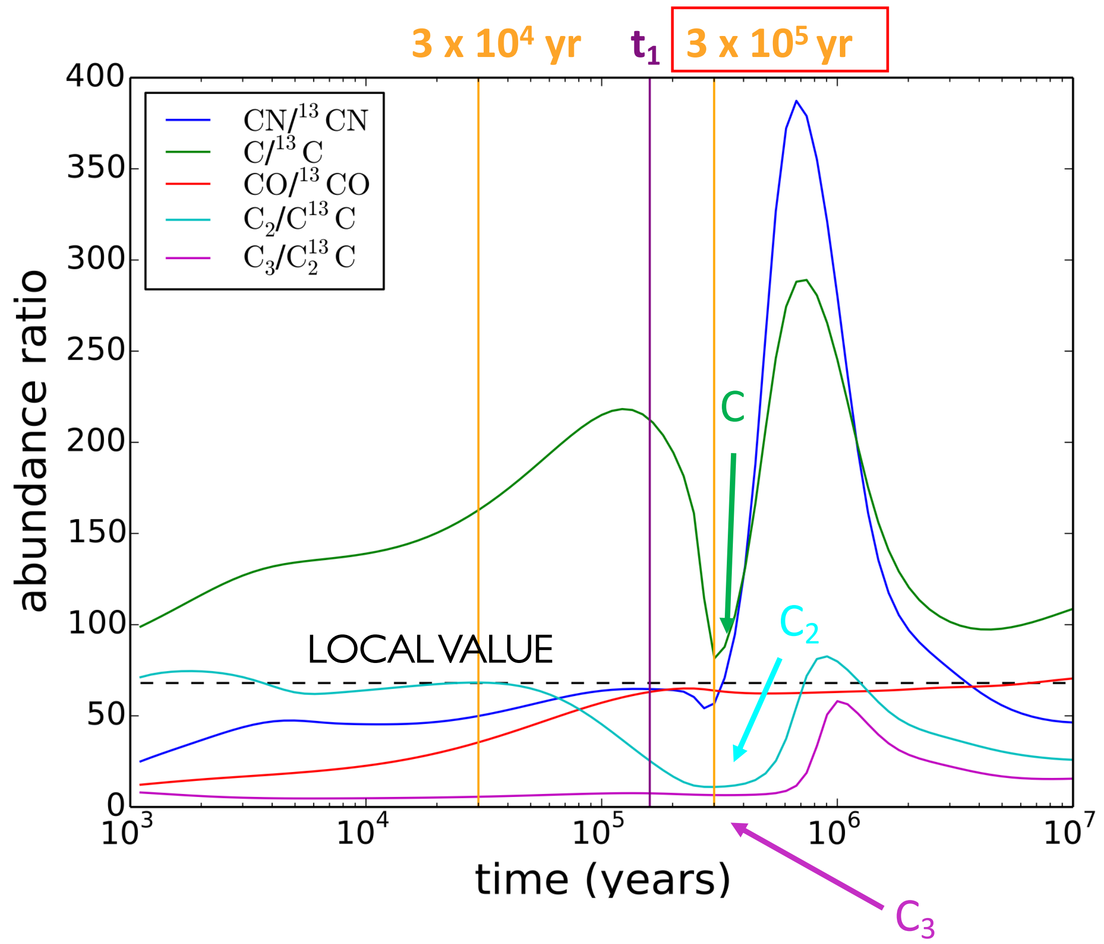
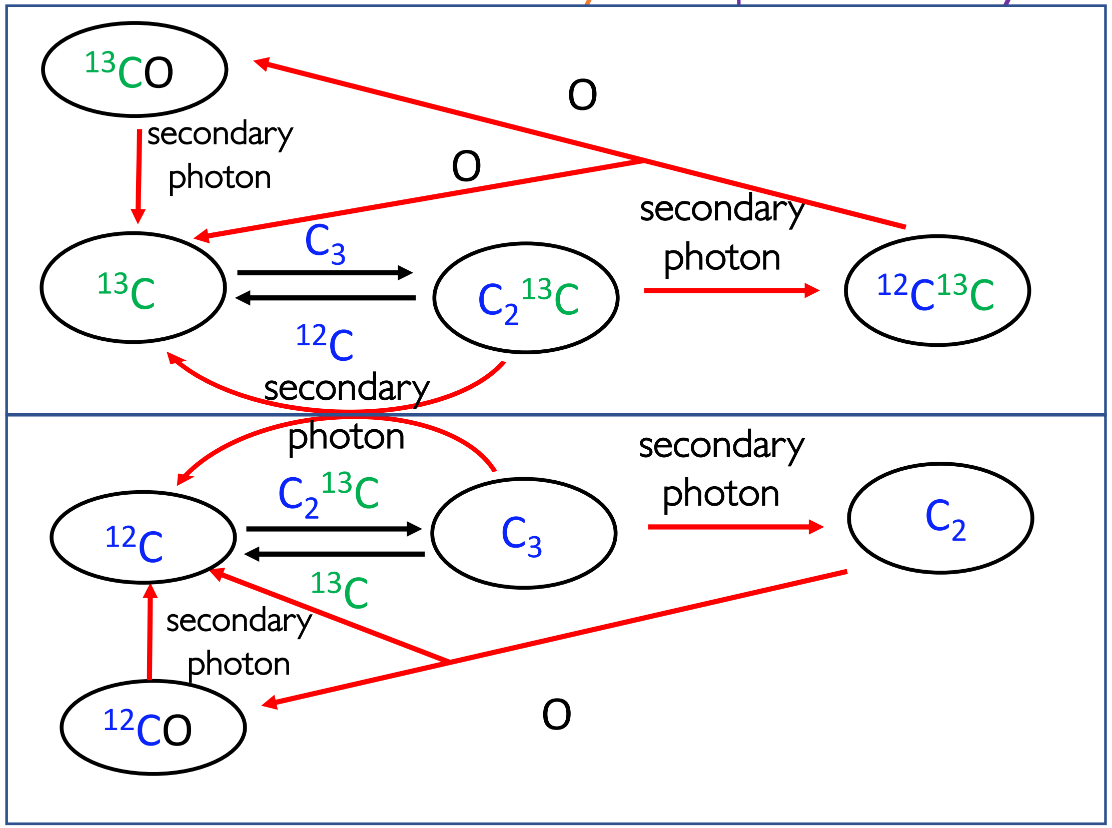


t = 3×10^5 yr > $t_I = 1.6\times10^5$ yr



Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays in our model

In gas-phase: → Wakelam+2015 (KIDA) and Heays+(2017)

DIRECT COSMIC-RAY IONIZATION REACTIONS $k_{\mathrm{CR}} = \gamma_2 \zeta$ ζ = cosmic-ray ionisation rate

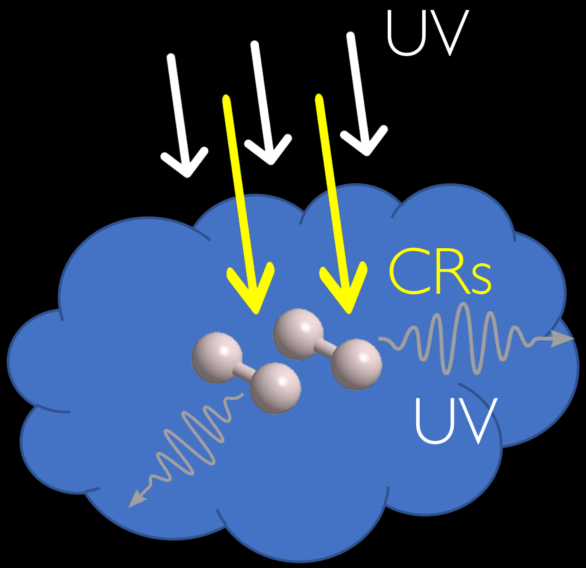
Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays in our model

In gas-phase: → Wakelam+2015 (KIDA) and Heays+(2017)

DIRECT COSMIC-RAY IONIZATION REACTIONS $k_{\mathrm{CR}} = \gamma_2 \zeta$

SECONDARY PHOTON REACTIONS $k_{\mathrm{SEC-PHOT}} = \dfrac{\alpha_{sec}\beta_{sec}\zeta}{1-\omega}$



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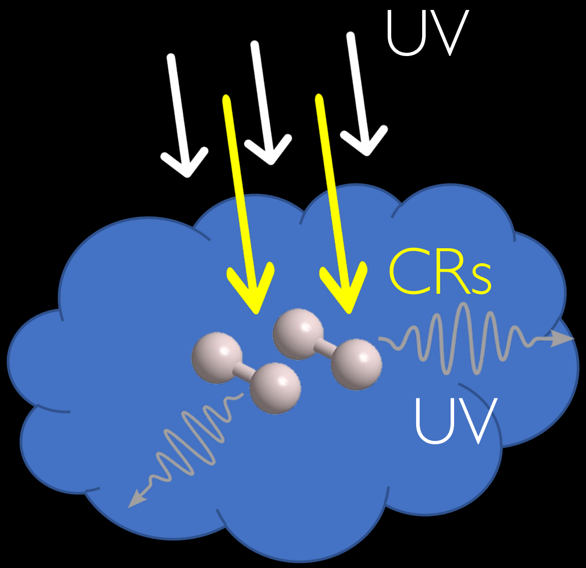
DIRECT COSMIC-RAY IONIZATION REACTIONS

$$k_{\mathrm{CR}} = \gamma_2 \zeta$$

SECONDARY PHOTON REACTIONS

$$k_{\mathrm{SEC-PHOT}} = \frac{\alpha_{sec}\beta_{sec}\zeta}{1-\omega}$$



Gas-grain interaction:

COSMIC-RAY DESORPTION

$$k_{\mathrm{i}}^{\mathrm{des,CR}} = 3.16 \times 10^{-19} \times (\,\zeta\,(\mathrm{s}^{-1})/1.3 \times 10^{-17}(\mathrm{s}^{-1}))\,k_{\mathrm{i}}^{\mathrm{des,th}}(70\mathrm{K})$$

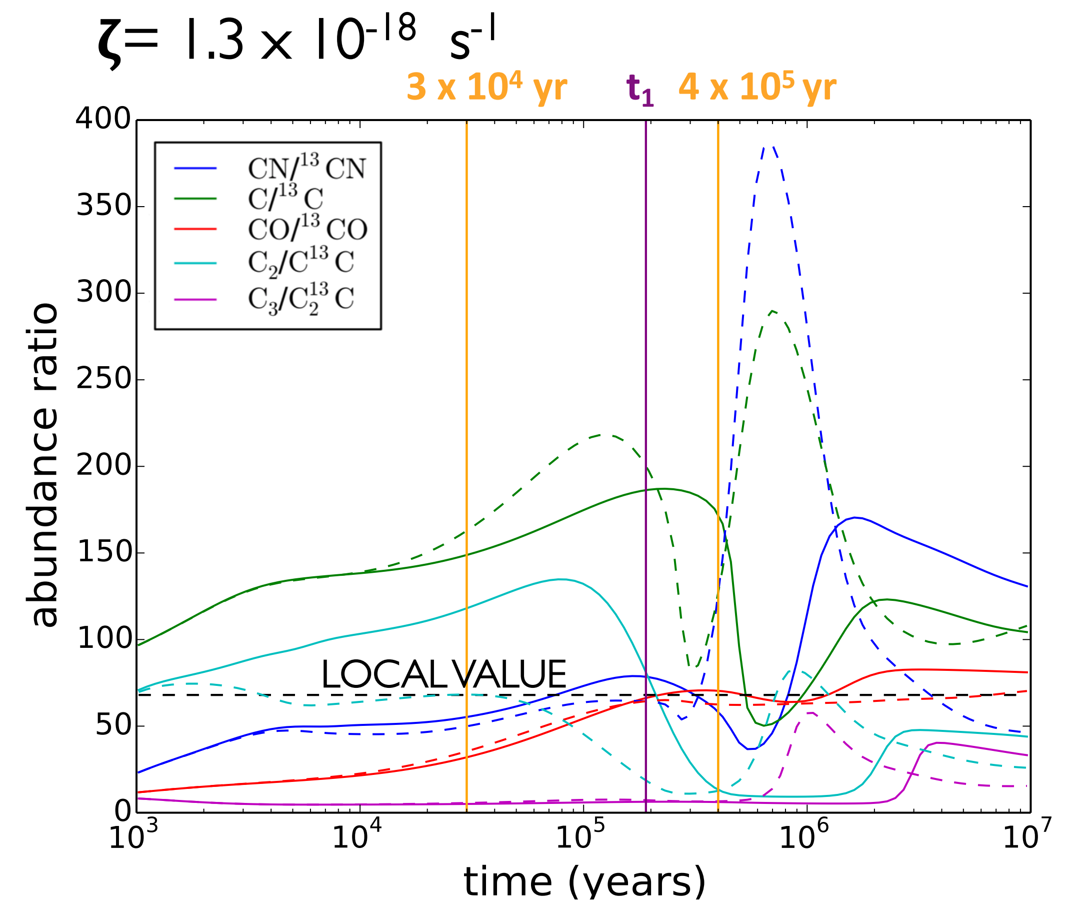
Where THERMAL DESORPTION:

$$k_{\mathrm{i}}^{\mathrm{des,th}} = \nu_{\mathrm{i}} \exp\left(-E_{\mathrm{i}}^{\mathrm{b}}/T_{\mathrm{dust}}\right)$$

→ Binding energies from Garrod and Herbst (2006)

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays in the fiducial model



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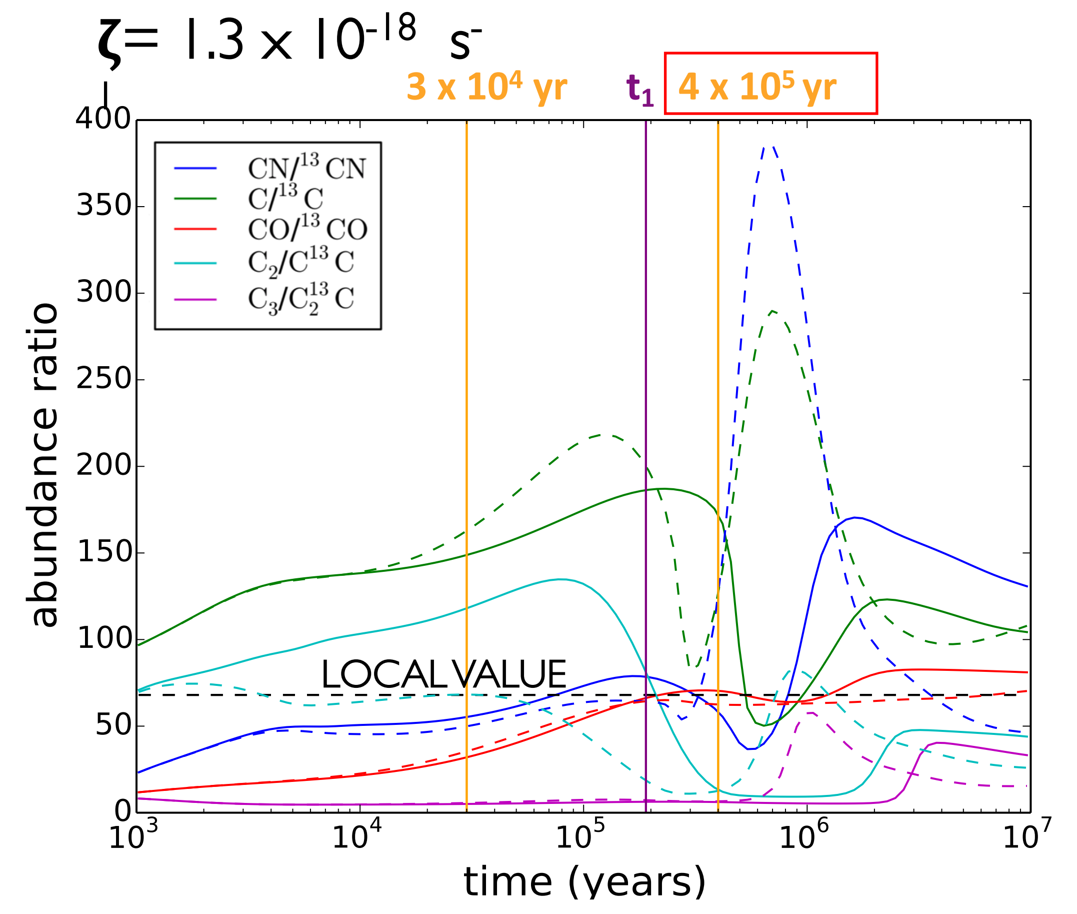
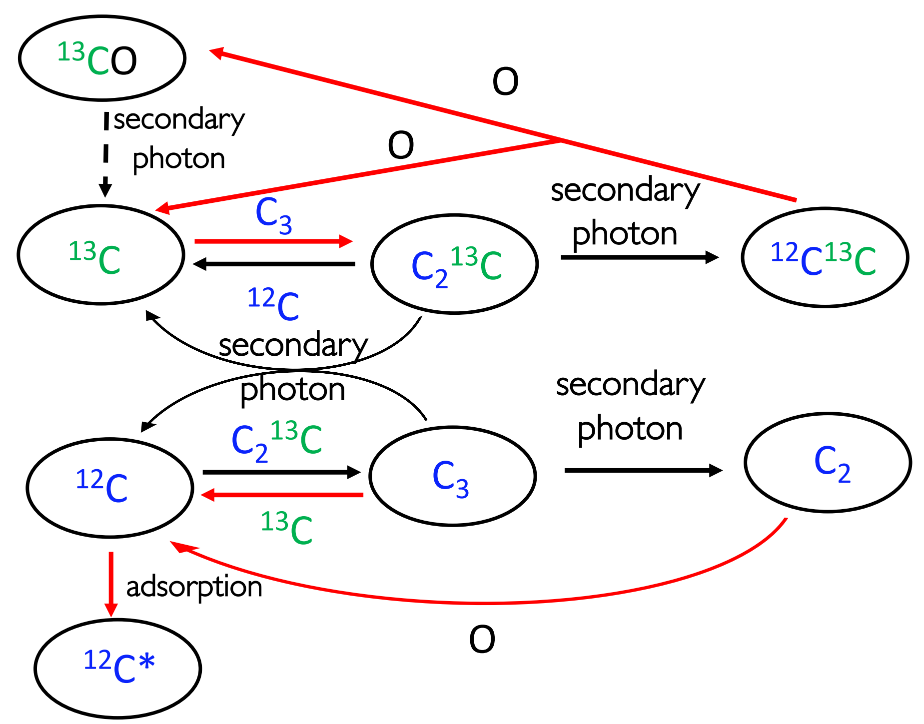


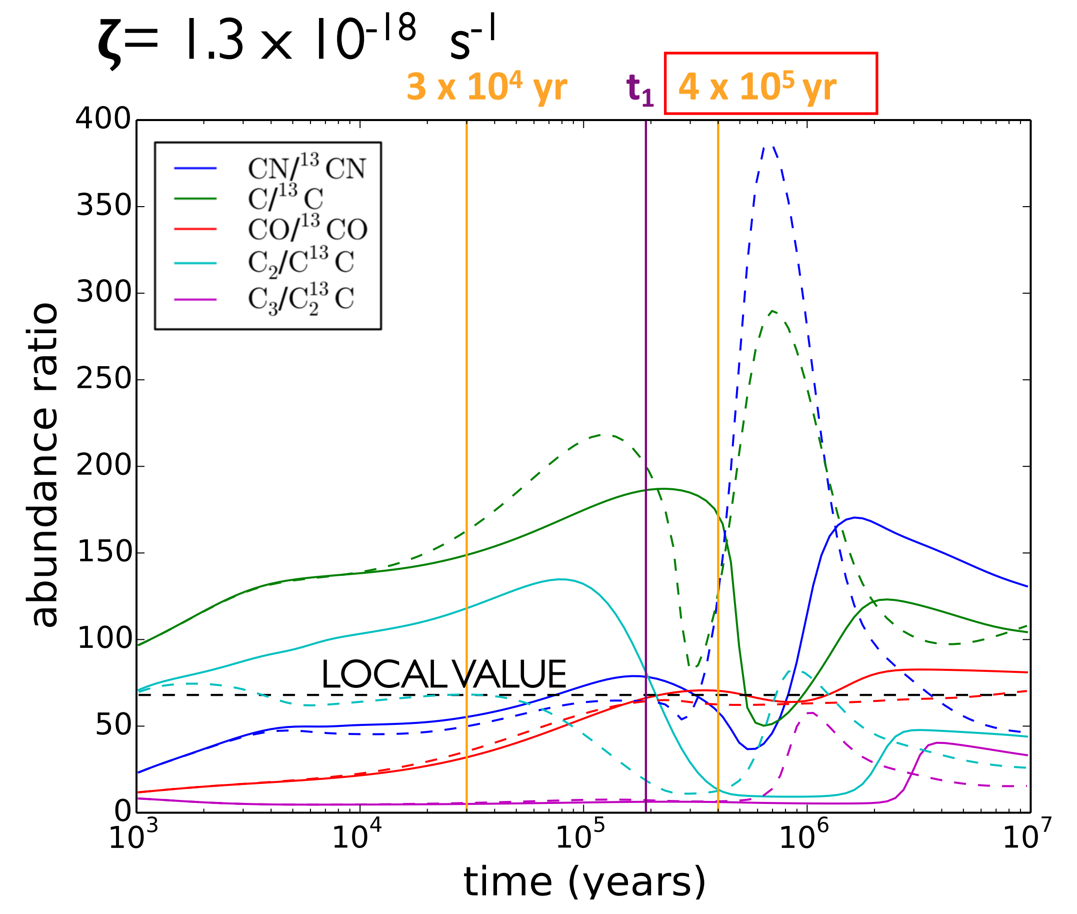
$t = 4\text{x}10^5$ yr > $t_1 = 1.9\text{x}10^5$ yr



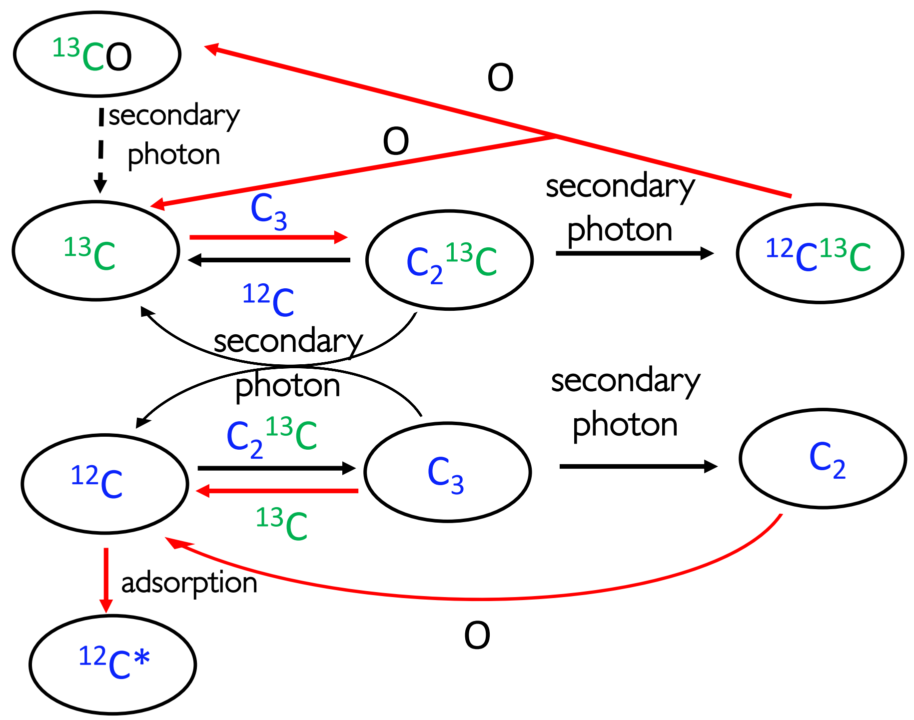
For long timescales: C_3 isotopic-exchange reaction still important: C_3 not efficiently destroyed, atomic ^{12}C abundance descrease and <u>atomic $^{12}C/^{13}C$ decreases</u>

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays in the fiducial model



t = 4x10^5 yr > t$_1$=1.9x10^5 yr

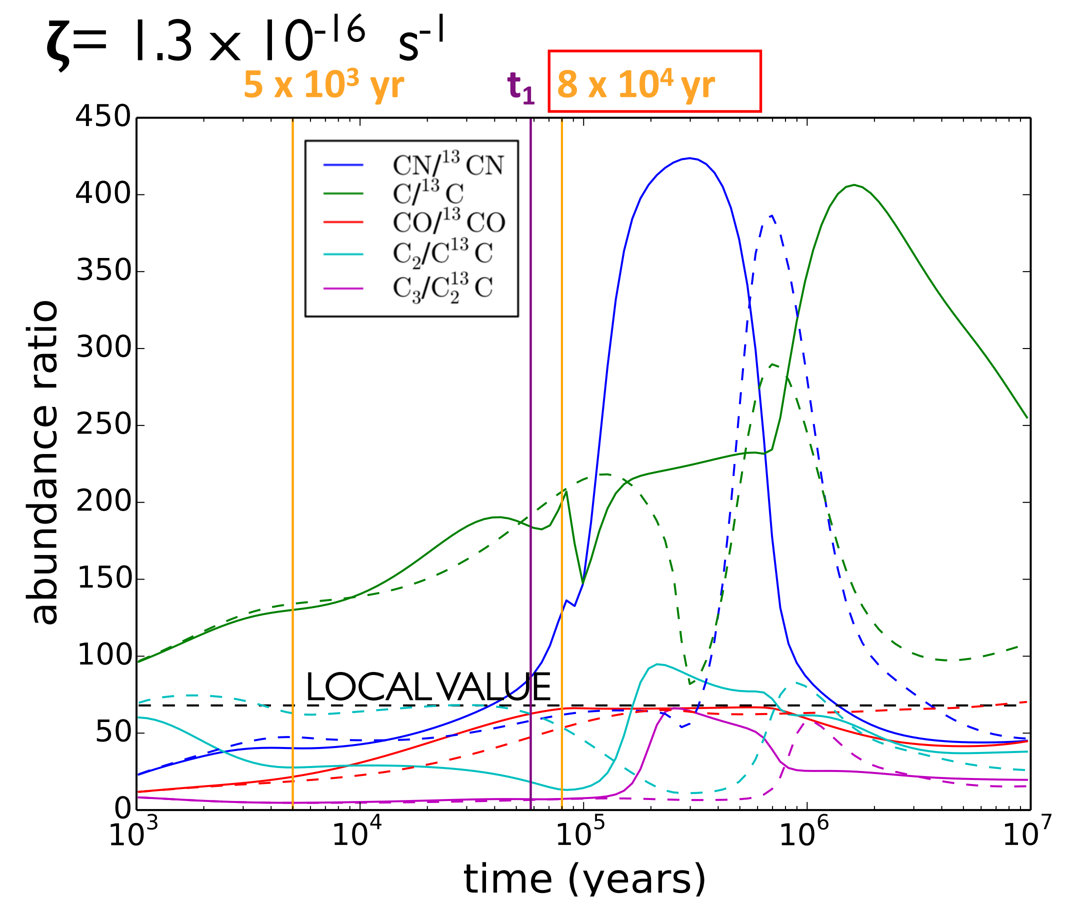


secondary-photon reactions not efficient → decrease of overall ^{12}C/^{13}C ratios

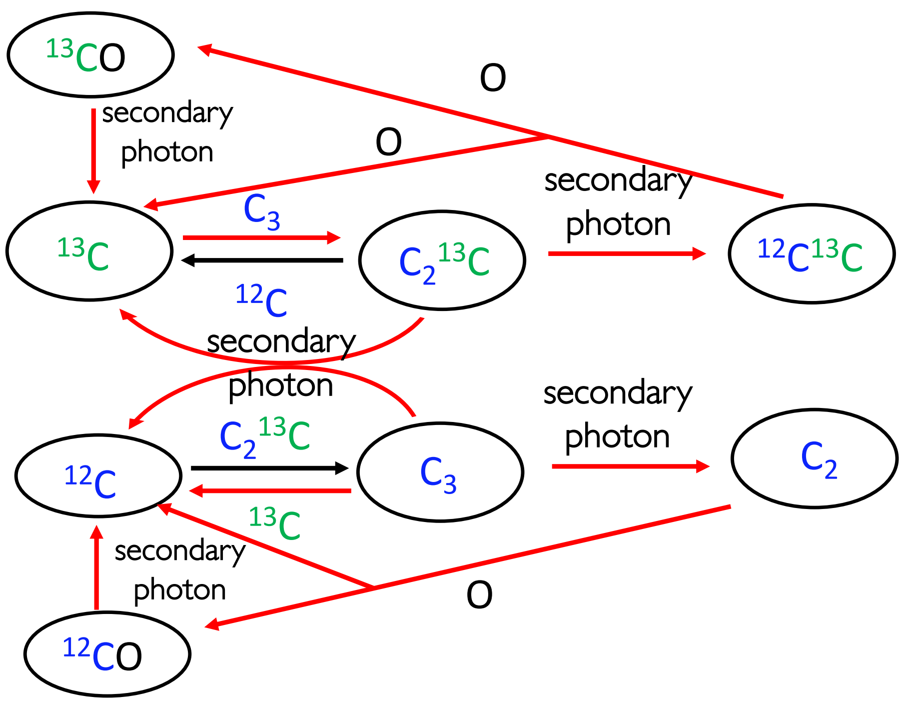
Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays in the fiducial model

$\zeta = 1.3 \times 10^{-16}\ s^{-1}$



$t = 8\times10^4$ yr $> t_1 = 5.8\times10^4$ yr



For long timescales: similar to the standard case BUT secondary-photon reactions more efficient → high atomic C abundance → C_3 isotopic-exchange reaction efficient → <u>atomic $^{12}C/^{13}C$ high</u>

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

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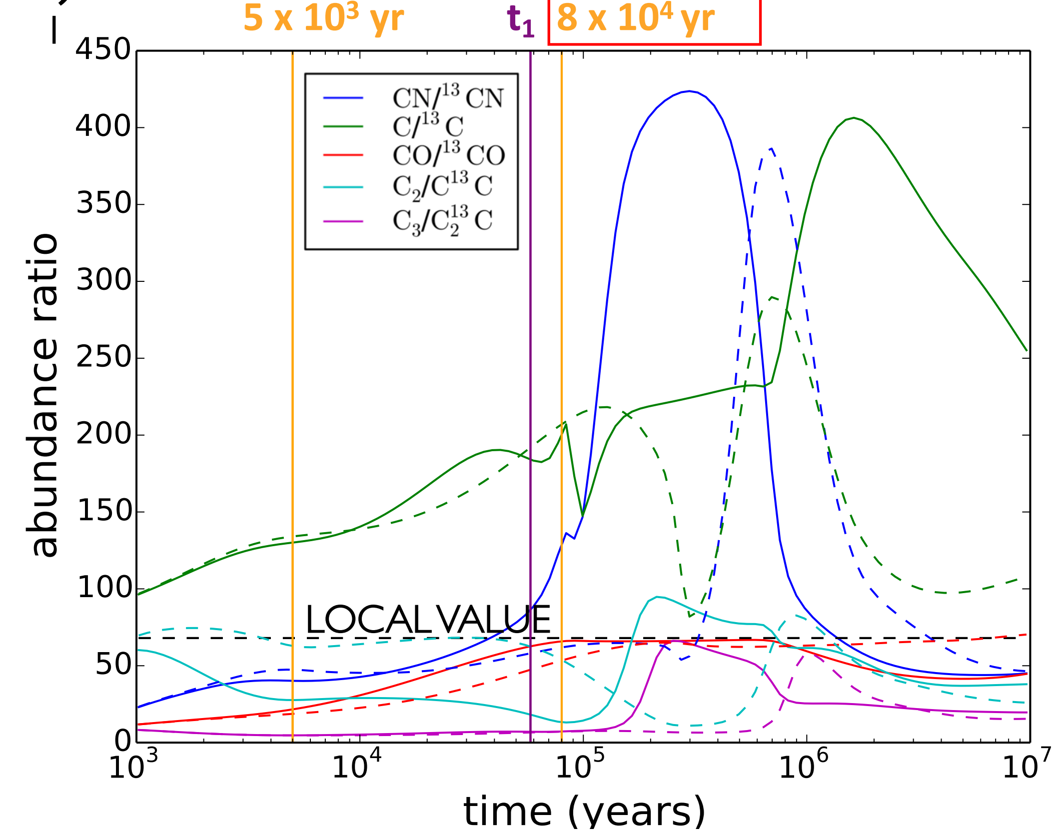

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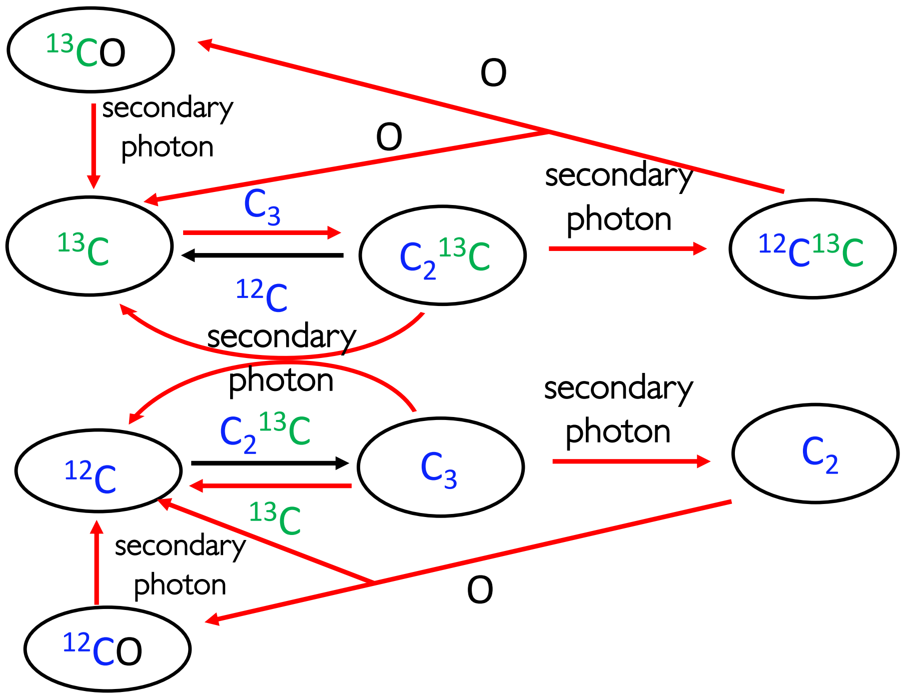
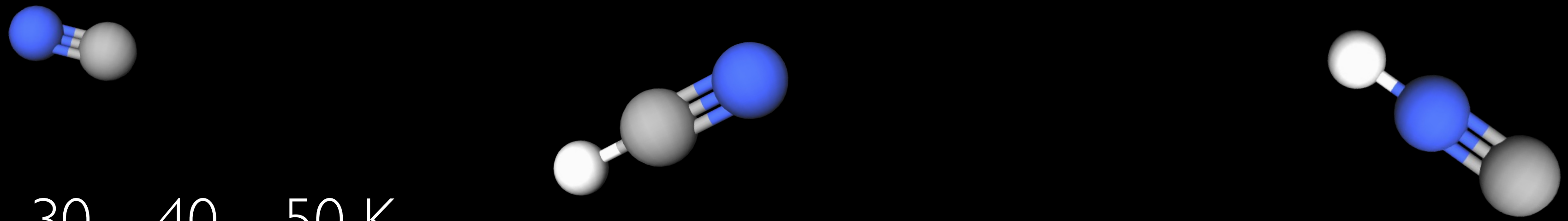


Secondary-photon reactions very efficient→ increase of overall ^{12}C/^{13}C ratios

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays: parameter space exploration



$T_{gas} = T_{dust}$ = 10 – 20 – 30 – 40 – 50 K

$n_H = 2 \times 10^4$ cm^{-3}

$\zeta = 1.3 \times 10^{-18} - 1.3 \times 10^{-17} - 1.3 \times 10^{-16}$ s^{-1} cosmic-ray ionization rate

ANALYSED TIMES:

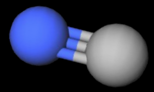
t_I = early-time chemistry

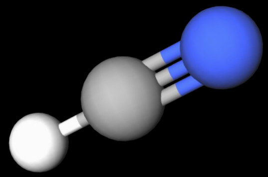
$2 \times t_I$

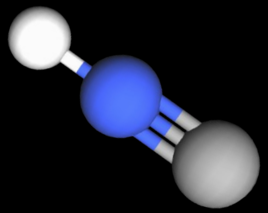
$10 \times t_I$

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays: parameter space exploration







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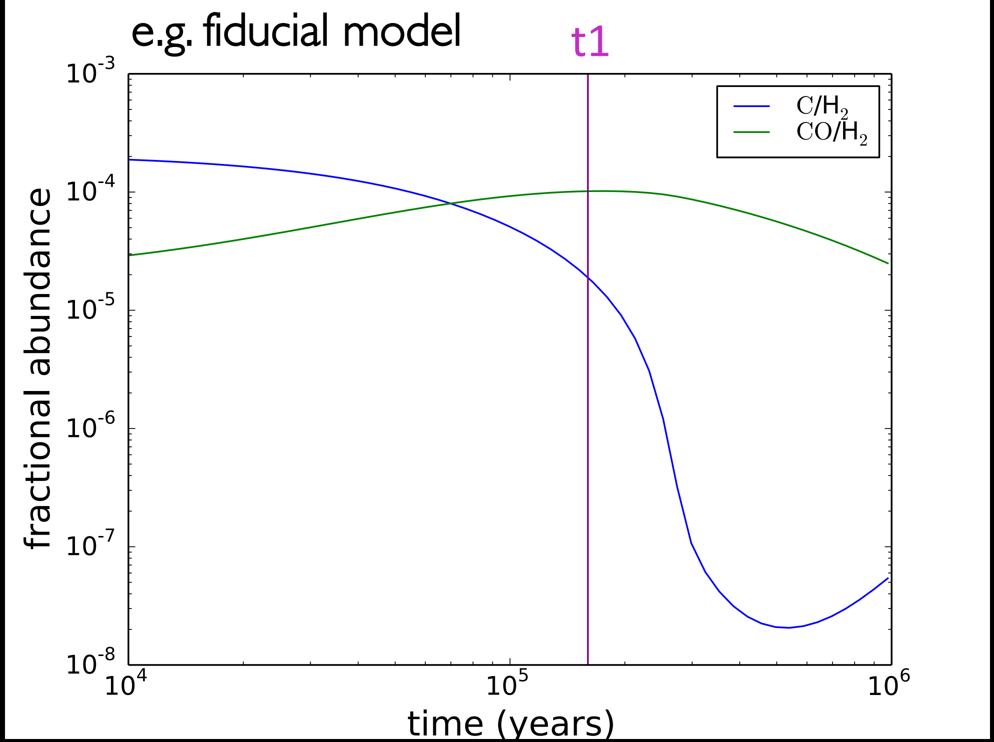

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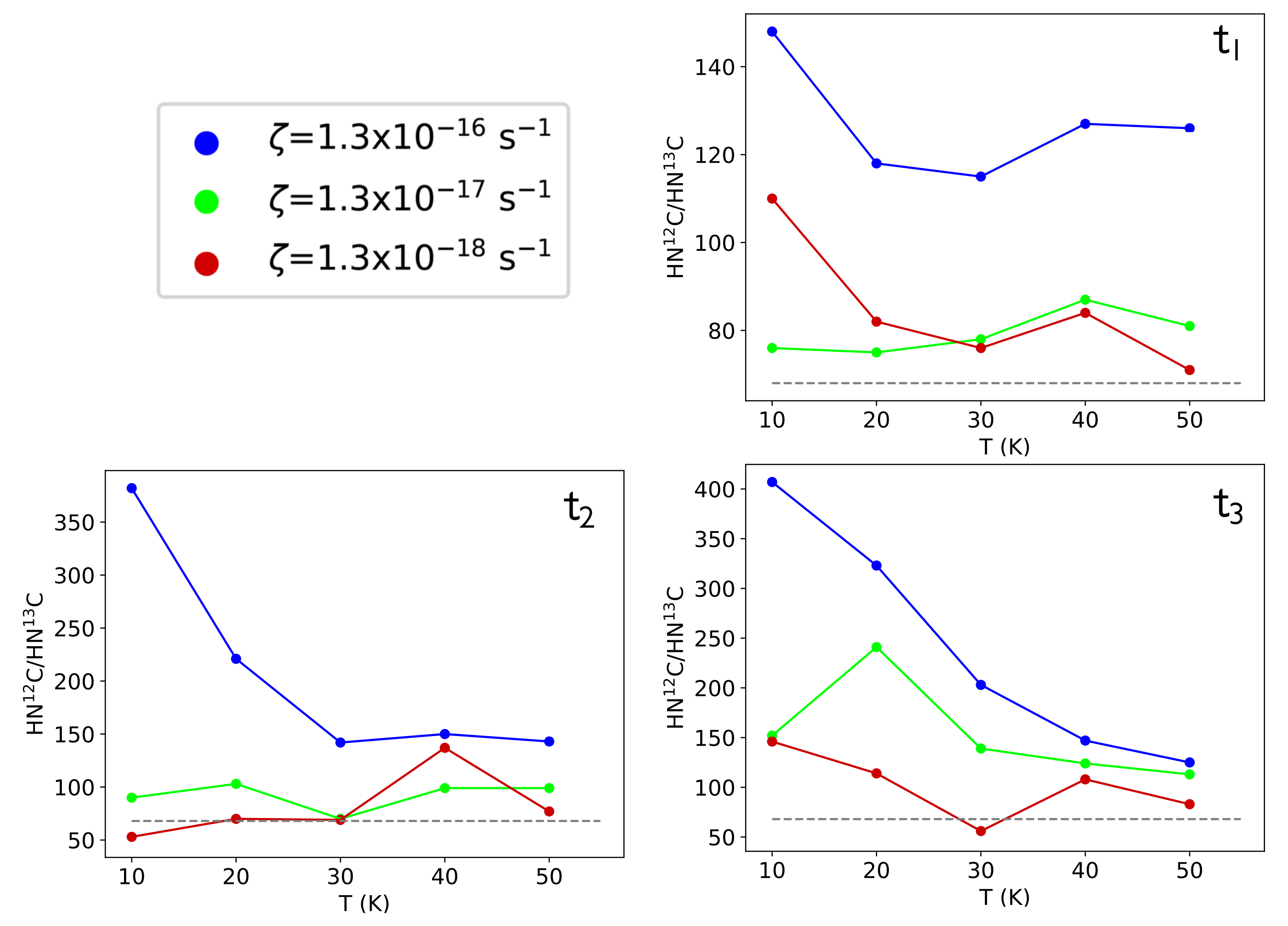
The effect of cosmic rays: parameter space exploration

HNC

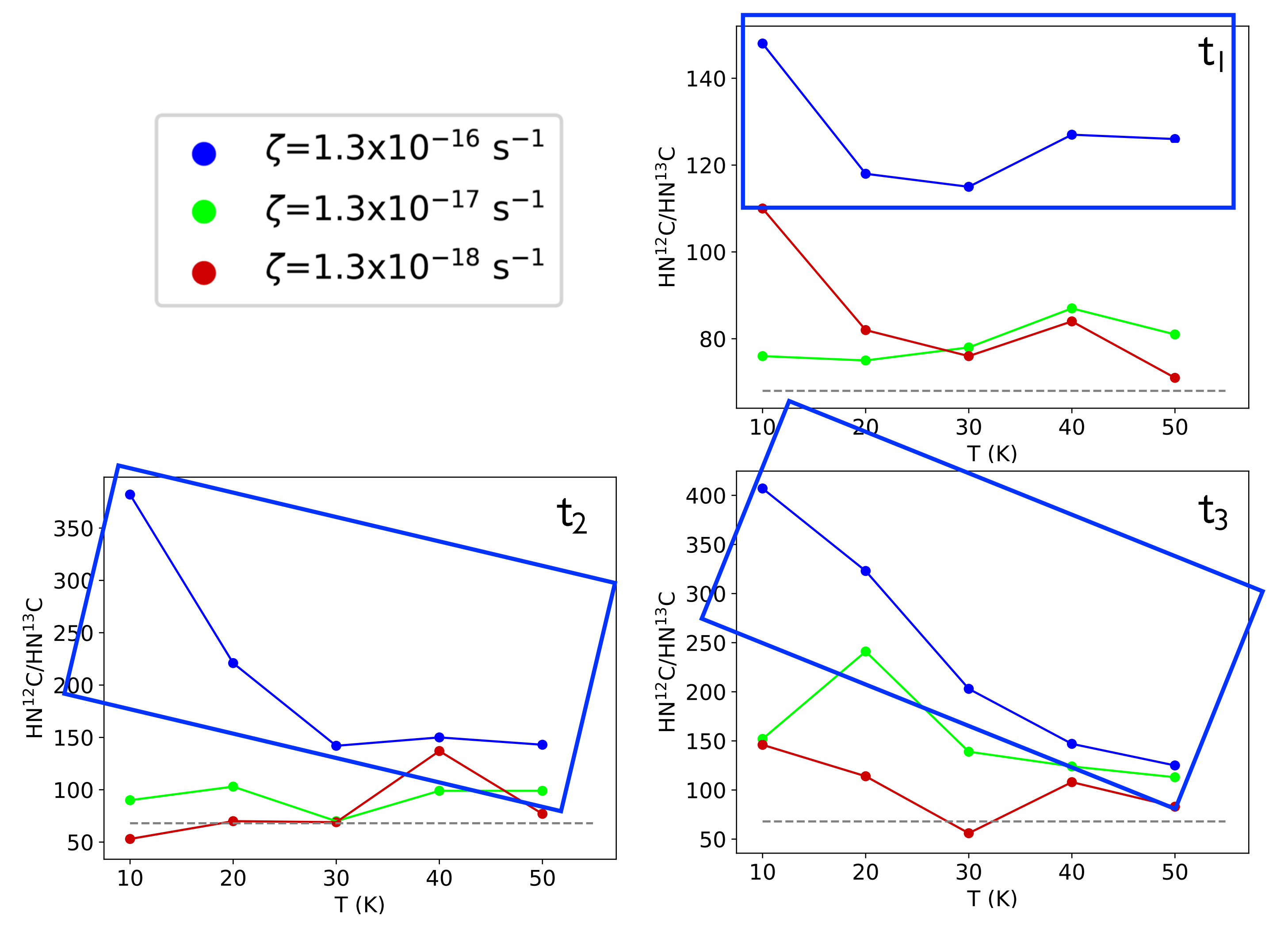


Reference: Colzi, L. , et al., 2020, A&A, 640, A51

The effect of cosmic rays: parameter space exploration

HNC

$^{12}C/^{13}C$ higher for higher cosmic-ray ionisation rate



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The effect of cosmic rays: parameter space exploration

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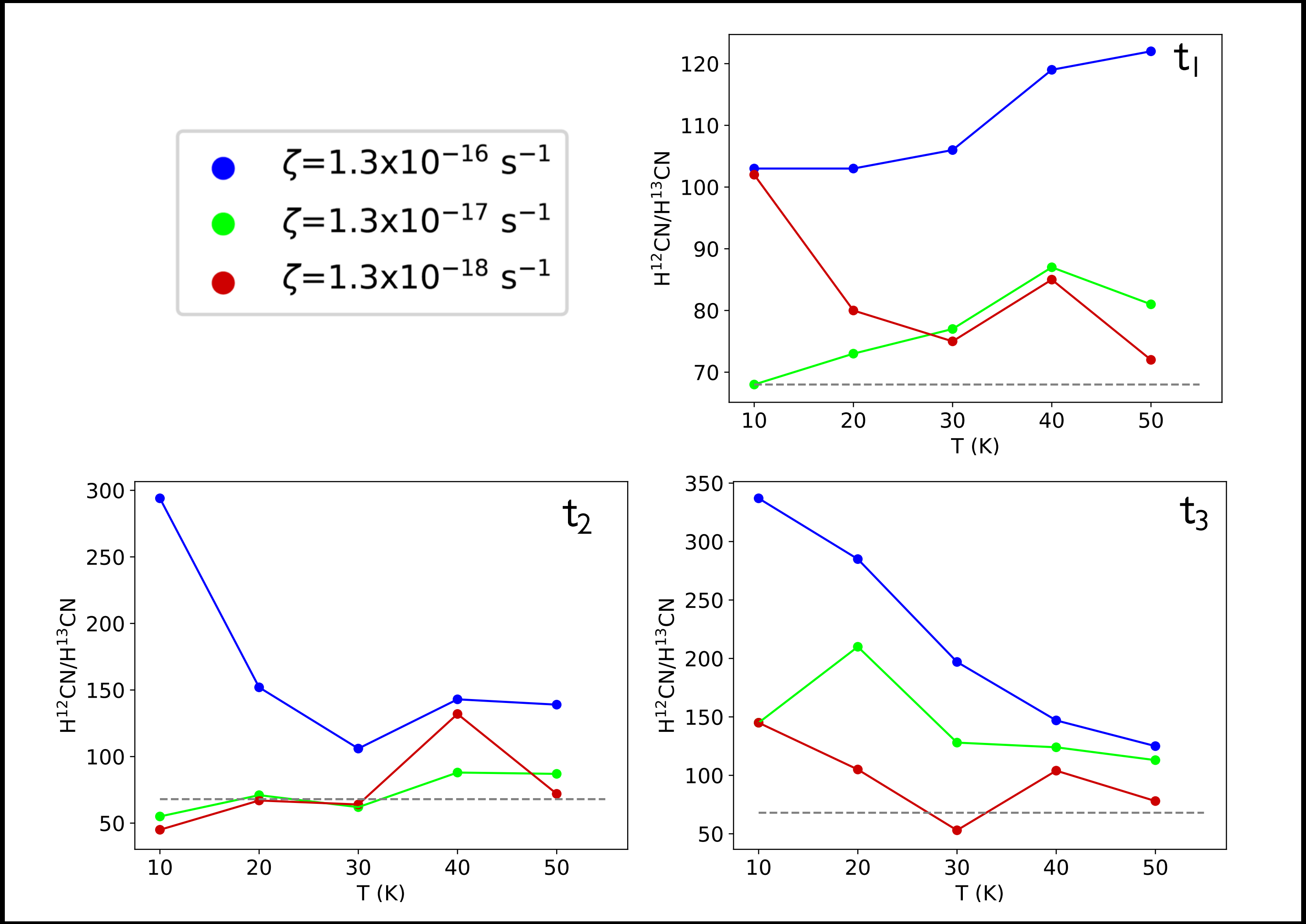

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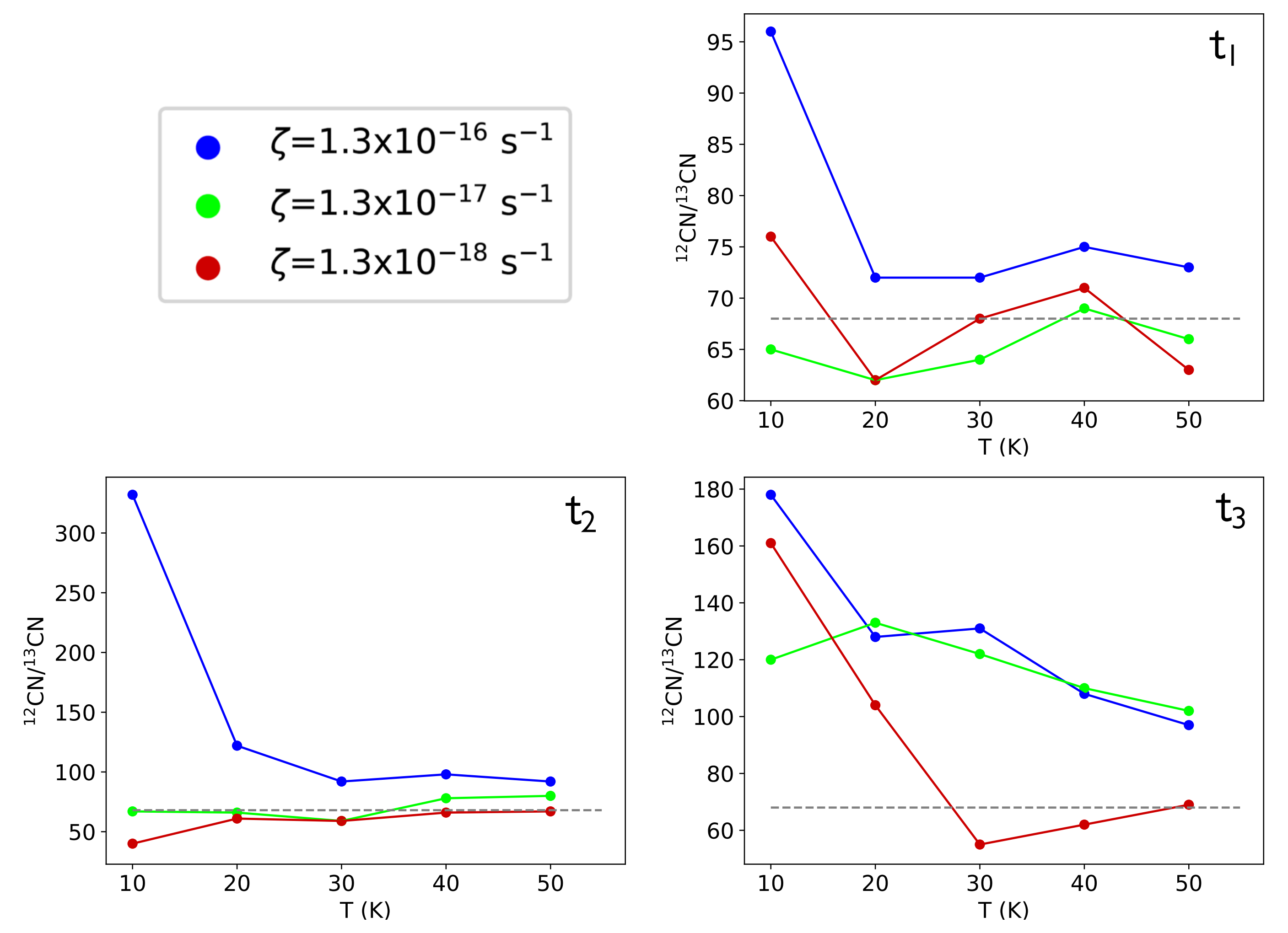
The effect of cosmic rays: parameter space exploration

CN



Laura Colzi

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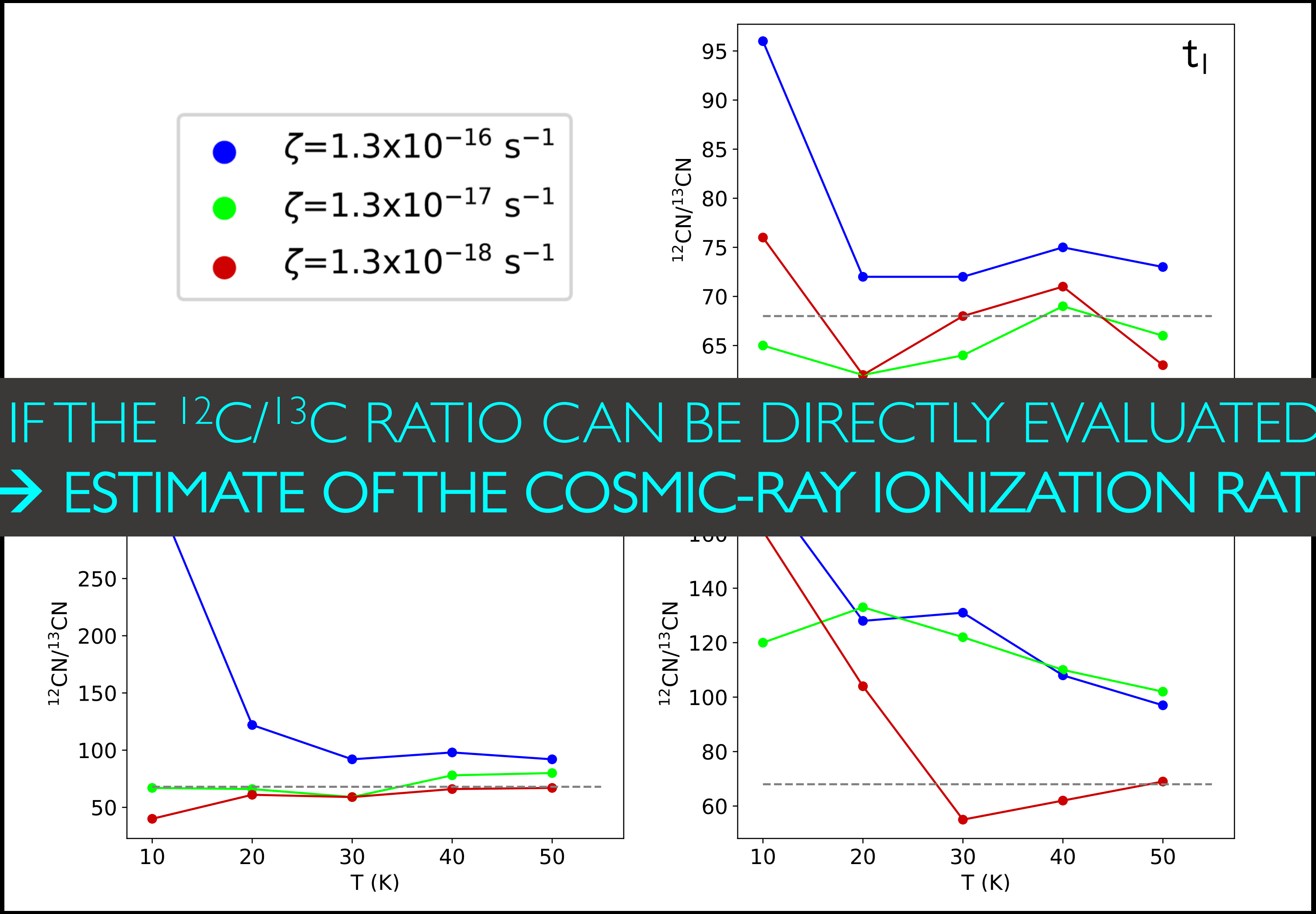

IF THE $^{12}C/^{13}C$ RATIO CAN BE DIRECTLY EVALUATED

→ ESTIMATE OF THE COSMIC-RAY IONIZATION RATE

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

How the $^{14}N/^{15}N$ ratios of nitriles could change…

PREDICTED VALUES $\zeta = 1.3 \times 10^{-16}\ s^{-1}$

$HNC/HN^{13}C$ = [120-350]

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Average $^{14}N/^{15}N$ ratio derived for HCN and HNC (Colzi et al. 2018a,b)

$$\longrightarrow \quad {}^{14}N/{}^{15}N = \left(\frac{330}{68}\right) \times [100\text{-}350] =$$

Assumed $^{12}C/^{13}C$ from Galactocentric trend

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→ IMPORTANT TO KNOW THE **EXACT** $^{12}C/^{13}C$ **RATIO** IF THE **DOUBLE-ISOTOPE METHOD IS USED!**

Reference: Colzi, L. , et al., 2020, A&A, 640, A51

CONCLUSIONS

We developed a **new chemical network** to study in detail how important are **isotopic exchange reactions for carbon fractionation**

☆ We suggested a possible **exchange between ^{13}C and C_3**

→ important for T < 30 K
→ leads to $^{12}C/^{13}C < 68$ for the fiducial model

*Loison+2020 found similar results.

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COSMIC RAYS 2

The salt of the star formation recipe

Florence, 8-10 November 2022

The effect of cosmic rays on carbon isotopic fractionation

Laura Colzi

(Centro de Astrobiología, CSIC-INTA)

9th November 2022

Olli Sipilä, Evelyne Roueff, Paola Caselli and Francesco Fontani

CENTRO DE ASTROBIOLOGÍA · CAB
ASOCIADO AL NASA ASTROBIOLOGY PROGRAM
CSIC INTA

AEI Retos project
PID2019-105552RB-C41