Tracing the production pathways of molecules by $^{12}C/^{13}C$ ratio

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$^{12}C/^{13}C$ Ratio in Molecular Cloud

- Optical depth estimation

  Interstellar $[^{12}C]/[^{13}C]$ Ratio＝60-70

  e.g.
  Lucas & Liszt (1998): 59, derived from HCO^+, HCN, & HNC
  Milam+(2005): 68, derived from CO, CN, & H_2CO

- "Chemical evolution" of galaxies

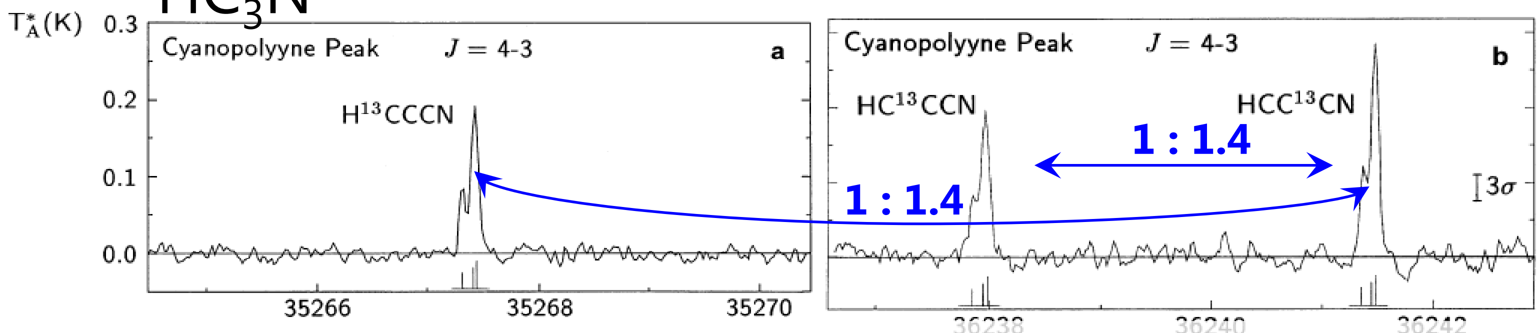
- "Fractionation" of ^{13}C species in cold clouds?

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

  (*c.f.* $H_3^+ + HD \rightarrow H_2D^+ + H_2 + 230\ K$)

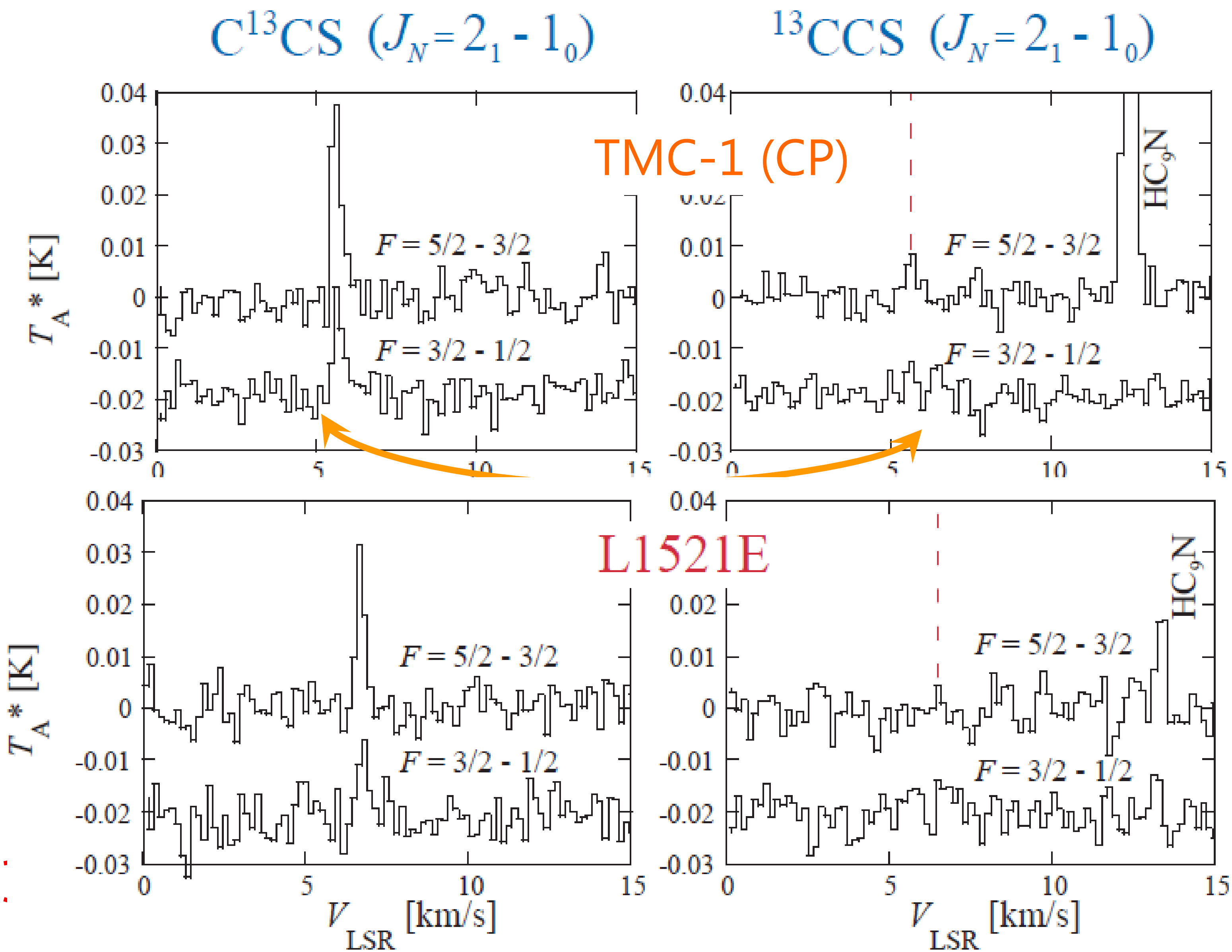
- Abundance anomaly in the same species?
  HC_3N

$[HC_3N]/[H^{13}CCCN]=79$
$[HC_3N]/[HC^{13}CCN]=75$
$[HC_3N]/[HCC^{13}CN]=55$



HCCH + CN would be the main reaction to produce HC_3N (Takano+1997)

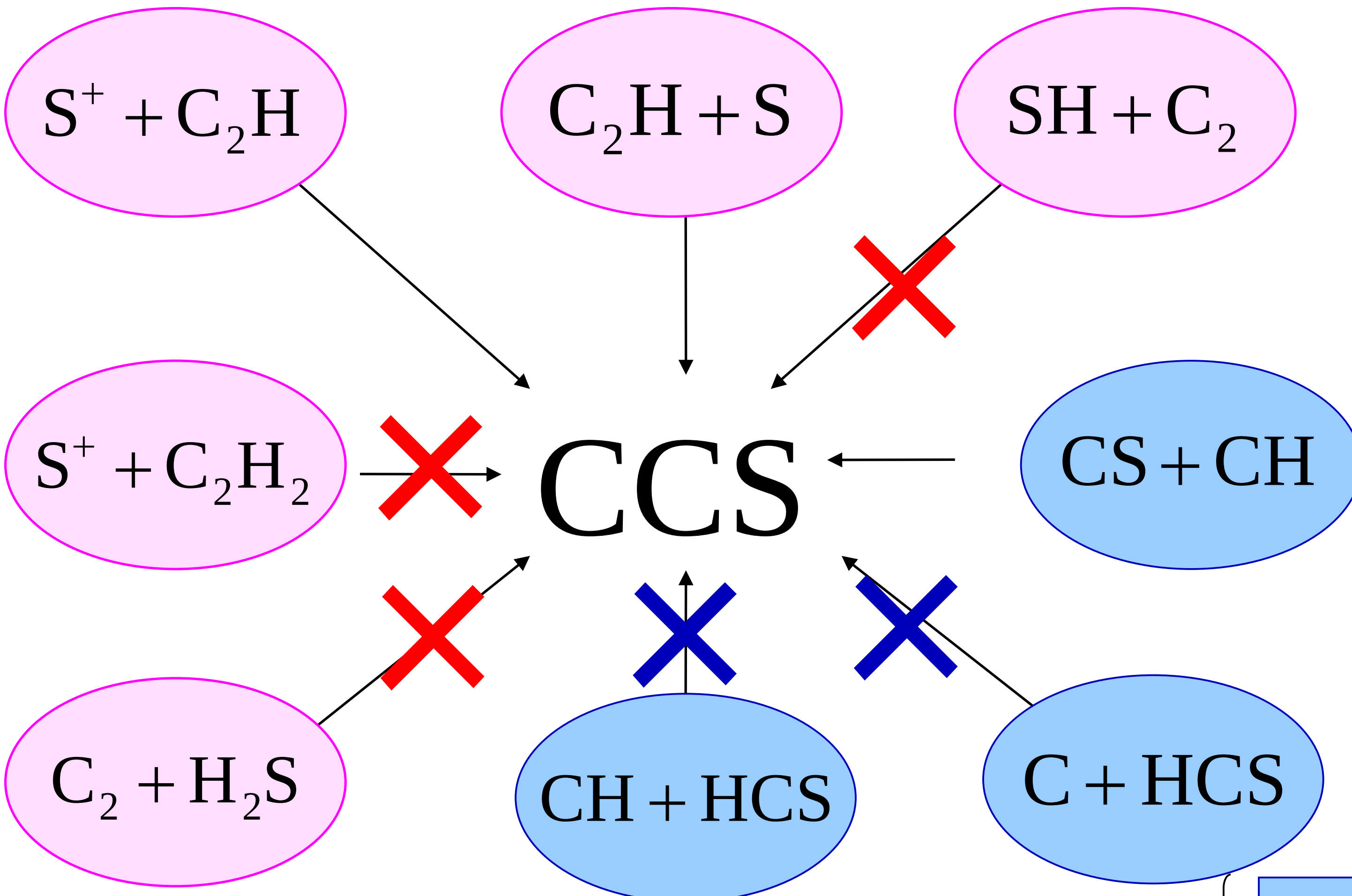
Abundance Anomaly: ^{13}C species of CCS



(Sakai+ 2007, ApJ 663, 1174)

Abundance Anomaly: ^{13}C species of CCS

Production Pathways of CCS



(Millar & Herbst.1990, Petrie+1996, Yamada+2002)

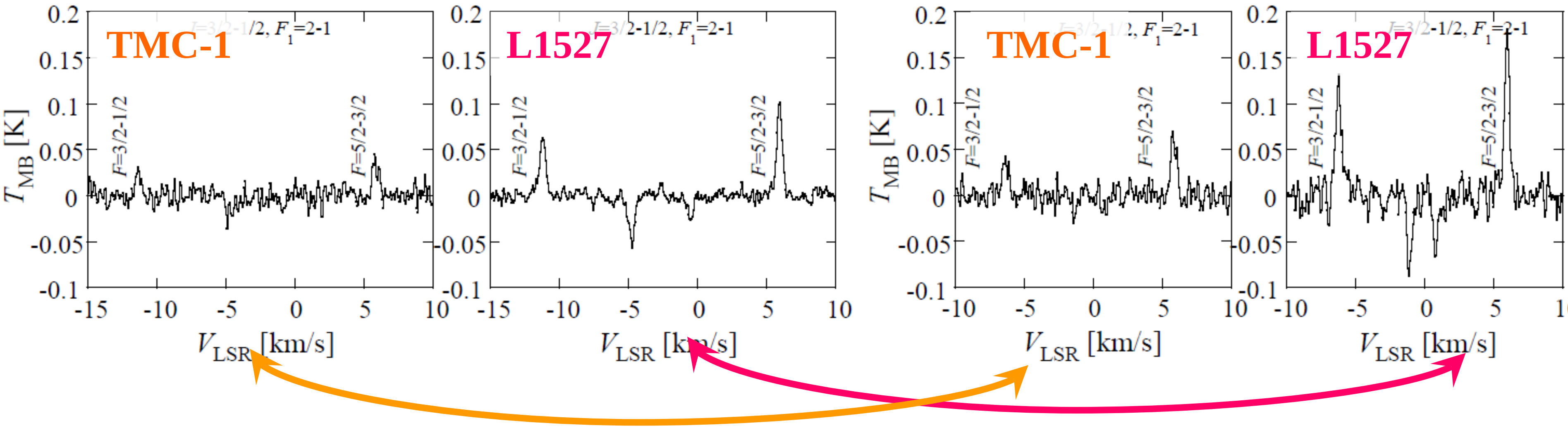
(Sakai+2007, ApJ 663, 1174)

Nonequivalent route

Equivalent routes

Abundance Anomaly: ^{13}C species of CCH

^{13}CCH   C^{13}CH



R = 1.6 ± 0.4 (3σ)   R = 1.6 ± 0.1 (3σ)

If CCS is formed via S$^+$ +CCH…

$S^+ + {}^{13}CCH \rightarrow C^{13}CS + H$

$S^+ + C^{13}CH \rightarrow {}^{13}CCS + H$

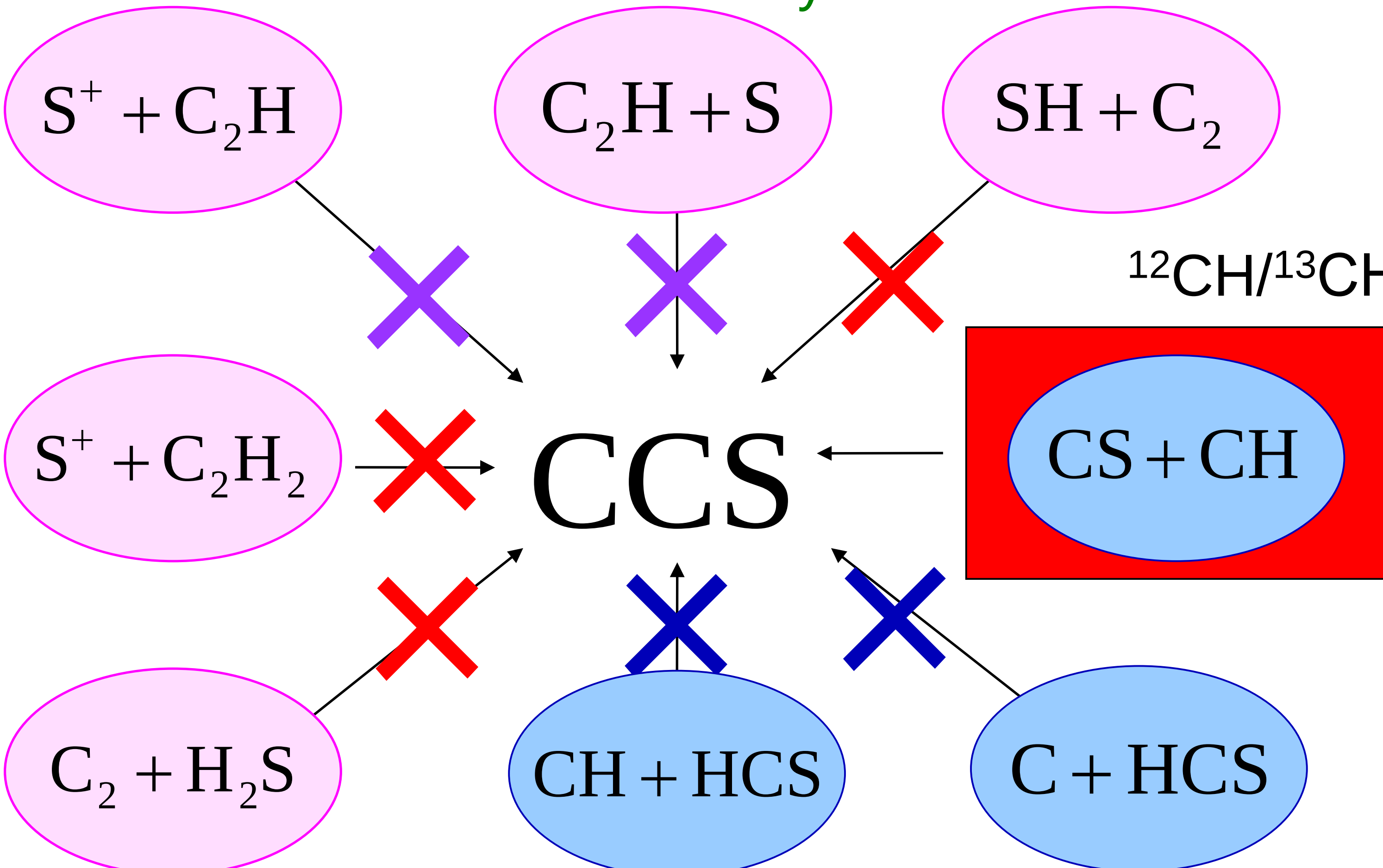
Opposite !

IRAM 30 m

(Sakai+2010, A&A, 512, A31)

Abundance Anomaly: ^{13}C species of CCS

Production Pathways of CCS



$^{12}CH/^{13}CH$ > 70 (3σ)
> 210 (1σ)

Most Probable Route

(Millar & Herbst.1990, Petrie+1996, Yamada+2002)

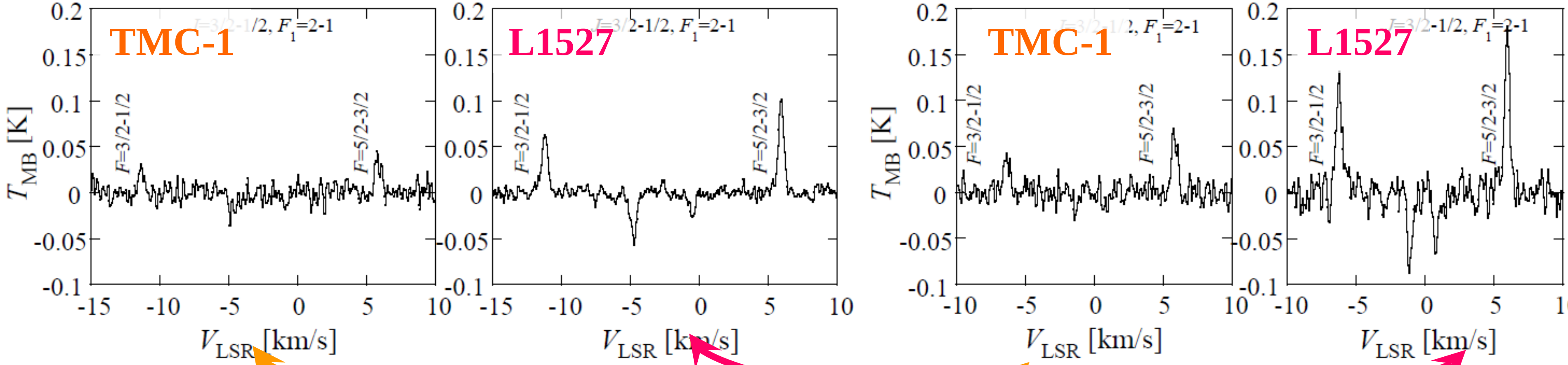
Nonequivalent route — 76%↑

~~Equivalent routes~~

(Sakai+2007, ApJ 663, 1174)

Abundance Anomaly: ^{13}C species of CCH

^{13}CCH | $C^{13}CH$



R = 1.6 ± 0.4 (3σ)

R = 1.6 ± 0.1 (3σ)

Production pathways of CCH

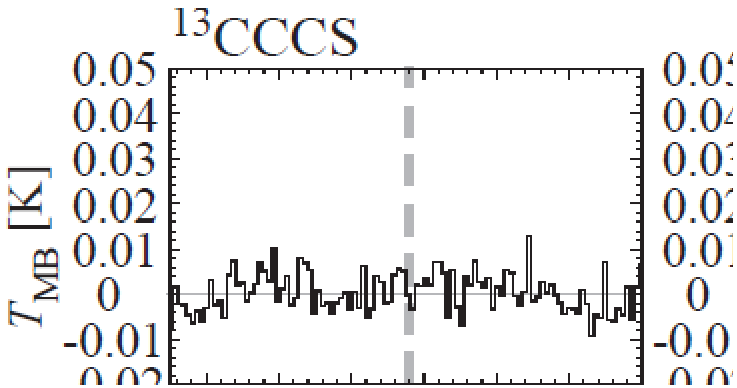
$HCCH^+ + e \rightarrow CCH + H$

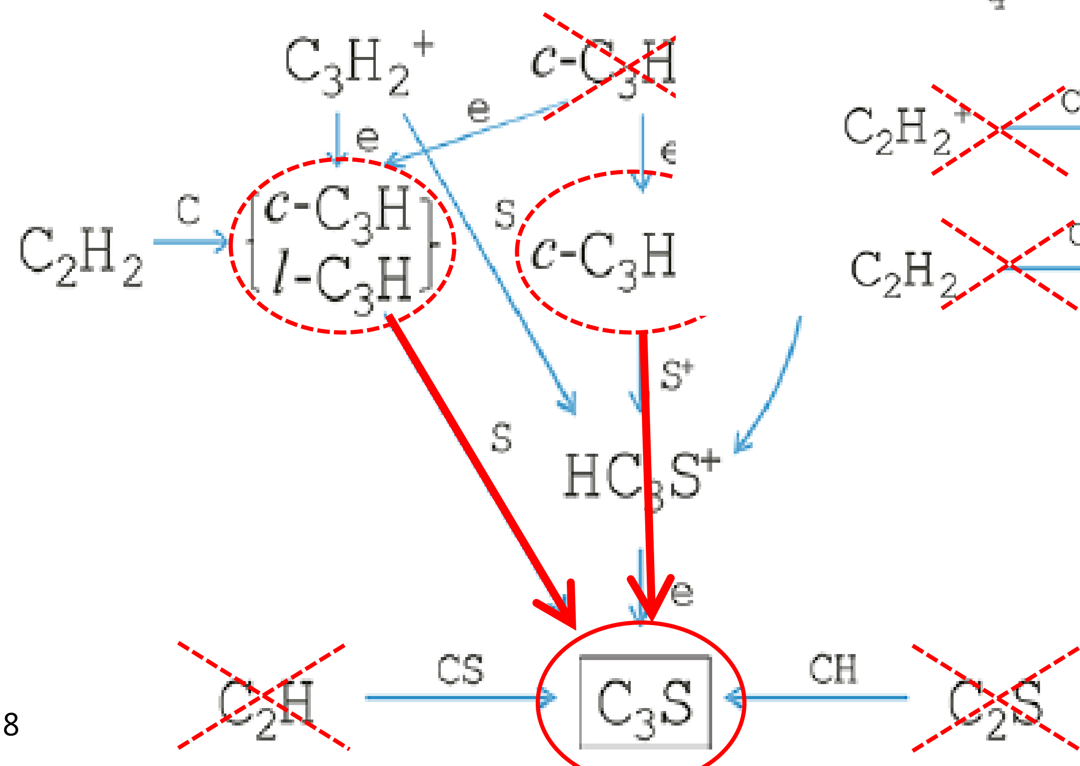
$C_2H_3^+ + e \rightarrow CCH + H_2$

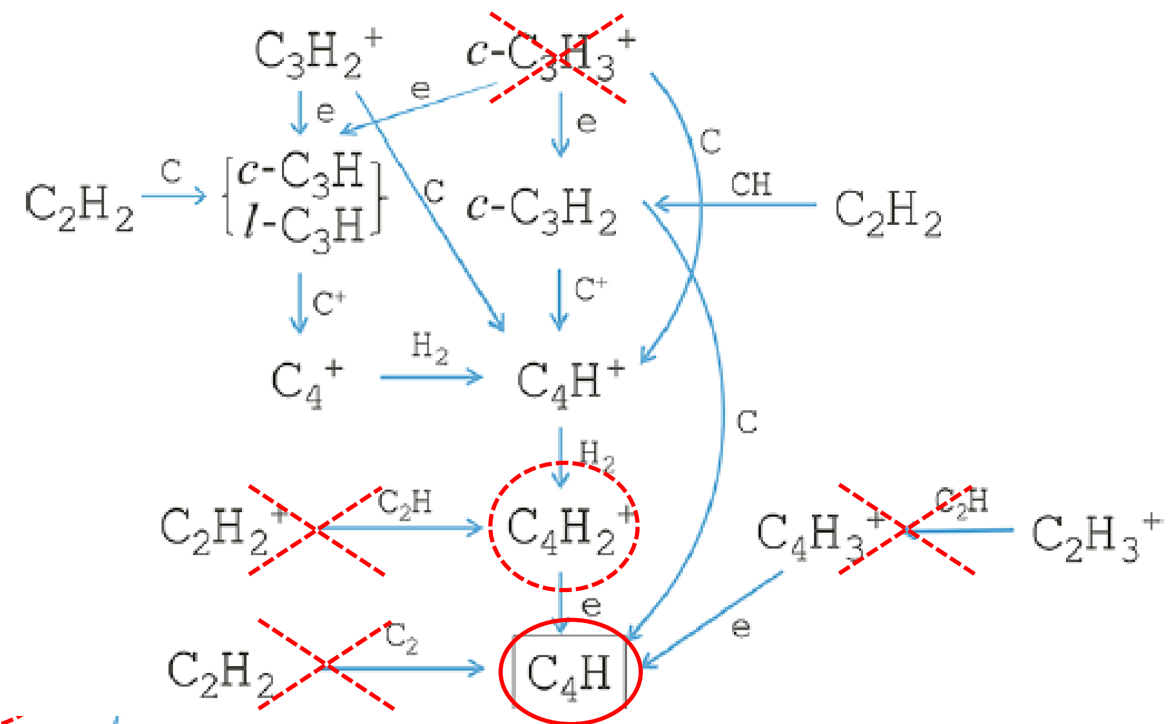
$CH_2 + C \rightarrow CCH + H$

(Sakai+2010, A&A, 512, A31)

Abundance Anomaly: ^{13}C species of C_3S&C_4H







:H= 1.0 : 1.5 : 1.7 : 1.2

By including the error,
there could be a symmetry.
[C13CCCH]~[CC13CCH]
[13CCCCH]~[CCC13CH]

(Sakai+2013, JPCA, 117, 9831)

How to constrain the pathways?

Chemical Models

~5000 reactions

~500 species

compare

Observations

abundances

Macroscopic Approach

Microscopic Approach (Isotopic Species)

Other Possibilities

Isotope exchange reactions??

CCH i) $\mathrm{H} + {}^{*}\mathrm{CCH} \rightarrow \mathrm{H}^{*}\mathrm{CC} + \mathrm{H}$ (ΔE=8 K)

1 : 1.6

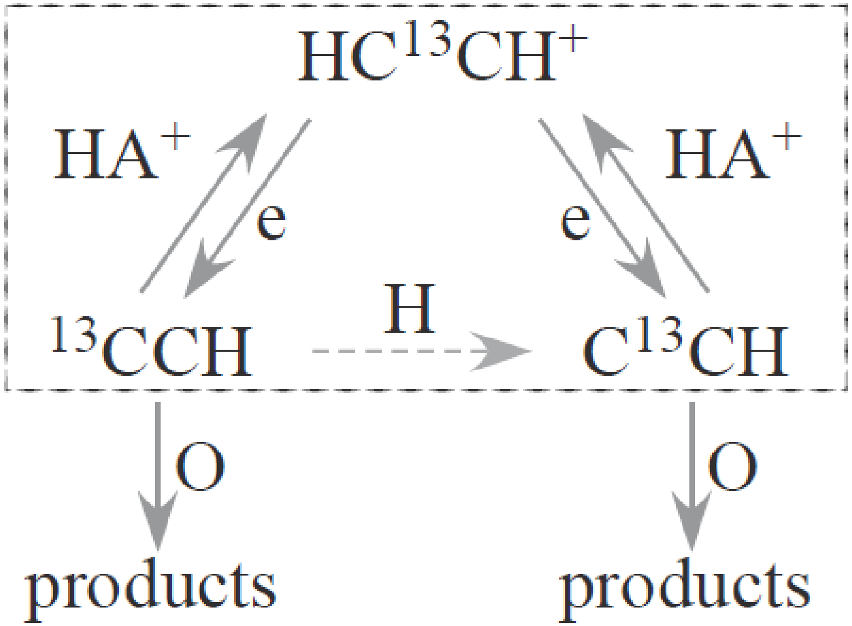
CCS ii) $\mathrm{S} + {}^{*}\mathrm{CCS} \rightarrow \mathrm{S}^{*}\mathrm{CC} + \mathrm{S}$ (ΔE=17 K)

1 : 4.2

S is less abundant than H.
Is this possible ???

(CCH: Tarroni, private communication)
(CCS: Osamura, private communication)

Exchange Reaction; CCH Case



R

$$\frac{[C^{13}CH]}{[^{13}CCH]} = \frac{2k_{ex}^{(f)}[H] + k_d[O]}{2k_{ex}^{(b)}[H] + k_d[O]}$$

$$k_{ex}^{(b)} = k_{ex}^{(f)} \exp\left(-\frac{\Delta G}{kT}\right)$$

	TMC-1			L1527	
$n(H_2)$/cm^{-3}	10^4	3×10^4	10^5	10^5	10^6
R	1.51	1.23	1.07	1.16	1.02
R(obs)	1.6 ±0.4 (3σ)			1.6 ±0.1 (3σ)	

Other Possibilities

Isotope exchange reactions??

CCH i) H + *CCH → H*CC + H (ΔE=8 K)

1 : 1.6

CCS ii) S + *CCS → S*CC + S (ΔE=17 K)

S is less abundant than H.
Is this possible ???

1 : 4.2

iii) H + *CCS → C*CS + H ???

The simplest catalyst !?!?

c−C_3H_2 ^{13}C on-axis : ^{13}C off axis =1:5 (expected to be 1:2)

Closed-shell molecule!

If it happens for C_3H_2, l-C_3H_2 ⇔ c-C_3H_2 would happen.

In this case, l-C_3H_2would be killed…..

(Yoshida+2015, ApJ, 807, 66)

$^{12}C/^{13}C$ ratios in Molecules

Anomaly of the ^{13}C Species in TMC-1(Starless cloud)

$CH/^{13}CH$	>71 (3σ)	$CCCCH/^{13}CCCCH$	141 ± 44 (3σ)
$CCH/^{13}CCH$	>250	$CCCCH/C^{13}CCCH$	97 ± 27 (3σ)
$CCH/C^{13}CH$	>170	$CCCCH/CC^{13}CCH$	82 ± 15 (3σ)
$CCS/^{13}CCS$	230 ± 130 (3σ)	$CCCCH/CCC^{13}CH$	118 ± 23 (3σ)
$CCS/C^{13}CS$	54 ± 5 (3σ)	$HCCCN/H^{13}CCCN$	79 ± 11 (1σ) (Takano+1997;Taniguchi+2016;Araki+2016)
$CCCS/^{13}CCCS$	>206 (3σ)	$HCCCN/HC^{13}CCN$	75 ± 10 (1σ) (Takano+1997;Taniguchi+2016;Araki+2016)
$CCCS/C^{13}CCS$	48 ± 15 (3σ)	$HCCCN/HCC^{13}CN$	55 ± 7 (1σ) (Takano+1997;Taniguchi+2016;Araki+2016)
$CCCS/CC^{13}CS$	30–206	HC_5N/HC_5N ^{13}C isotopomers	82-103 (Takano+1990;Taniguchi+2016)
		HC_7N/average ^{13}C isotopomers	87^{+35}_{-19} (1σ) (Langston & Turner 2007)

Interstellar $^{12}C/^{13}C$ ratio : 60-70

Dilution of ^{13}C !

(*e.g.* Sakai et al. 2013, JPC, 117, 9831)

$^{12}C/^{13}C$ Ratio in Molecular Cloud

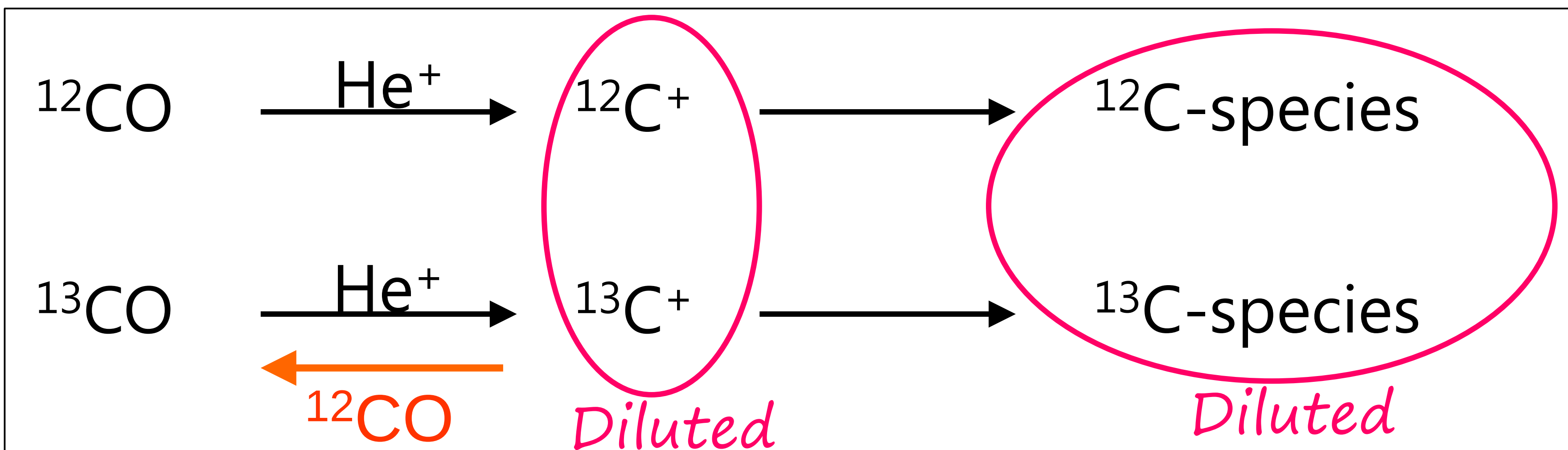
- Main reservoir of ^{13}C in molecular cloud → ^{13}CO
- Source of $^{13}C^+$ for production of molecules

  $CO + He^+ \rightarrow C^+ + O + He$ (→Original $^{12}C^+/^{13}C^+$=60-70)

- Main loss process of $^{13}C^+$

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

  ⇨ High $^{12}C/^{13}C$ ratio in various molecules



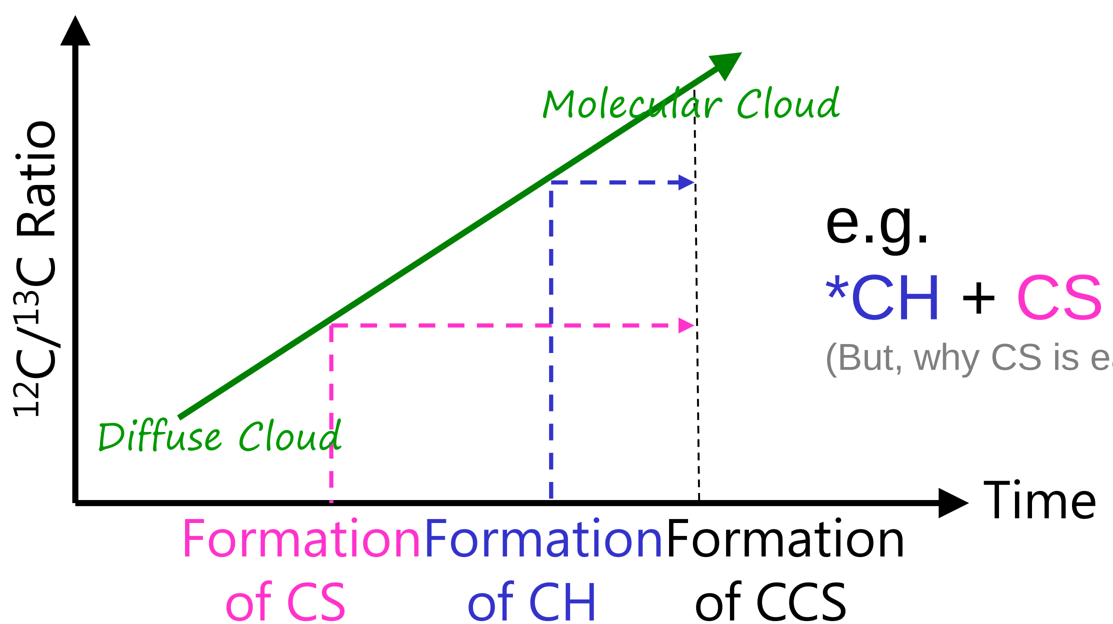
R ~ 60-70 R > 60-70 R > 60-70

(c.f. Langer+1984, ApJ, 277, 581).

$^{12}C/^{13}C$ Ratio in Diffuse Cloud

- Main reservoir of ^{13}C in diffuse cloud → $^{13}C^+$
- $^{12}C^+/^{13}C^+$ ratio remains to be 60-70, even if the $^{13}C^+$ + CO reaction proceeds. (In diffuse cloud, CO is a minor species)
- Various species have the $^{12}C/^{13}C$ ratio of 60-70.

^{13}C is diluted in molecules as cloud evolution!



e.g.
*CH + CS → *CCS
(But, why CS is earlier than CH??)

$^{12}C/^{13}C$ Ratio in CH_3OH

Gas phase Formation

$CH_3^+ + H_2O \rightarrow CH_3OH_2^+ + h\nu$

$CH_3OH_2^+ + e \rightarrow CH_3OH + H$

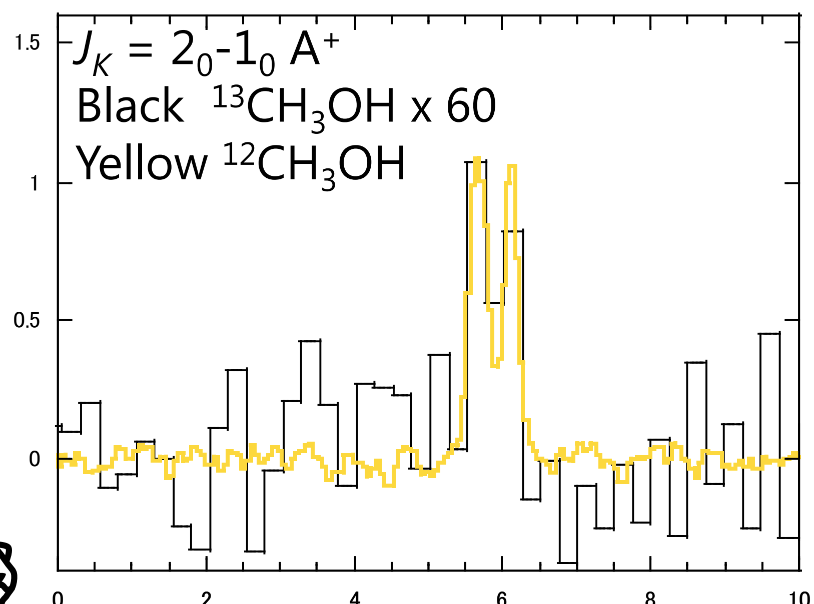
$^{12}C/^{13}C >> 60\text{-}70$

Formation on Grains

$CO \rightarrow HCO \rightarrow H_2CO$

$\rightarrow CH_3O \rightarrow CH_3OH$

$^{12}C/^{13}C = 60\text{-}70$



TMC-1(CP): Starless core

$^{13}CH_3OH$:

$J_K = 1_0\text{-}0_0\ A^+,\ 2_0\text{-}1_0\ A^+,\ 2_{-1}\text{-}1_{-1}\ E$

$^{12}CH_3OH$:

$J_K = 1_0\text{-}0_0\ A^+,\ 2_0\text{-}1_0\ A^+,\ 2_{-1}\text{-}1_{-1}\ E,$
$3_0\text{-}2_0\ A^+,\ 3_{-1}\text{-}2_{-1}\ E$

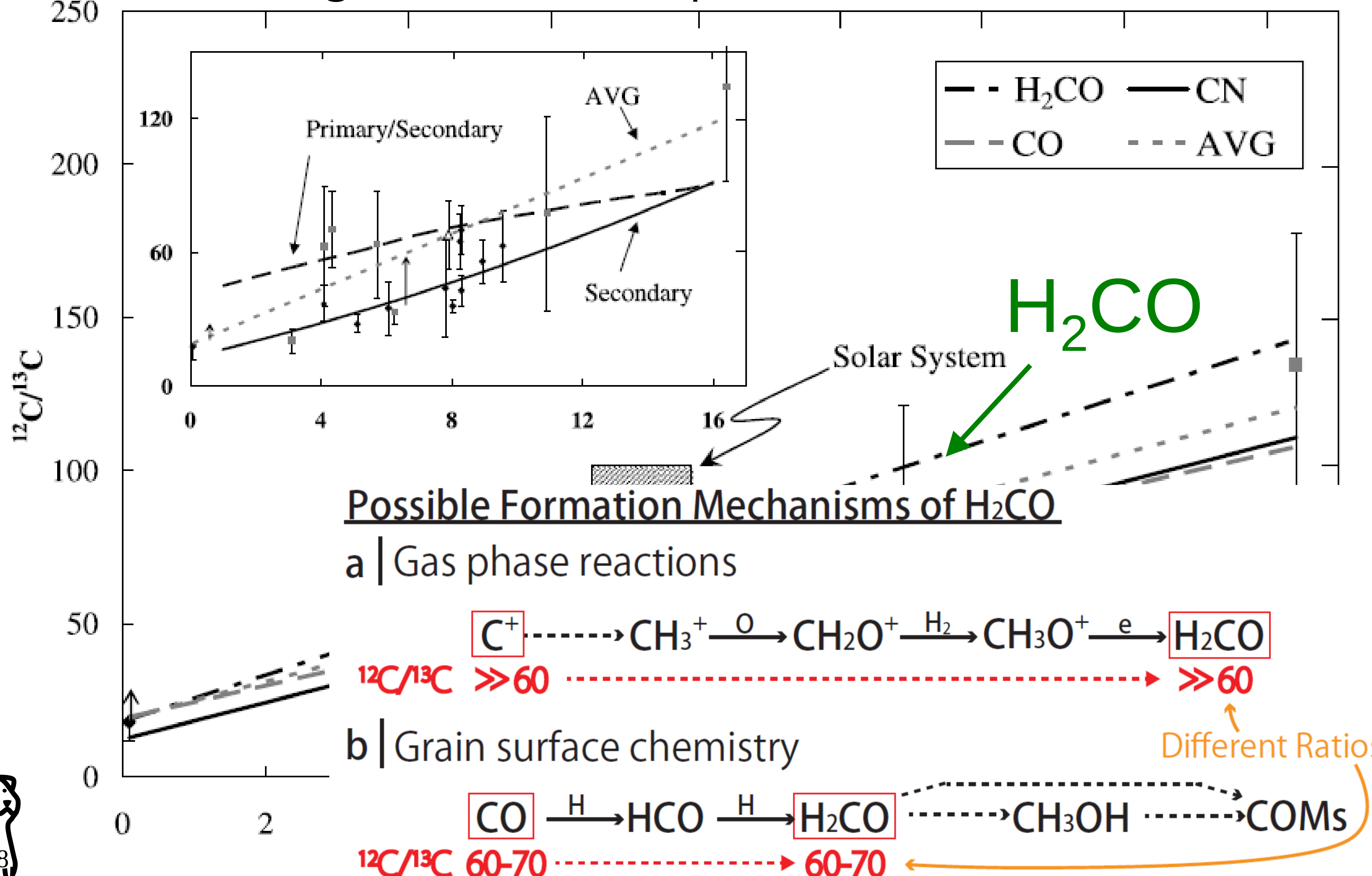
$^{12}C/^{13}C = 62 \pm 10$ (LVG)

Non-thermal Desorption

(Soma, Sakai+2015, ApJ, 802, 74)

$^{12}C/^{13}C$ Ratio in H_2CO?

e.g. Milam et al. ApJ, 634, 1126 (2005)



Summary

- Abundance anomalies are observed in ^{13}C isotopomers in the same species. (HC_3N, HC_5N, CCS, C_3S, CCH, c-C_3H_2, C_4H)

  →It would reflect production pathways, although isotope exchange reactions after the formation of molecules may affect the ratio.

- Various ^{13}C species are found to be diluted in molecules.

  →Molecules formed from C^+ (but not via CO) can have higher $^{12}C/^{13}C$ ratio

- $^{12}C/^{13}C$ ratio would becomes higher along cloud evolution.

  →We can learn formation pathways not only for carbon-chain molecules but also for other C-bearing species.
  (ex; CH_3OH, H_2CO, and many other COMs)
  ($^{12}C/^{13}C$ ratio could be a tracer of cloud evolution?)

AAS

Postdoctoral Positions in Astrophysics and Astrochemistry in Japan - JRID55814

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Submission Dates