Chemical exchange between isotopes of carbon and oxygen in a T-Tauri disk

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Outline of the talk

- Modelling disk chemistry

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- ^{13}C isotope chemistry in disks

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- Modelling disk chemistry
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- Modelling disk chemistry
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- Small species - HCN and C_2H_2

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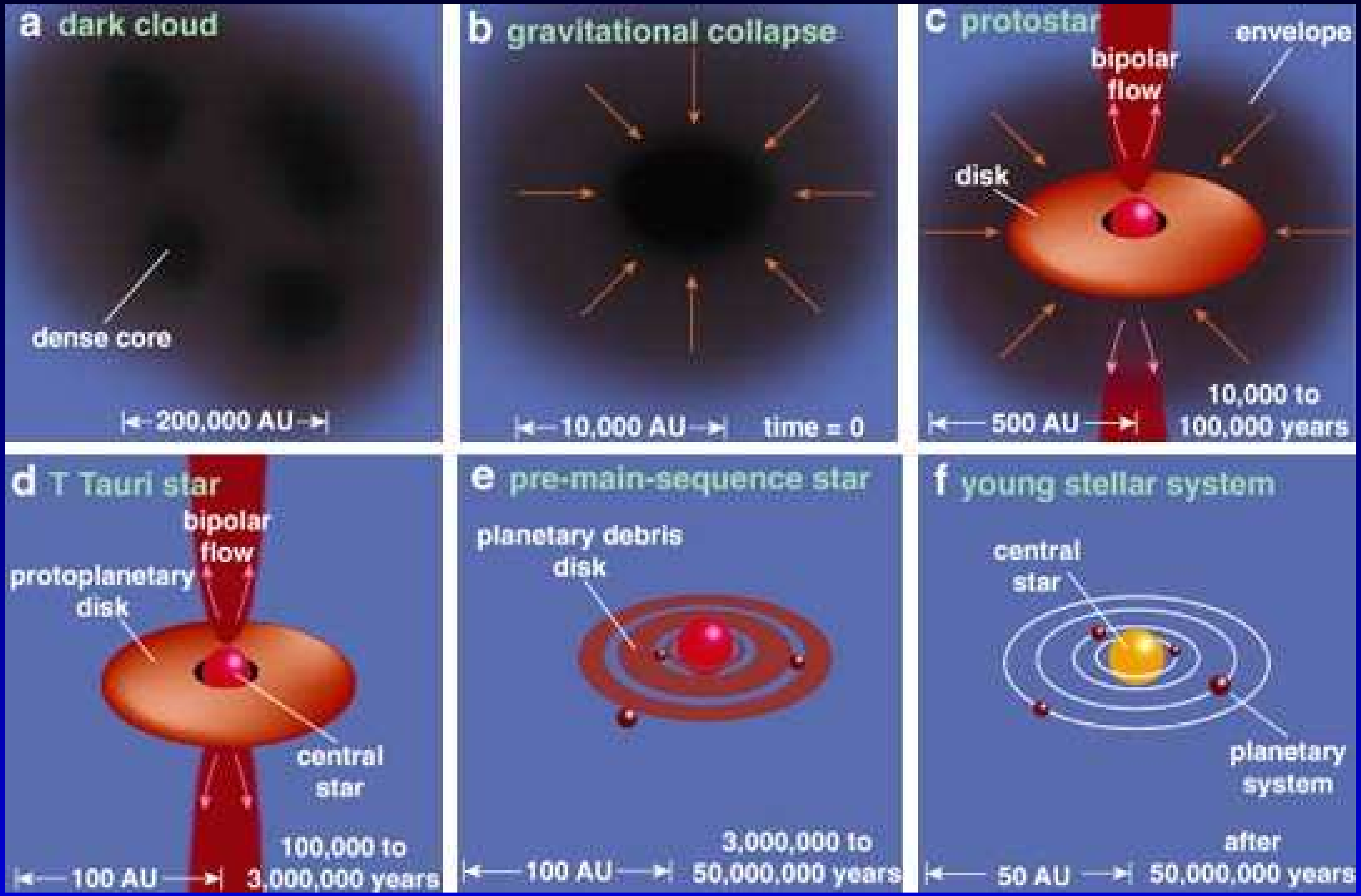
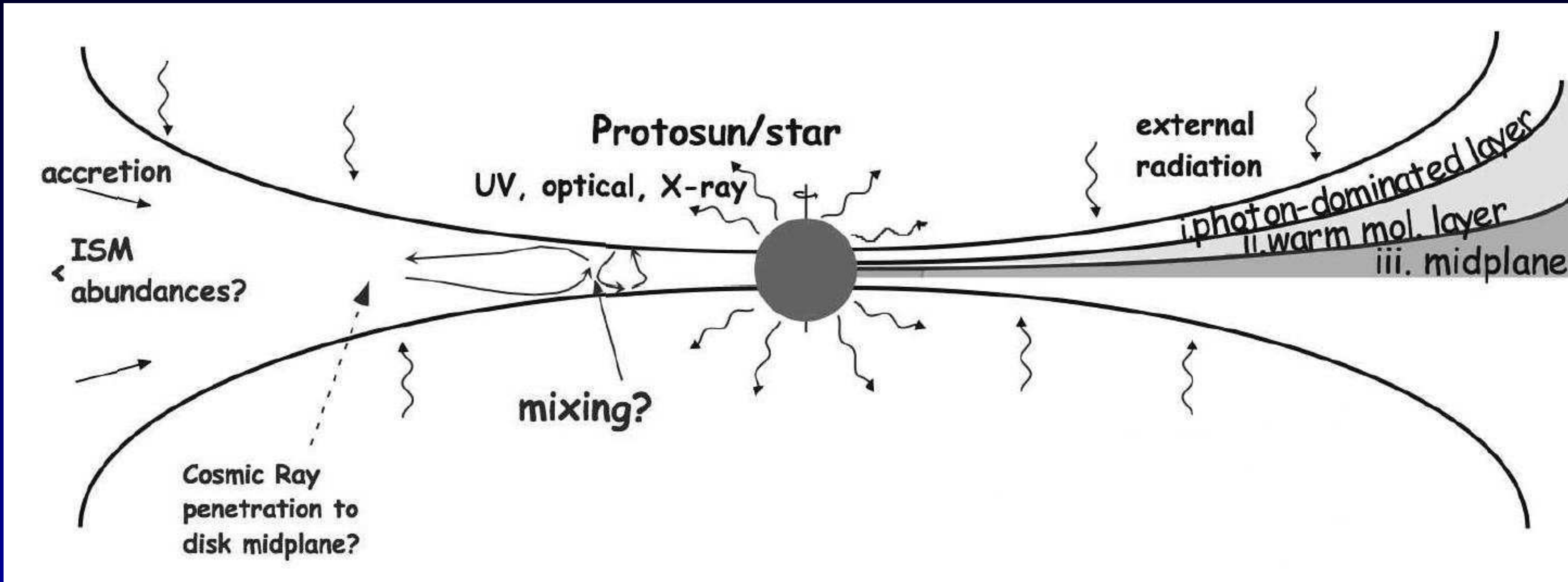
Low-mass star formation



Greene (2001)

A chemical view of disks



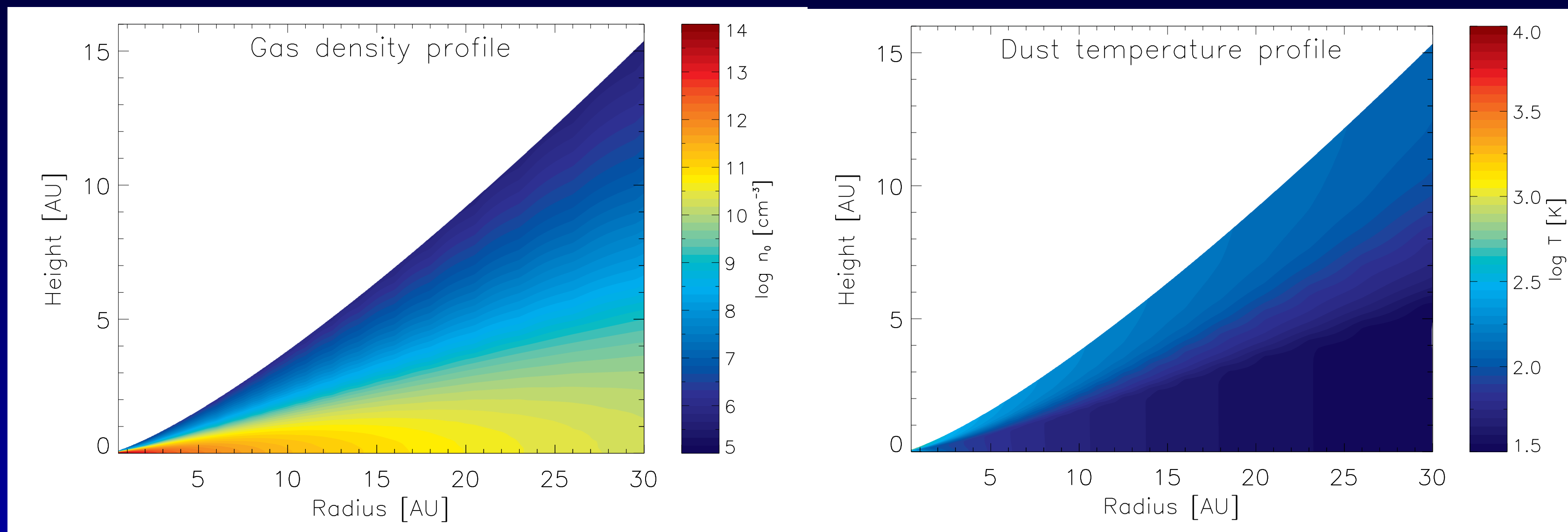
i) Photon-dominated layer - mostly ions and radicals, e.g. C^+

ii) Warm molecular layer - many species in the gas phase, interactions between ions and neutrals

iii) Midplane - most species frozen out onto grains

Disk model

Model of D'Alessio et al. for a typical T Tauri disk



$\dot{M} = 10^{-8}\,\mathrm{M_\odot yr^{-1}}$, $\alpha = 0.01$, $M_\star = 0.5\,\mathrm{M_\odot}$,
$R_\star = 2\,\mathrm{R_\odot}$, $T_\star = 4\,000\,\mathrm{K}$, $L_\star = 0.9\,\mathrm{L_\odot}$, $\eta = 1$

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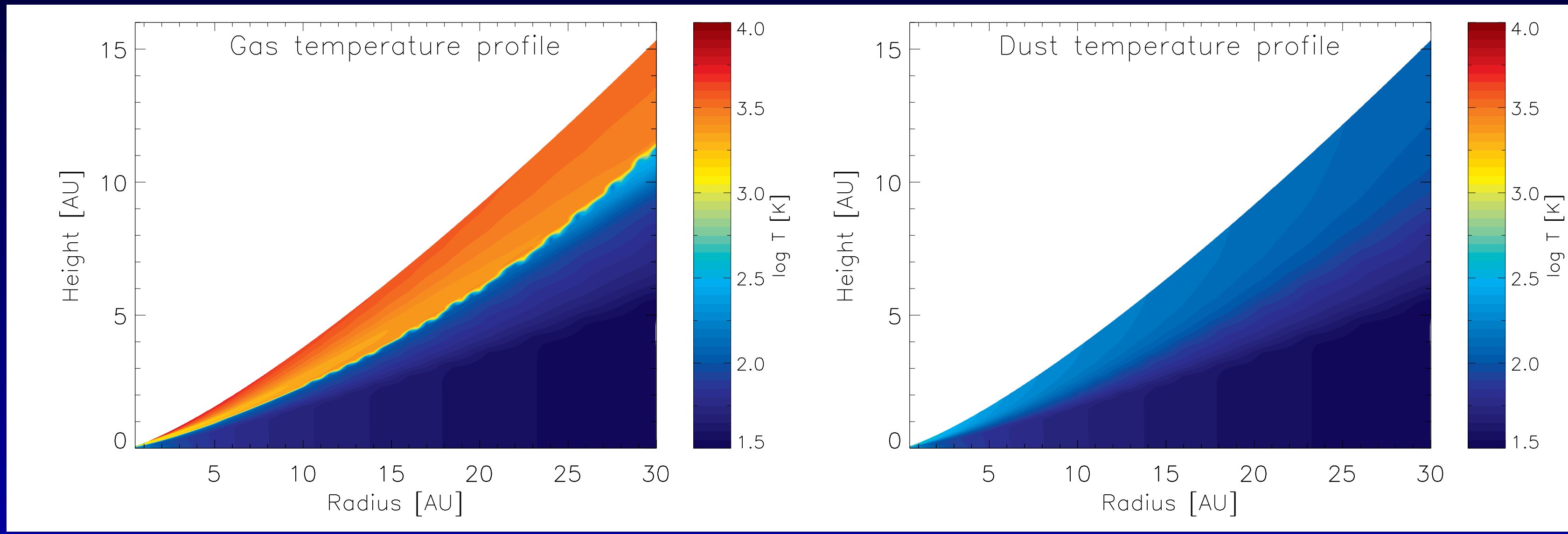
Disk model

Model of D'Alessio et al. for a typical T Tauri disk



$\dot{M} = 10^{-8}\,\mathrm{M}_\odot \mathrm{yr}^{-1}$, $\alpha = 0.01$, $M_\star = 0.5\,\mathrm{M}_\odot$,
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Chemical model

A subset of the UMIST Ratefile
(www.udfa.net)
+ grain surface reactions
+ X-ray ionisation reactions
= around 8000 reactions
between 475 species
incorporating 6 elements
Interstellar initial abundances
3 or 4 days to run on a 3 GHz PC

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- ^{13}C isotope chemistry in disks

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What can isotopes of C tell us?

- Trace the origin and evolution of molecules
  - Formation environment
  - Types of chemical processing
- Trace vertical temperature structure of disks (Piétu et al. 2007, Dartois et al. 2003)
- Allow us to trace molecules which may be optically thick (^{12}CO vs. ^{13}CO)
- Label various regions of the disk
- Indicate grain chemistry in action? (Charnley et al. 2004)

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Carbon isotope chemistry

$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E(35\,\mathrm{K})$$

Rate measured by Watson et al. (1976), Smith & Adams (1980)
Rate calculated by Langer et al. (1984), Lohr (1998)

$$\mathrm{H}^{12}\mathrm{CO}^{+} + ^{13}\mathrm{CO} \rightleftharpoons \mathrm{H}^{13}\mathrm{CO}^{+} + ^{12}\mathrm{CO} + \Delta E(9\,\mathrm{K})$$

Rate measured by Smith & Adams (1980)
Rate calculated by Langer et al. (1984), Lohr (1998)

Carbon isotope chemistry

$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E(35\,\mathrm{K})$$

$$\begin{aligned} k_{\mathrm{for}} &= 3.3 \times 10^{-10} (T/300\,\mathrm{K})^{-0.448} \\ k_{\mathrm{rev}} &= k_{\mathrm{for}} \exp(-35\,\mathrm{K}/T) \end{aligned}$$

Woods & Willacy (2008)

$$\mathrm{H}^{12}\mathrm{CO}^{+} + ^{13}\mathrm{CO} \rightleftharpoons \mathrm{H}^{13}\mathrm{CO}^{+} + ^{12}\mathrm{CO} + \Delta E(9\,\mathrm{K})$$

$$\begin{aligned} k_{\mathrm{for}} &= 2.6 \times 10^{-10} (T/300\,\mathrm{K})^{-0.277} \\ k_{\mathrm{rev}} &= k_{\mathrm{for}} \exp(-9\,\mathrm{K}/T) \end{aligned}$$

Woods & Willacy (2008)

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Carbon isotope chemistry

-

$$\mathrm{HO^{13}C^{+} + ^{12}CO \rightleftharpoons ^{13}CO + HO^{12}C^{+}} + \Delta E(2.5\,\mathrm{K})$$

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Carbon isotope chemistry

- $$\mathrm{HO^{13}C^{+} + ^{12}CO \rightleftharpoons ^{13}CO + HO^{12}C^{+}} + \Delta E(2.5\,\mathrm{K})$$

- $$\mathrm{^{13}C^{+} + ^{12}CN \rightleftharpoons ^{13}CN + ^{12}C^{+}} + \Delta E(34\,\mathrm{K})$$

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Carbon isotope chemistry

- $$\mathrm{HO^{13}C^{+} + ^{12}CO \rightleftharpoons ^{13}CO + HO^{12}C^{+}} + \Delta E(2.5\,\mathrm{K})$$
- $$\mathrm{^{13}C^{+} + ^{12}CN \rightleftharpoons ^{13}CN + ^{12}C^{+}} + \Delta E(34\,\mathrm{K})$$
- $$\mathrm{^{13}C^{+} + ^{12}CS \rightleftharpoons ^{13}CS + ^{12}C^{+}} + \Delta E$$

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Carbon isotope chemistry

- $$\mathrm{HO^{13}C^{+}} +^{12}\mathrm{CO} \rightleftharpoons^{13}\mathrm{CO} + \mathrm{HO^{12}C^{+}} + \Delta E(2.5\,\mathrm{K})$$
- $$^{13}\mathrm{C^{+}} +^{12}\mathrm{CN} \rightleftharpoons^{13}\mathrm{CN} +^{12}\mathrm{C^{+}} + \Delta E(34\,\mathrm{K})$$
- $$^{13}\mathrm{C^{+}} +^{12}\mathrm{CS} \rightleftharpoons^{13}\mathrm{CS} +^{12}\mathrm{C^{+}} + \Delta E$$
- $$^{13}\mathrm{C^{+}} +^{12}\mathrm{CH_3} \rightleftharpoons^{13}\mathrm{CH_3} +^{12}\mathrm{C^{+}} + \Delta E$$

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Carbon isotope chemistry

- $$\mathrm{HO^{13}C^+ + ^{12}CO \rightleftharpoons ^{13}CO + HO^{12}C^+} + \Delta E (2.5\,\mathrm{K})$$
- $$\mathrm{^{13}C^+ + ^{12}CN \rightleftharpoons ^{13}CN + ^{12}C^+} + \Delta E (34\,\mathrm{K})$$
- $$\mathrm{^{13}C^+ + ^{12}CS \rightleftharpoons ^{13}CS + ^{12}C^+} + \Delta E$$
- $$\mathrm{^{13}C^+ + ^{12}CH_3 \rightleftharpoons ^{13}CH_3 + ^{12}C^+} + \Delta E$$
- $\Longrightarrow$ Rates unknown?

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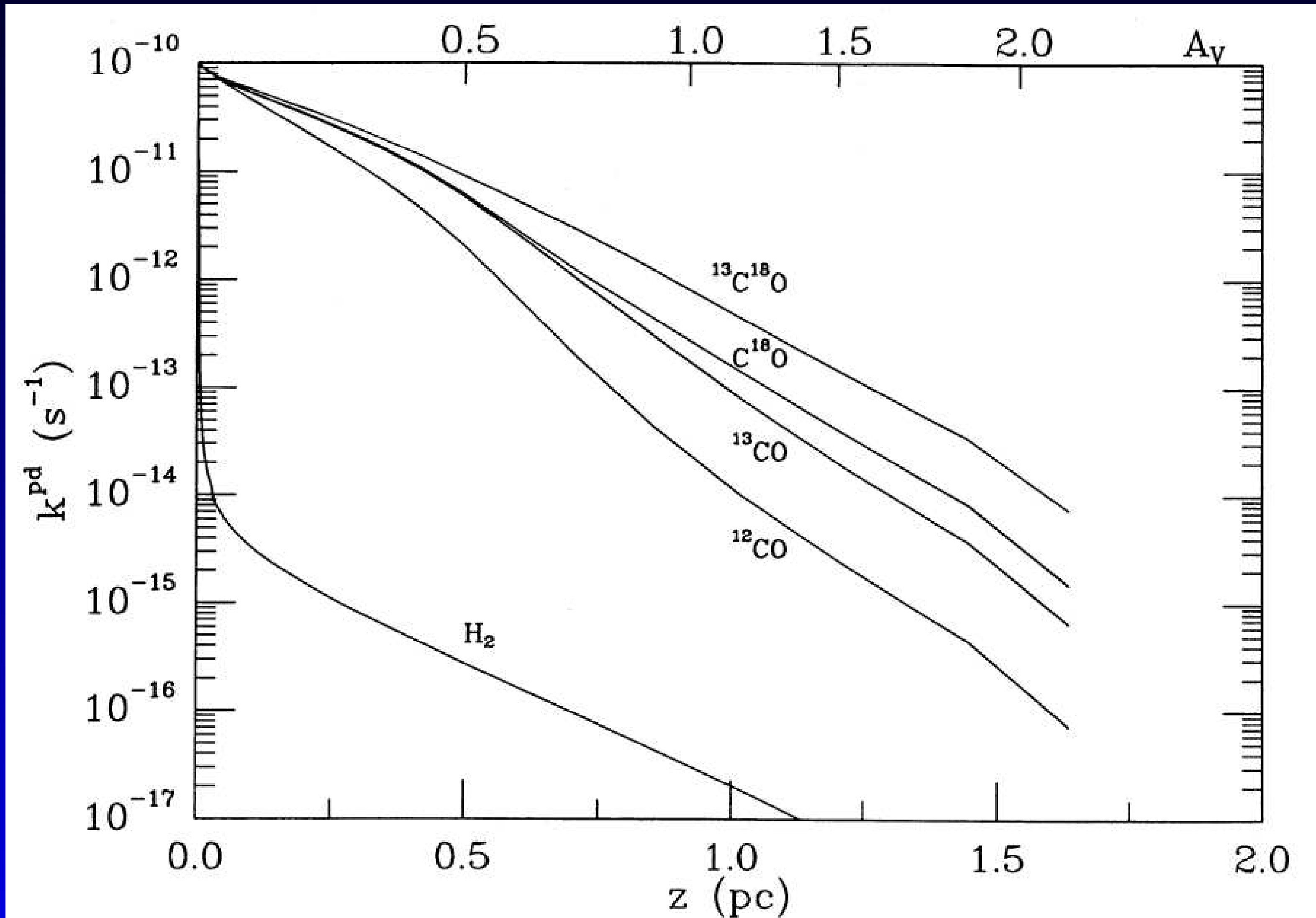
Selective photodissociation



van Dishoeck & Black (1988)

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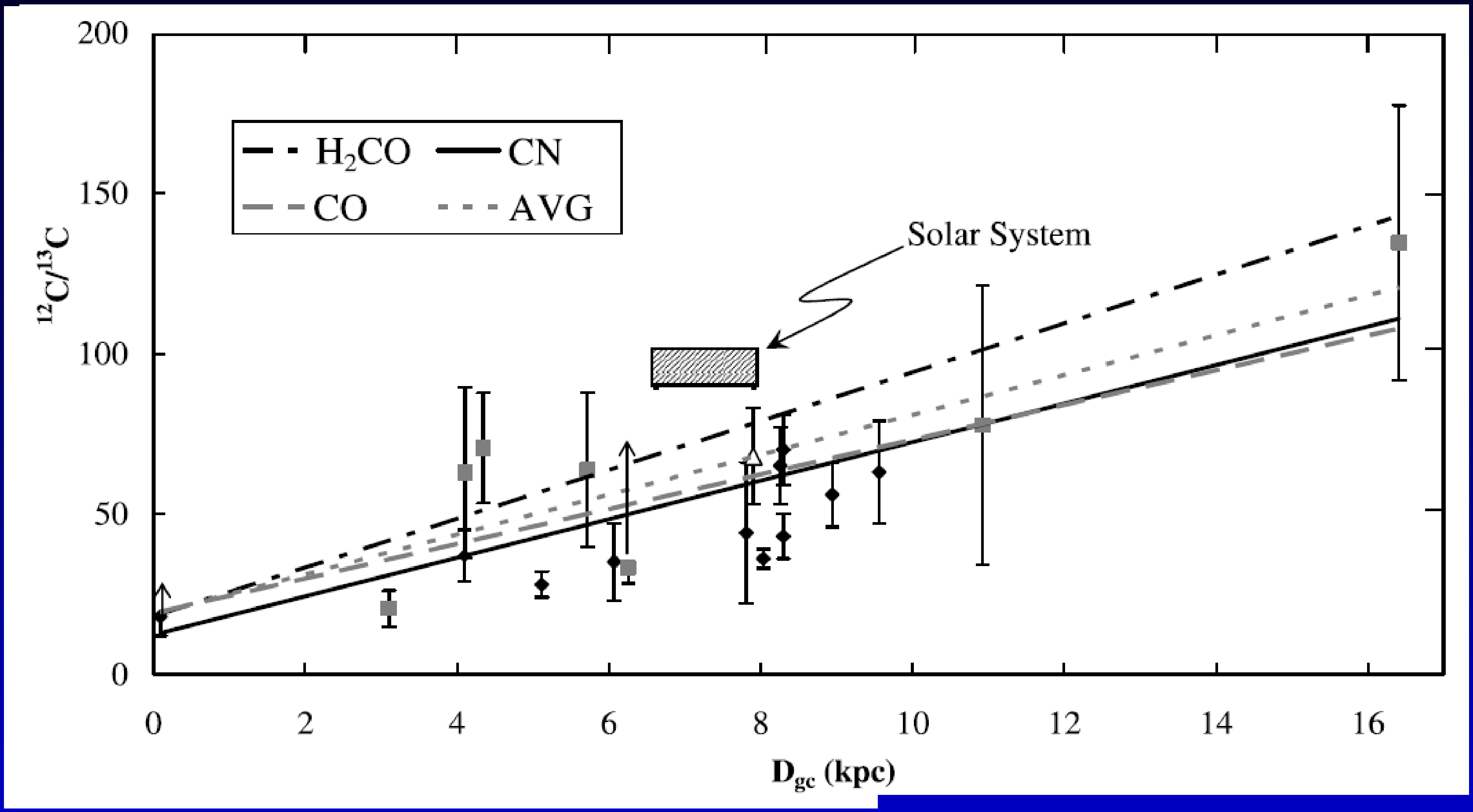
Inputs: the local $^{12}C/^{13}C$ ratio

Hawkins & Jura (1987)	43 ± 4
Goto et al. (2003)	57 ± 5
Langer & Penzias (1993)	62 ± 4
Langer & Penzias (1990)	~70
Stahl & Wilson (1992)	71 ± 3
Stahl et al. (1983)	77 ± 3
Goto et al. (2003)	86 ± 49
Penzias (1983)	100 ± 14
Vladilo et al. (1993)	98–120
Goto et al. (2003)	137 ± 9
Goto et al. (2003)	158

Galactic $^{12}C/^{13}C$ ratio



Milam et al. (2005)

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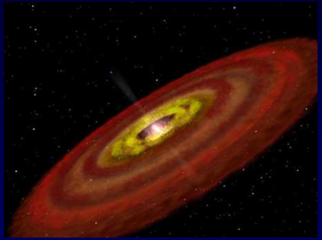
Input abundances

$\frac{^{12}C+}{^{13}C+}$=77 $\Rightarrow$

10^6 yr

$\Rightarrow$ $\frac{^{12}CO}{^{13}CO}$ =56, $\frac{^{12}C}{^{13}C}$ =93 $\Rightarrow$, $\frac{H_2^{12}CO}{H_2^{13}CO}$=108

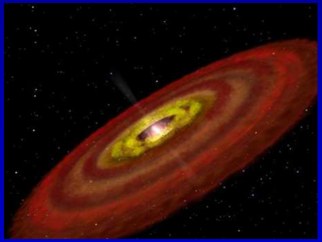


$\Rightarrow$?

$\frac{^{12}C+}{^{13}C+}$=89 $\Rightarrow$

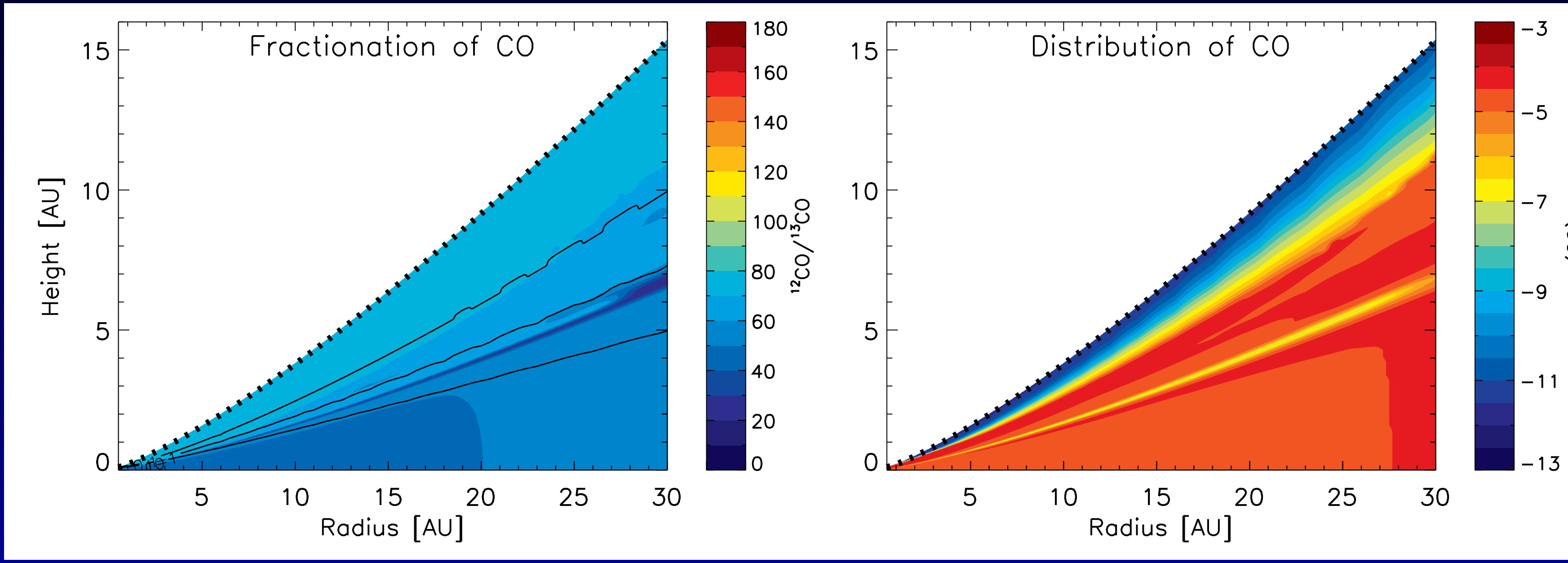
10^6 yr

$\Rightarrow$ $\frac{^{12}CO}{^{13}CO}$ =64, $\frac{^{12}C}{^{13}C}$ =108 $\Rightarrow$, $\frac{H_2^{12}CO}{H_2^{13}CO}$=125



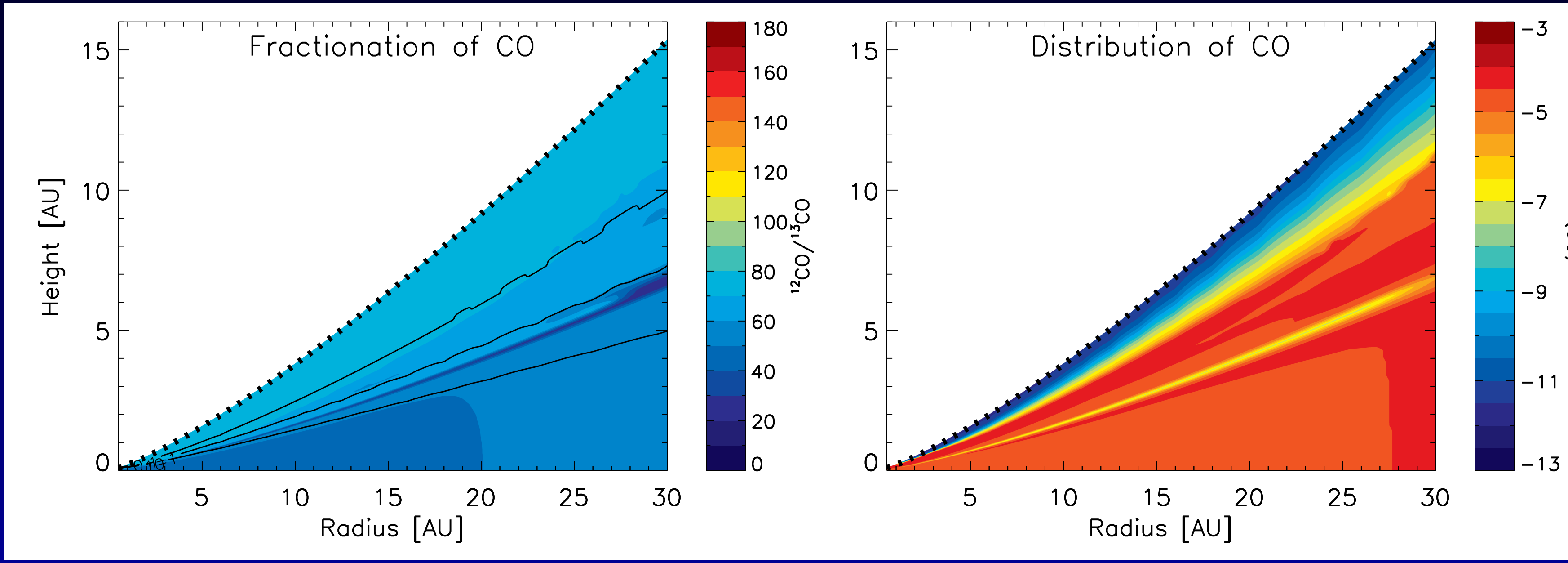
$\Rightarrow$?

Carbon isotopes - CO



$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E$$

Carbon isotopes - CO



Gibb et al. (2007), GV Tau:

$T(^{12}CO) \approx 240\,K$ $\qquad$ $^{12}CO/^{13}CO = 54 \pm 15$

Brittain et al. (2005), HL Tau:

$T(^{12}CO) \approx 100\,K$ $\qquad$ $^{12}CO/^{13}CO = 76 \pm 9$

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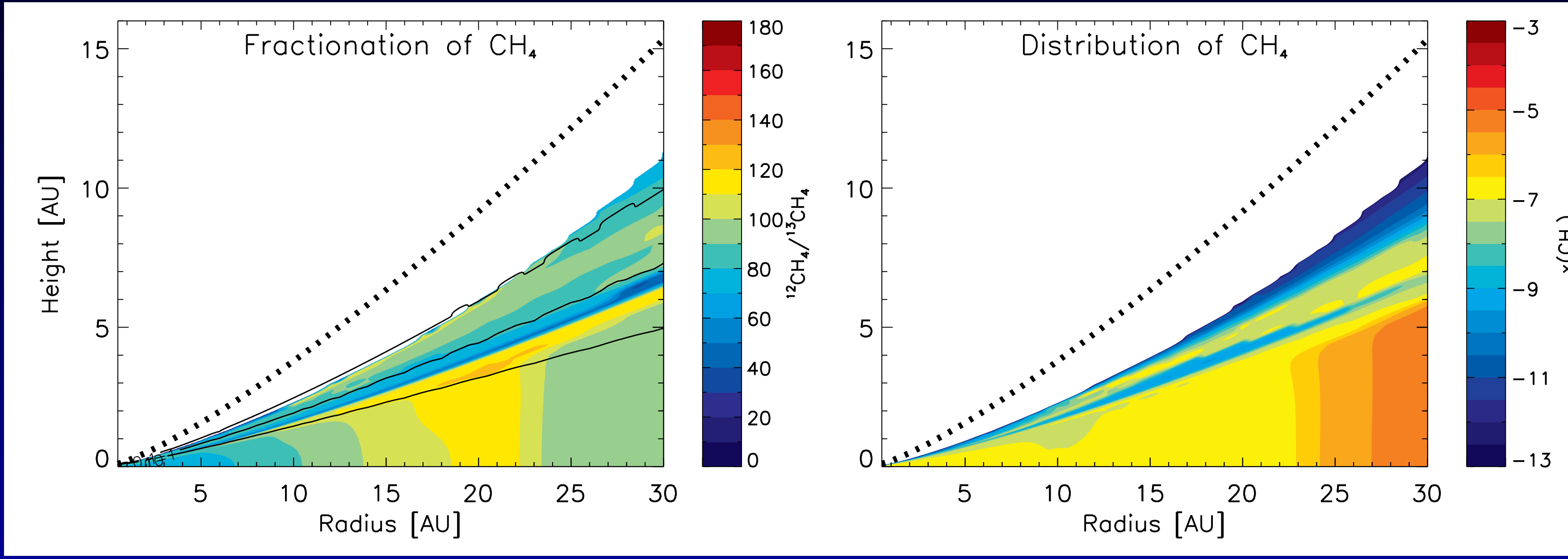
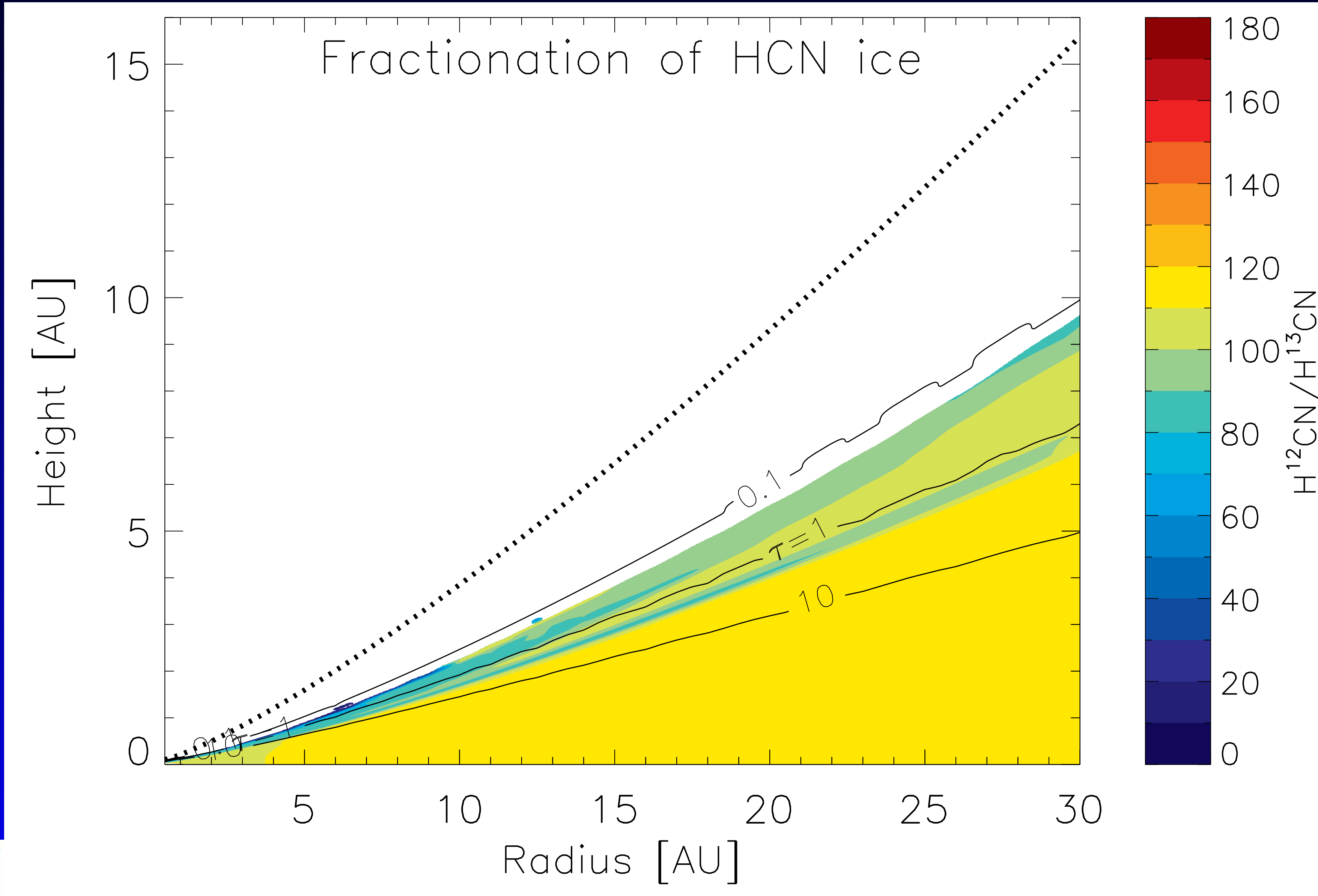
Carbon isotopes - CH_4



$$^{13}\mathrm{C}^{+} + ^{12}\mathrm{CO} \rightleftharpoons ^{13}\mathrm{CO} + ^{12}\mathrm{C}^{+} + \Delta E$$

Carbon isotopes - HCN



Points to note

- Fractionation varies with species
- Fractionation varies with radius
  - for gaseous species
  - some ices retain interstellar fractionation
- Fractionation varies with height

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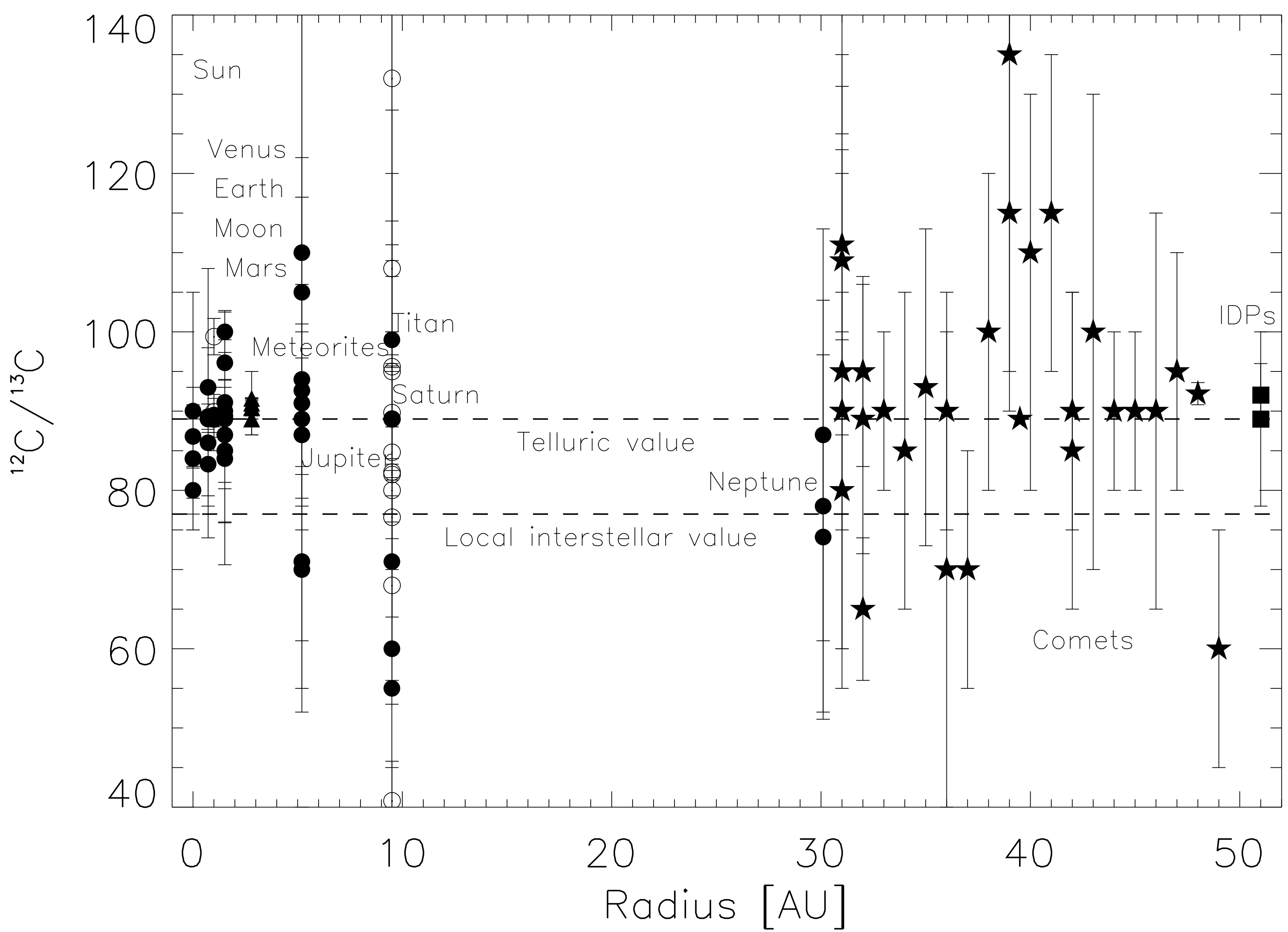
Solar System comparison



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Oxygen isotope chemistry

$$\begin{aligned}
{}^{13}\mathrm{C}^{+} + \mathrm{C}^{18}\mathrm{O} &\rightleftharpoons {}^{13}\mathrm{C}^{18}\mathrm{O} + \mathrm{C}^{+} + \Delta E(36\,\mathrm{K}) \\
\mathrm{HCO}^{+} + \mathrm{C}^{18}\mathrm{O} &\rightleftharpoons \mathrm{HC}^{18}\mathrm{O}^{+} + \mathrm{CO} + \Delta E(14\,\mathrm{K}) \\
\mathrm{HCO}^{+} +^{13}\mathrm{C}^{18}\mathrm{O} &\rightleftharpoons \mathrm{H}^{13}\mathrm{C}^{18}\mathrm{O}^{+} + \mathrm{CO} + \Delta E(22\,\mathrm{K}) \\
\mathrm{H}^{13}\mathrm{CO}^{+} + \mathrm{C}^{18}\mathrm{O} &\rightleftharpoons \mathrm{HC}^{18}\mathrm{O}^{+} +^{13}\mathrm{CO} + \Delta E(5\,\mathrm{K}) \\
\mathrm{H}^{13}\mathrm{CO}^{+} +^{13}\mathrm{C}^{18}\mathrm{O} &\rightleftharpoons \mathrm{H}^{13}\mathrm{C}^{18}\mathrm{O}^{+} +^{13}\mathrm{CO} + \Delta E(13\,\mathrm{K}) \\
\mathrm{HC}^{18}\mathrm{O}^{+} +^{13}\mathrm{C}^{18}\mathrm{O} &\rightleftharpoons \mathrm{H}^{13}\mathrm{C}^{18}\mathrm{O}^{+} + \mathrm{C}^{18}\mathrm{O} + \Delta E(8\,\mathrm{K})
\end{aligned}$$

Rates measured by Smith & Adams (1980)

Rates calculated by Langer et al. (1984), Lohr (1998)

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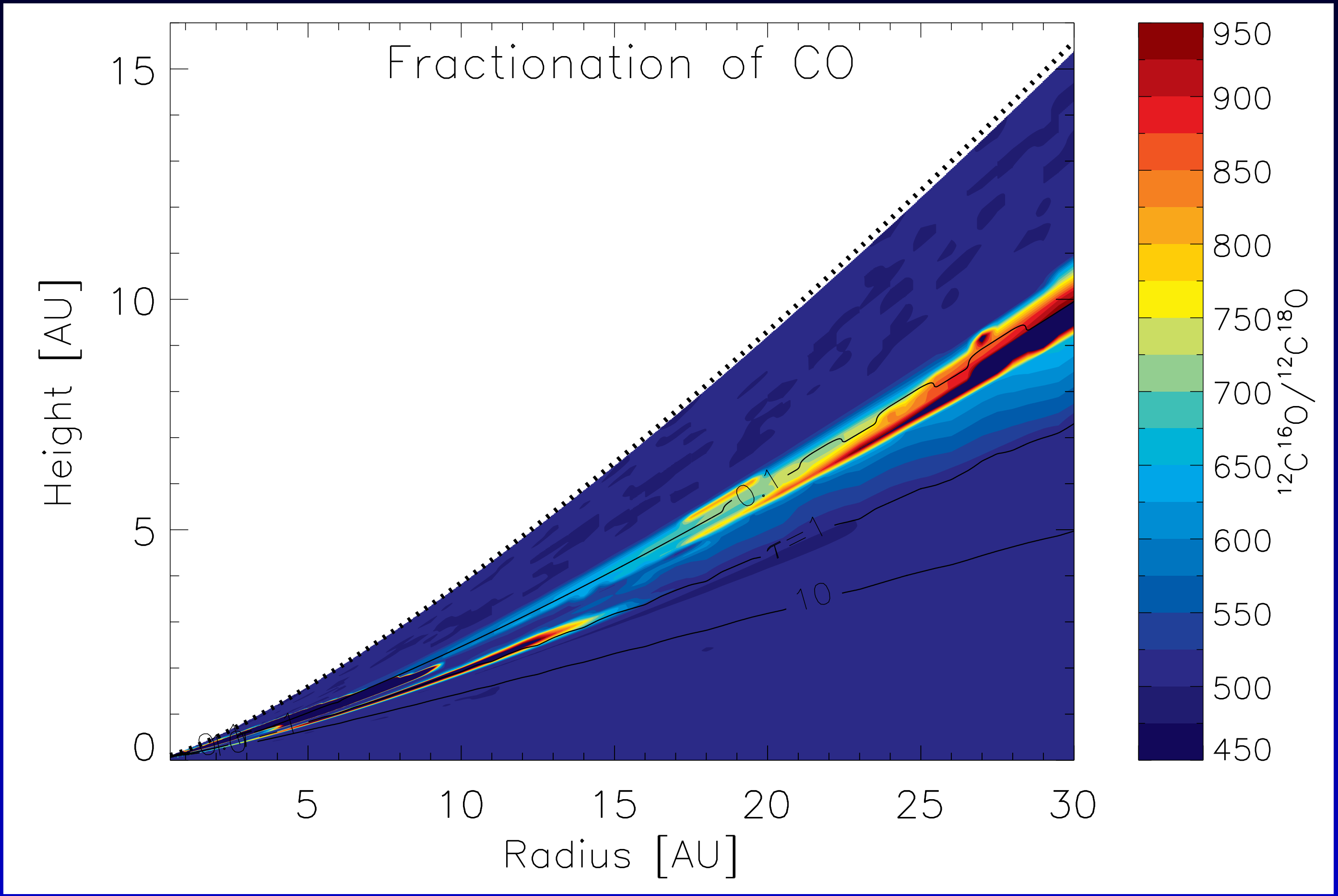
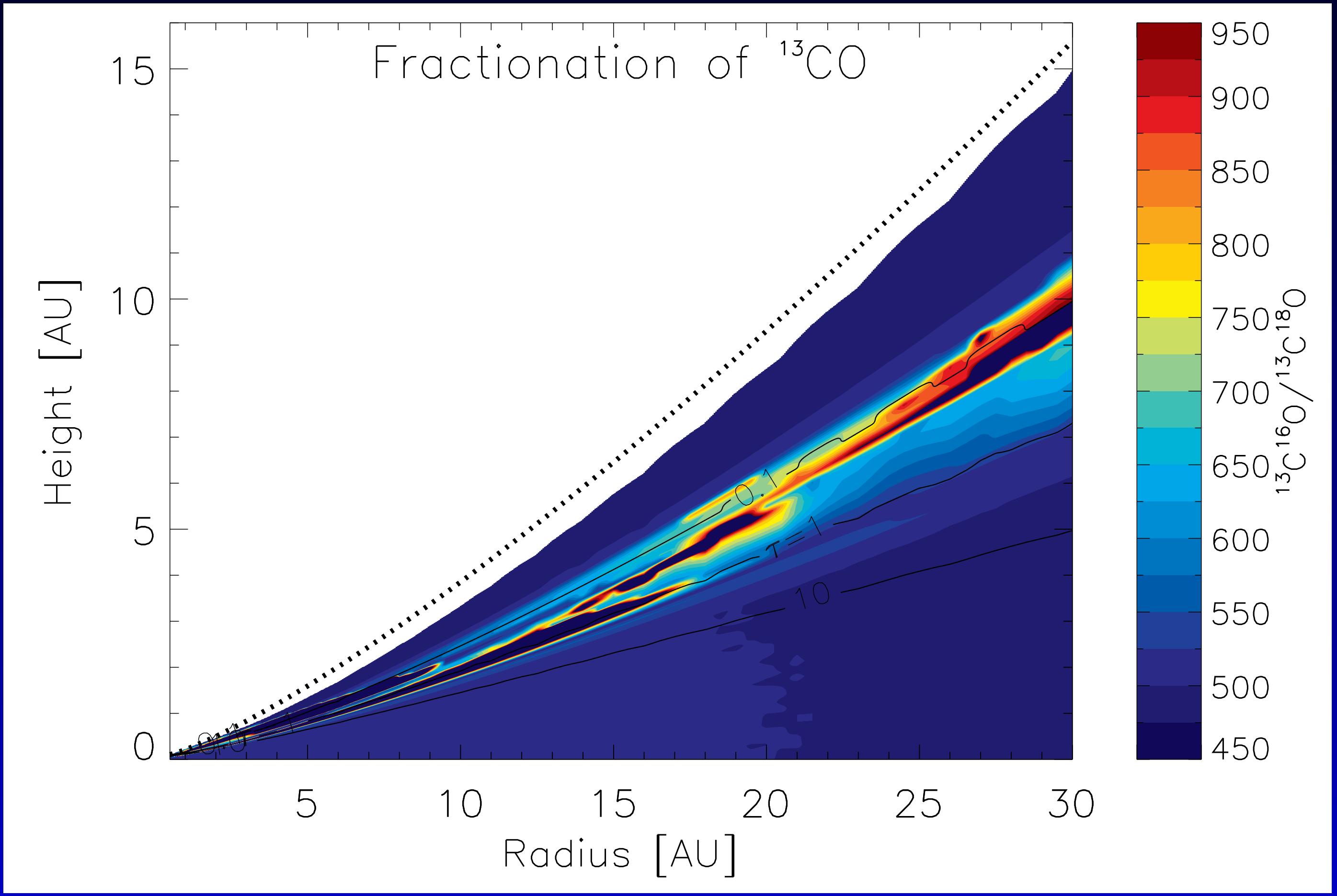
Initial results



Input ratio $^{16}O/^{18}O = 500$.

Initial results



Input ratio $^{16}O/^{18}O = 500$.

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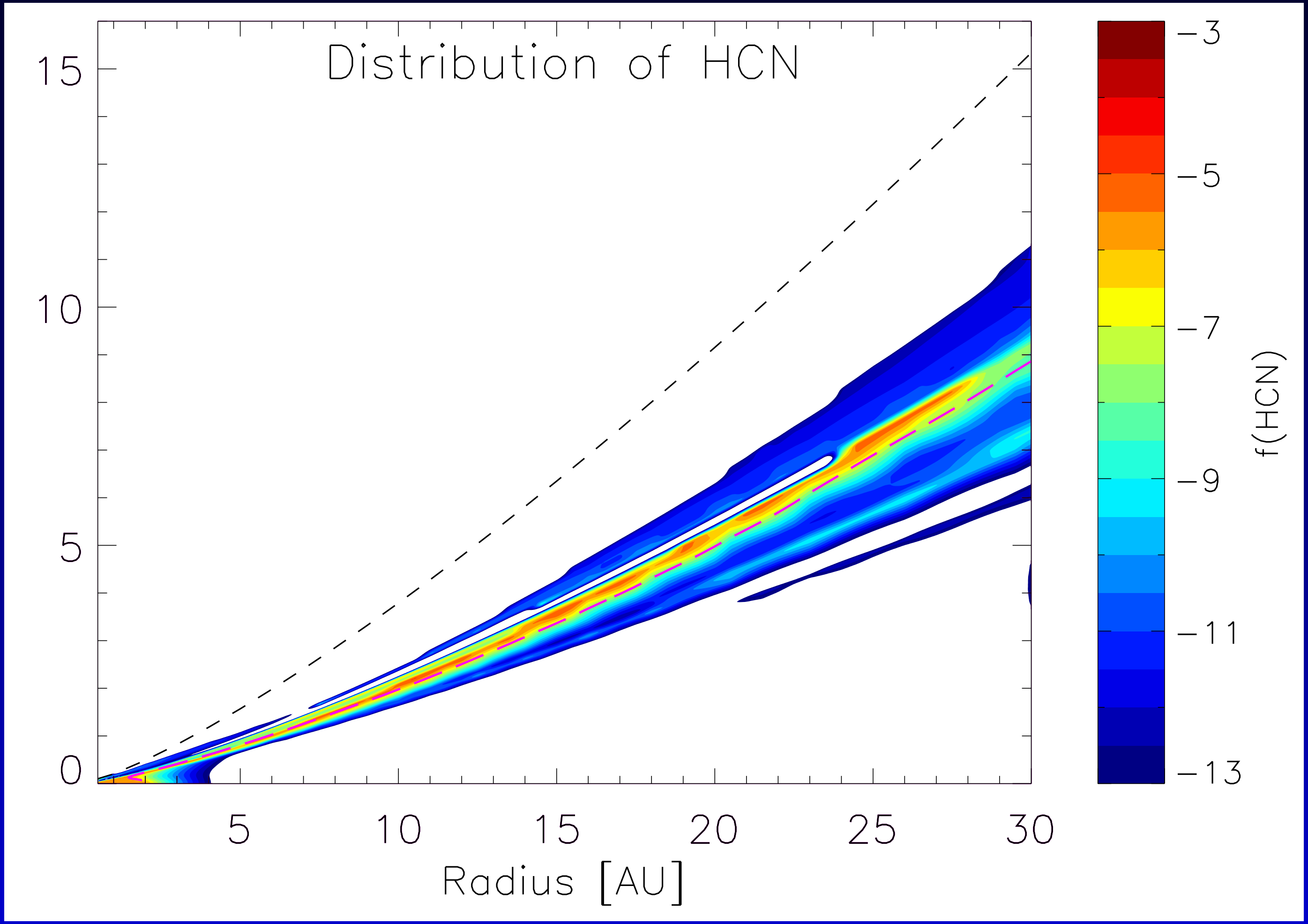
Simple molecules - HCN, C_2H_2



GV Tau: T(HCN) $\sim$ 115 K (Gibb et al. 2007)

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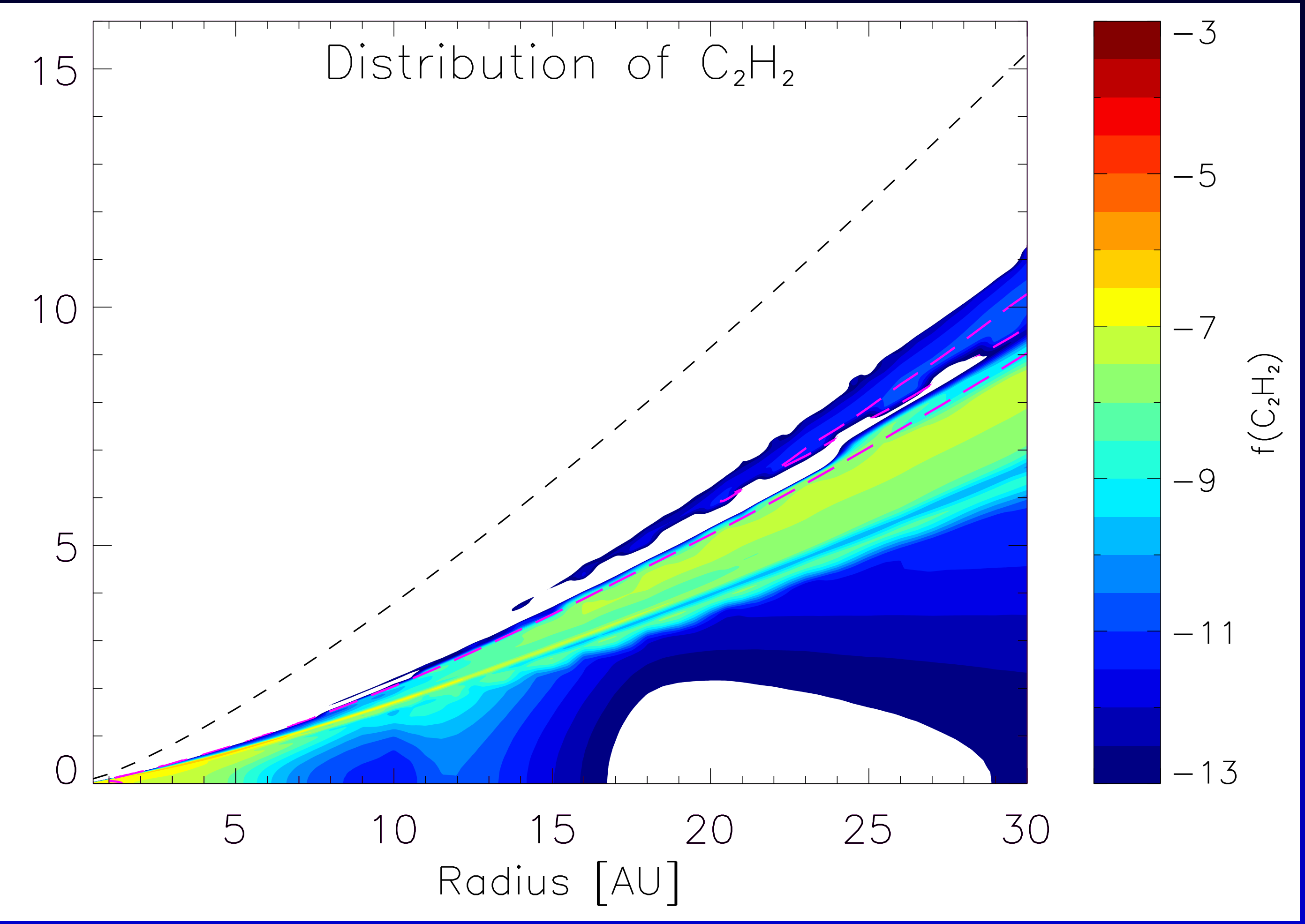
Simple molecules - HCN, C_2H_2



GV Tau: $T(C_2H_2) \sim 170\,K$ (Gibb et al. 2007)

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- ^{13}C isotope chemistry in disks
- Small species - HCN and C_2H_2
- Complex species - benzene and PAHs

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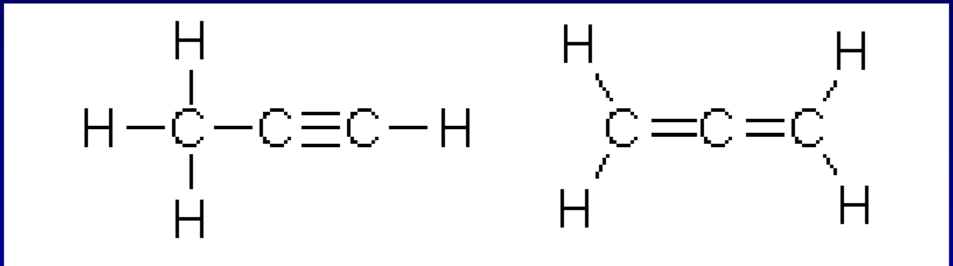
Forming complex species

$$CH_4 + C_2H_3^+ \longrightarrow C_3H_5^+ + H_2$$
$$C_3H_5^+ + e^- \longrightarrow C_3H_4 + H$$



Forming complex species

$$CH_4 + C_2H_3^+ \longrightarrow C_3H_5^+ + H_2$$
$$C_3H_5^+ + e^- \longrightarrow C_3H_4 + H$$

$$C_3H_4 + C^{(+)} \longrightarrow C_4H^{(+)} + H_2$$
$$C_3H_4 + C_2H_4^+ \longrightarrow C_4H_5^+ + CH_3$$
$$C_3H_4 + C_2H_2^+ \longrightarrow C_5H_4^+ + H_2$$
$$C_3H_4 + C_2H_3^+ \longrightarrow C_5H_5^+ + H_2$$
$$C_3H_4 + C_3X^+ \longrightarrow C_6X^+ + \text{H or } H_2$$
$$C_3H_4 + C_4X^+ \longrightarrow C_7X^+ + \text{H or } H_2$$
$$C_3H_4 + C_5X^+ \longrightarrow C_8X^+ + \text{H or } H_2$$

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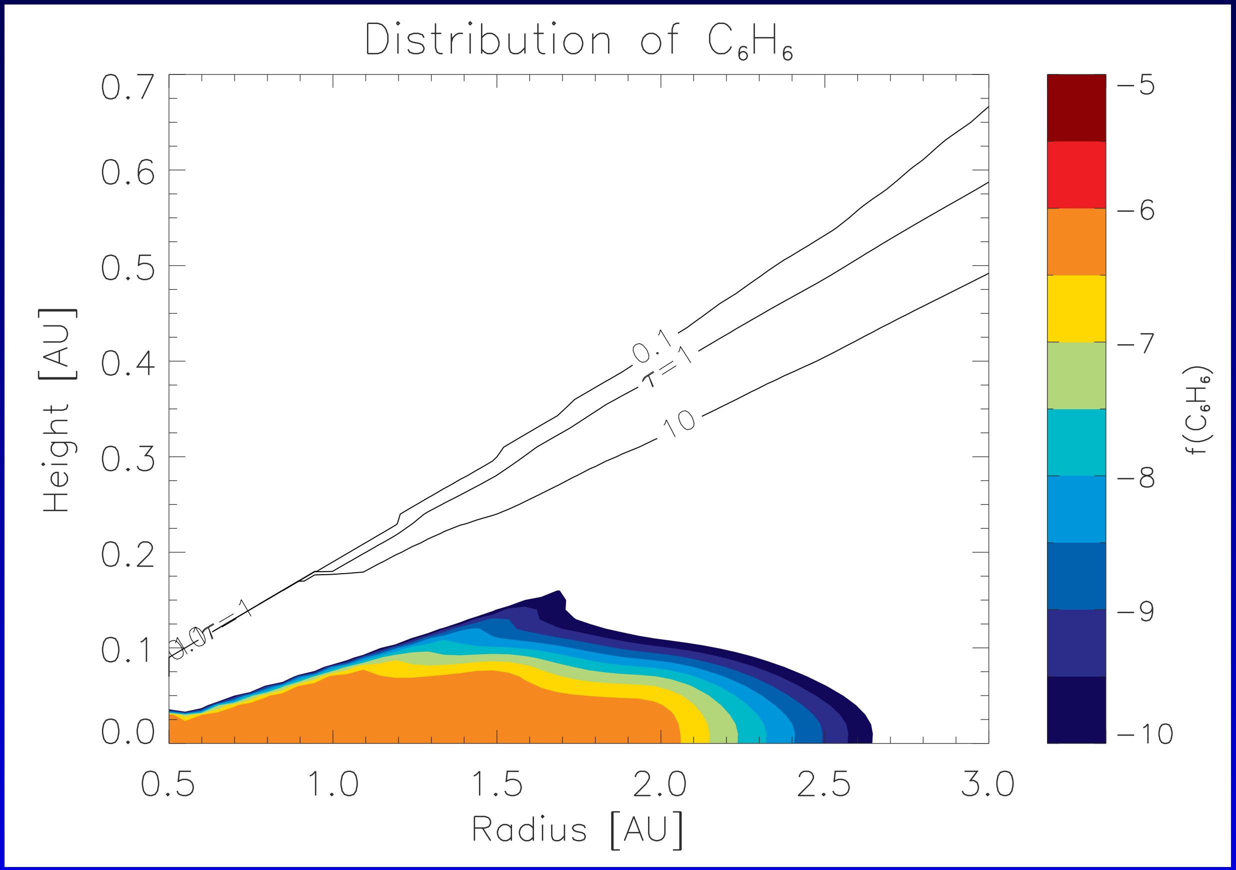
Complex species - C_6H_6

$$C_3H_4 + C_3H_4^+ \longrightarrow c{-}C_6H_7^+ + H$$

$$c{-}C_6H_7^+ + \text{grain} \longrightarrow g{-}C_6H_6 + g{-}H$$



Woods & Willacy, 2007, ApJ, 655, L49

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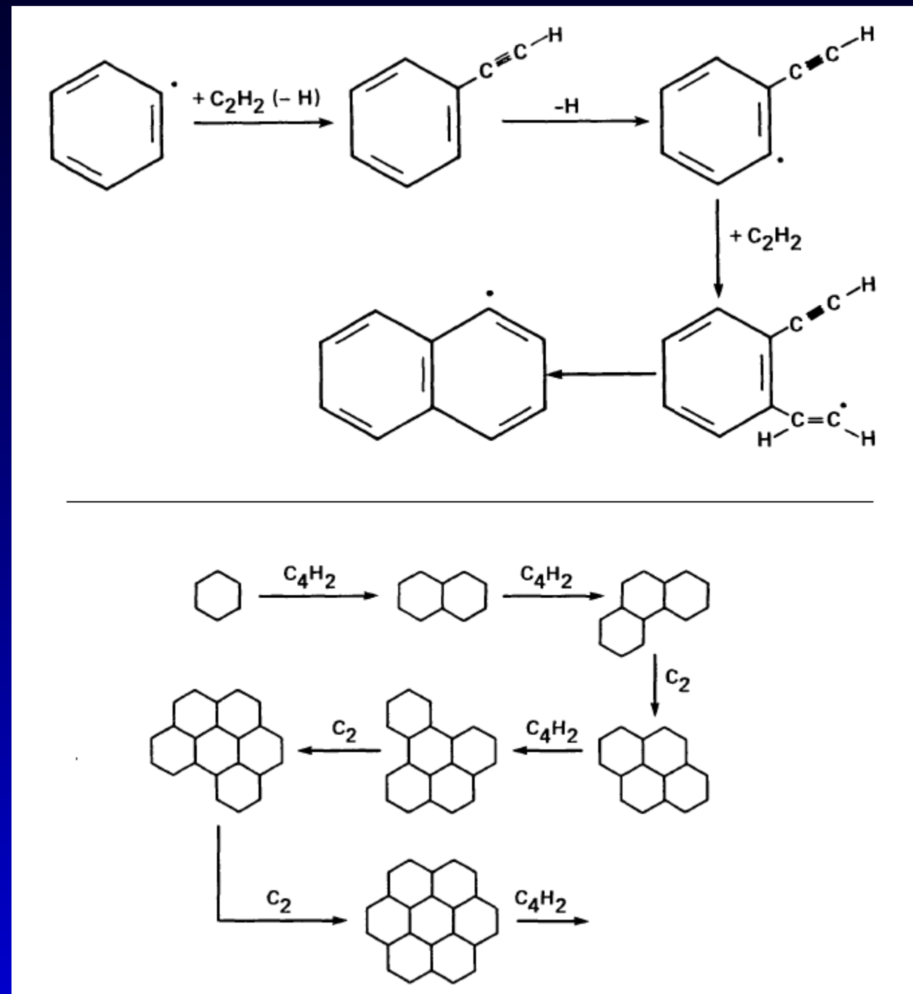
PAHs



Allamandola et al. (1989)

PAHs

PAHs have been observed in T Tauri disks:
e.g., Geers et al. (2006)

PAHs may form in the gas phase in AGB stars:
e.g., Frenklach & Feigelson (1989), Cherchneff et al. (1992)

Regions of high density with long residency times occur in the inner regions of disks. Do the right ingredients (benzene, acetylene) mix at the right temperatures (700–1 100 K)?

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Impact of ALMA on chemistry

- ALMA will allow us to resolve different chemical regions - both vertically and radially
- Sub-arcsecond resolution at the distance of local star-forming regions such as Taurus and Orion will let us probe inside 10 AU
- ALMA will be able to probe the cold gas at R<30 AU, and discover the chemically important regions where molecules come off grains
- High spectral resolution that will help us to separate very narrow lines in the line forest
- Observers will be able to map species and physical conditions at a much higher resolution than currently possible, and help modellers to refine their models.
- Models will give observers densities, temperatures, and more importantly, the location of species of interest

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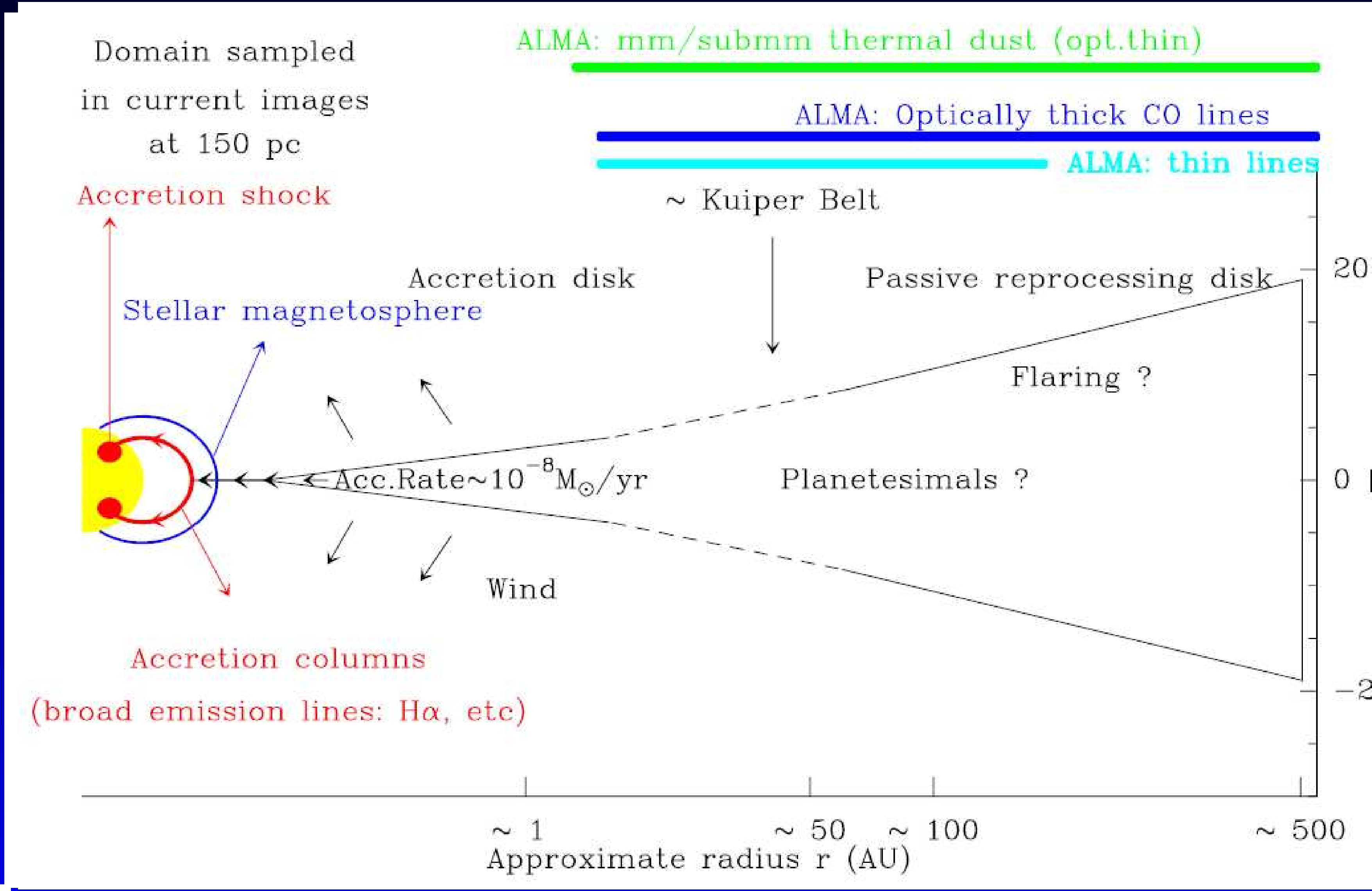
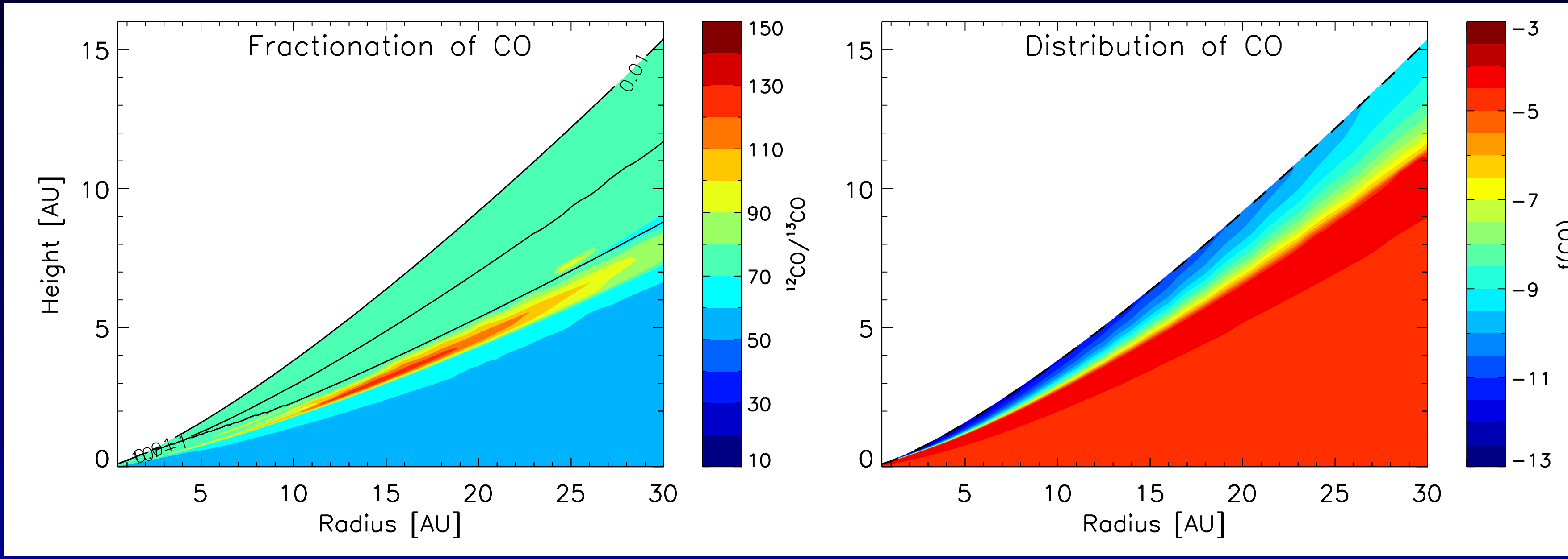
Impact of ALMA on chemistry

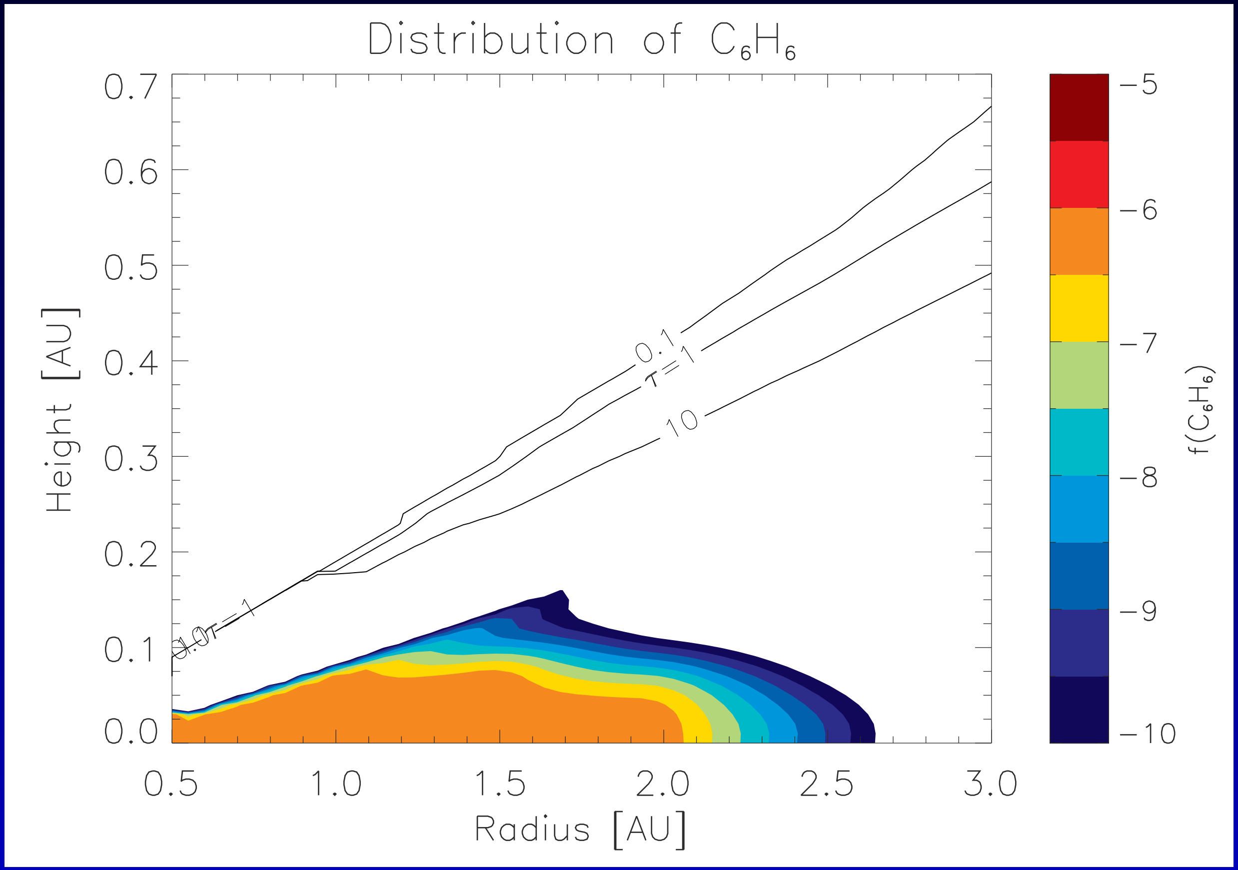


Dutrey et al. (2005)

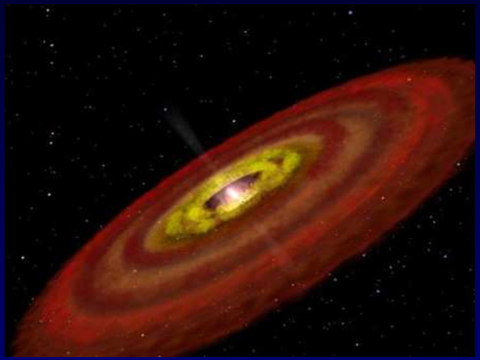
Carbon isotopes - CO



Complex species - C_6H_6



What happens next?



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