Carbon Chemistry – Fractionation in PDRs

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Carbon Chemistry – Fractionation in PDRs

- KOSMA-τ PDR model allows for modular setup of the chemical network, i.e. chemical species are easily added/removed from the chemistry.
- KOSMA-τ includes isotopes in the energy balance (e.g. cooling lines, etc.) and chemistry (e.g. shielding for CO isotopologues, isotope chemistry, etc.)
- Chemical databases do not contain isotopes/isotopologues.

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Introducing isotopologues into chem. databases is tedious.

$$\mathrm{H + CH \longrightarrow C + H_2}$$

becomes

$$\mathrm{H + {}^{12}CH \longrightarrow {}^{12}C + H_2}$$
$$\mathrm{H + {}^{13}CH \longrightarrow {}^{13}C + H_2}$$

$$\mathrm{C + HCO^+ \longrightarrow CO + CH^+}$$

becomes

$$\mathrm{C + HC^{18}O^+ \longrightarrow C^{18}O + CH^+}$$
$$\mathrm{C + H^{13}CO^+ \longrightarrow {}^{13}CO + CH^+}$$
$$\mathrm{C + H^{13}C^{18}O^+ \longrightarrow {}^{13}C^{18}O + CH^+}$$
$$\mathrm{{}^{13}C + HCO^+ \longrightarrow CO + {}^{13}CH^+}$$
$$\mathrm{{}^{13}C + HC^{18}O^+ \longrightarrow C^{18}O + {}^{13}CH^+}$$

Introducing isotopologues into chem. databases is tedious.

Keeping functional groups intact.

$$\mathrm{CH_2CN^+ + e^- \longrightarrow CN + CH_2}$$
$$\mathrm{CH_2{}^{13}CN^+ + e^- \longrightarrow {}^{13}CN + CH_2}$$
$$\mathrm{{}^{13}CH_2CN^+ + e^- \longrightarrow CN + {}^{13}CH_2}$$

But not

$$\mathrm{CH_2{}^{13}CN^+ + e^- \longrightarrow CN + {}^{13}CH_2}$$

Carbon Chemistry – Fractionation in PDRs

Introducing isotopologues into chem. databases is tedious.

Many assumptions involved (e.g. *minimal scrambling*)

$$\mathrm{CH_3OH + C_3H^+ \longrightarrow HC_3O^+ + CH_4}$$
$$\mathrm{CH_3OH + C_2{}^{13}CH^+ \longrightarrow HC_2{}^{13}CO^+ + CH_4}$$
$$\mathrm{CH_3{}^{18}OH + C_3H^+ \longrightarrow HC_3{}^{18}O^+ + CH_4}$$
$$\mathrm{CH_3{}^{18}OH + C_2{}^{13}CH^+ \longrightarrow HC_2{}^{13}C{}^{18}O^+ + CH_4}$$
$$\mathrm{{}^{13}CH_3OH + C_3H^+ \longrightarrow HC_3O^+ + {}^{13}CH_4}$$
$$\mathrm{{}^{13}CH_3{}^{18}OH + C_3H^+ \longrightarrow HC_3{}^{18}O^+ + {}^{13}CH_4}$$

But not

$$\mathrm{{}^{13}CH_3OH + C_3H^+ \longrightarrow HC_2{}^{13}CO^+ + CH_4}$$

Carbon Chemistry – Fractionation in PDRs

Isotopization is done by an automatic routine, that can be applied to updated/different databases and takes care of proper reaction rate scaling.

$$\mathrm{C} + \mathrm{O_2} \longrightarrow \mathrm{CO} + \mathrm{O} \qquad \alpha = 4.7(-11)$$

Assuming equal branching ratios leads to:

$$\mathrm{C} + \mathrm{O^{18}O} \longrightarrow \mathrm{CO} + {}^{18}\mathrm{O} \qquad \alpha = 2.35(-11)$$

$$\mathrm{C} + \mathrm{O^{18}O} \longrightarrow \mathrm{C^{18}O} + \mathrm{O} \qquad \alpha = 2.35(-11)$$

$$^{13}\mathrm{C} + \mathrm{O_2} \longrightarrow {}^{13}\mathrm{CO} + \mathrm{O} \qquad \alpha = 4.7(-11)$$

$$^{13}\mathrm{C} + \mathrm{O^{18}O} \longrightarrow {}^{13}\mathrm{CO} + {}^{18}\mathrm{O} \qquad \alpha = 2.35(-11)$$

$$^{13}\mathrm{C} + \mathrm{O^{18}O} \longrightarrow {}^{13}\mathrm{C^{18}O} + \mathrm{O} \qquad \alpha = 2.35(-11)$$

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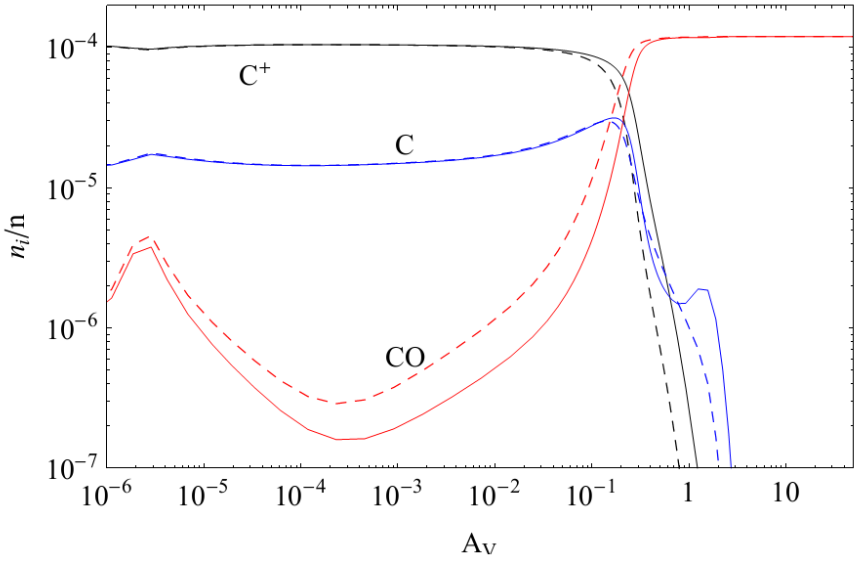
Most important reactions are still fractionation reactions with different back and forth reaction rates. These reactions channel isotopes into some preferred species.

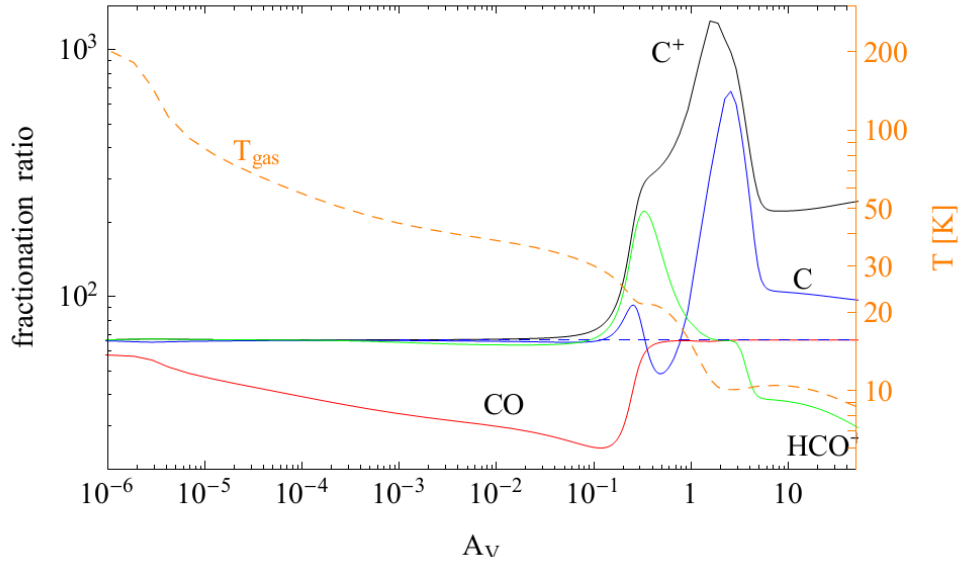
$$^{13}C^{+} + CO \rightleftharpoons C^{+} + {}^{13}CO + \Delta E = 35\,K$$

$$HCO^{+} + {}^{13}CO \rightleftharpoons H{}^{13}CO^{+} + CO + \Delta E = 9\ K$$

Whenever the chemistry of one of the involved species is dominated by the respective fractionation reaction, that species will show considerable fractionation, i.e. a deviation from the elemental abundance ratio (ER).

Carbon Chemistry – Fractionation in PDRs

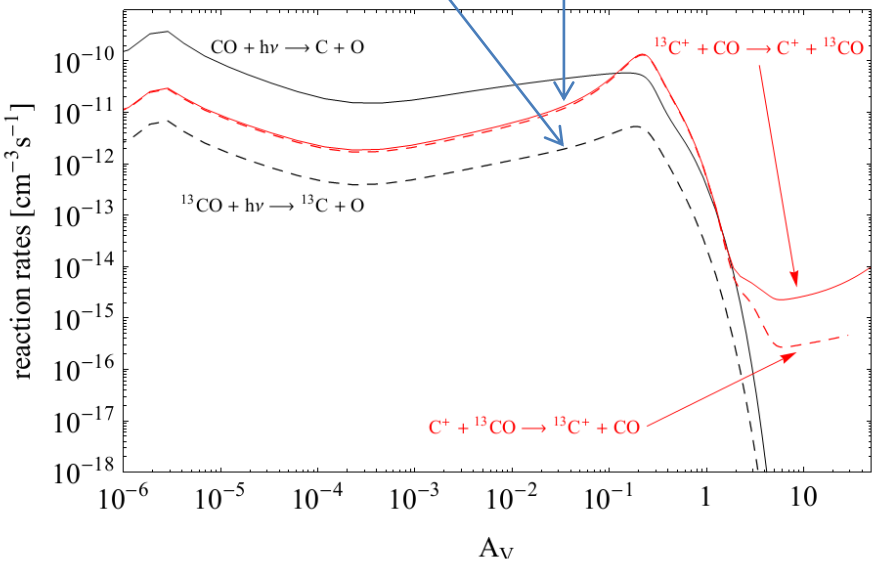




Standard behavior of carbon isotopologues in PDRs:

^{13}CO recombines at lower A_V compared to ^{12}CO despite the weaker shielding capabilities of ^{13}CO.

^{13}CO photo-dissociation is always weaker than the chemical channels.



Röllig & Ossenkopf, 2012, submitted to A&A

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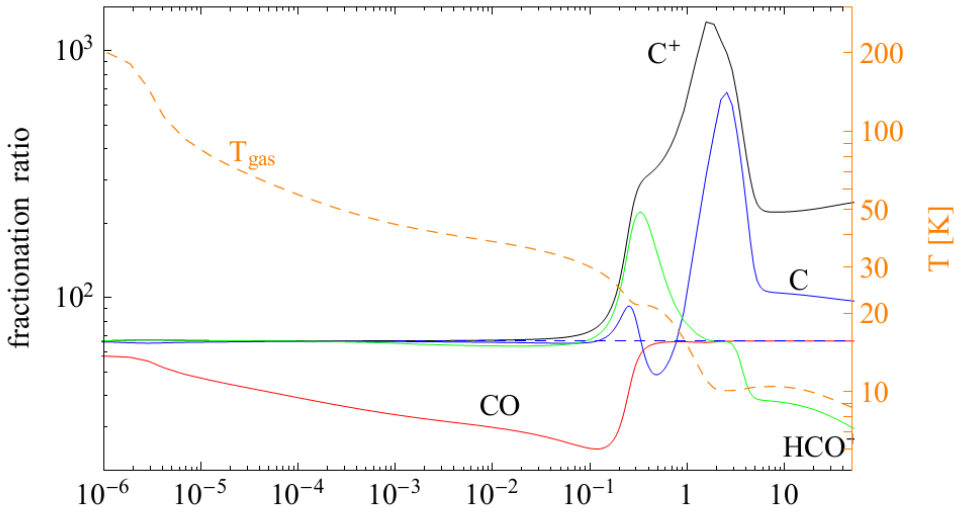
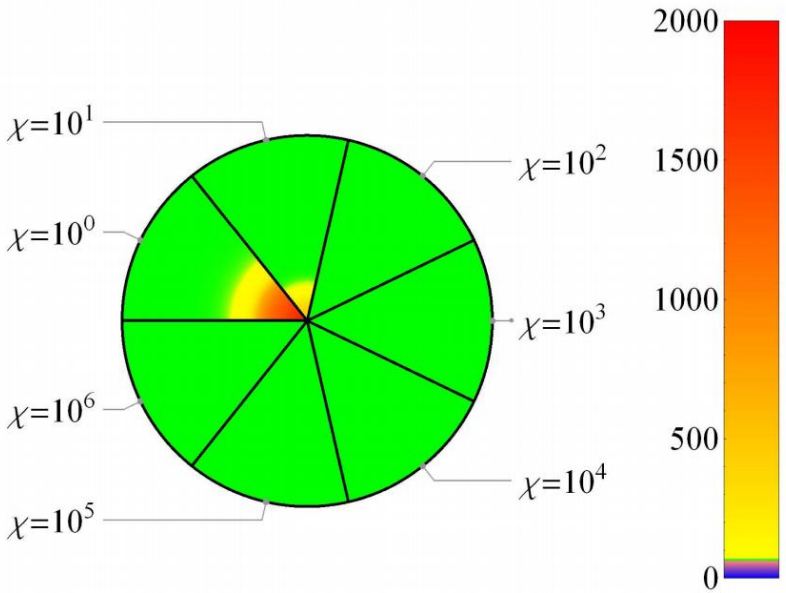


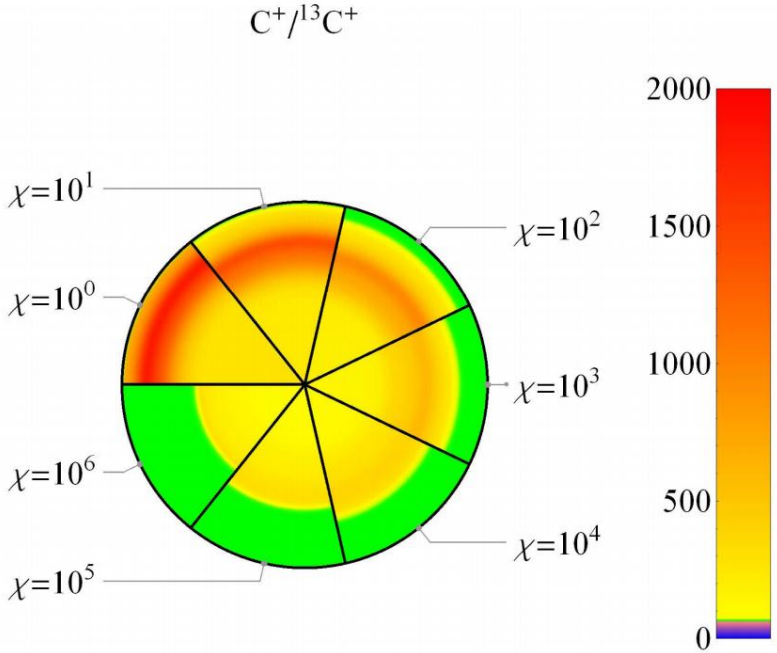
Standard behavior of carbon isotopologues in PDRs:

- C^+ fractionation ratio (FR) is always ≥ ER
- C^+ FR ≈ ER at low A_V
- C^+ FR increases significantly with A_V

C^+ fractionation needs cool, shielded C^+ gas (weak column density effect)

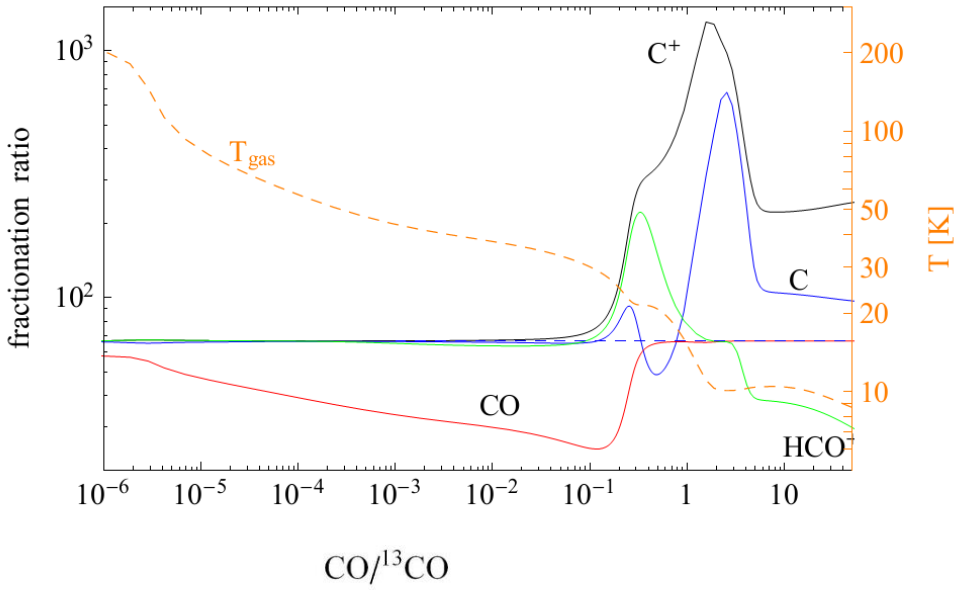


$n=10^3$ cm^{-3}, M=1 $M_\odot$



$n=10^5$ cm^{-3}, M=1 $M_\odot$

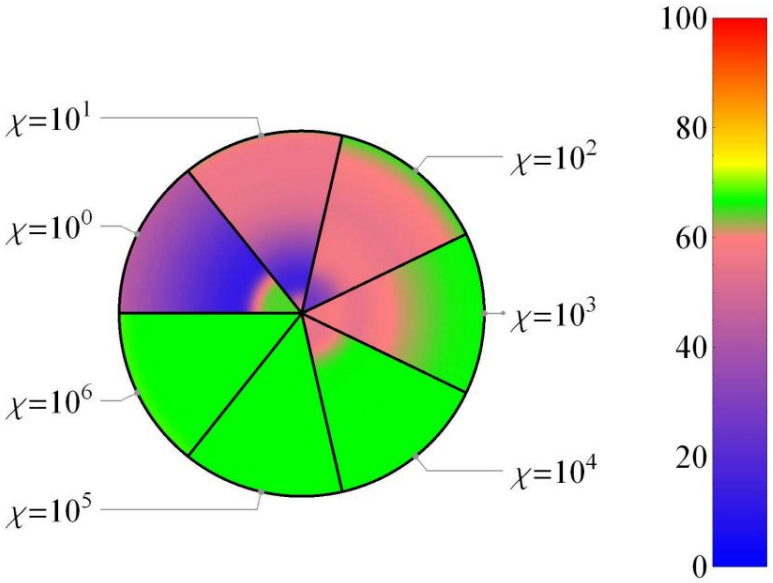
Carbon Chemistry – Fractionation in PDRs



Standard behavior of carbon isotopologues in PDRs:

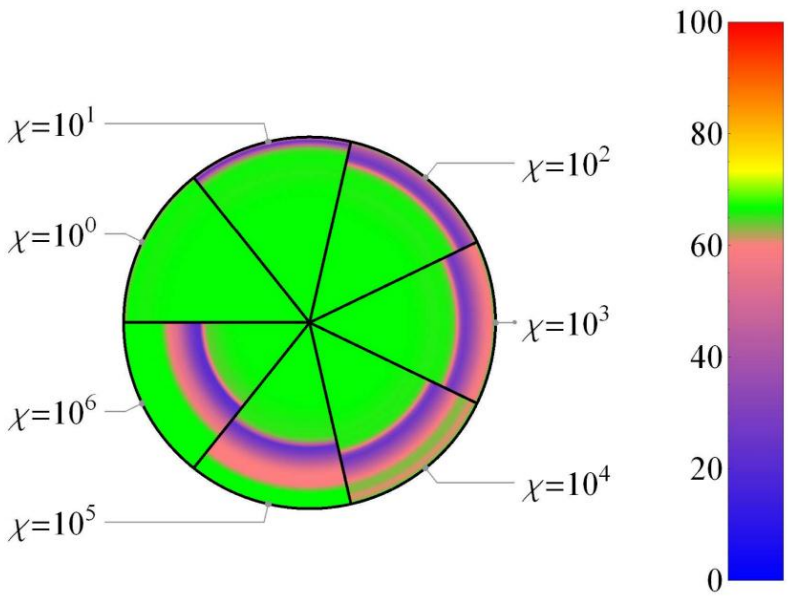
- CO fractionation ratio (FR) is always ≤ ER
- CO FR ≈ ER at high A_V
- CO FR < ER at $A_V << 1$

CO fractionation needs hot, unshielded CO gas (weak column density effect)



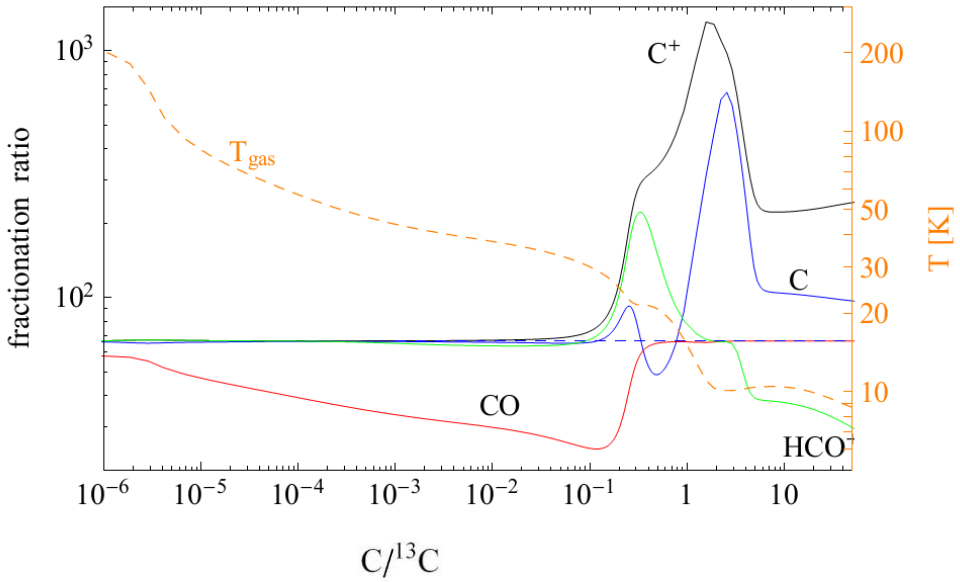
$n=10^3$ cm^{-3}, M=1 $M_\odot$

$CO/^{13}CO$



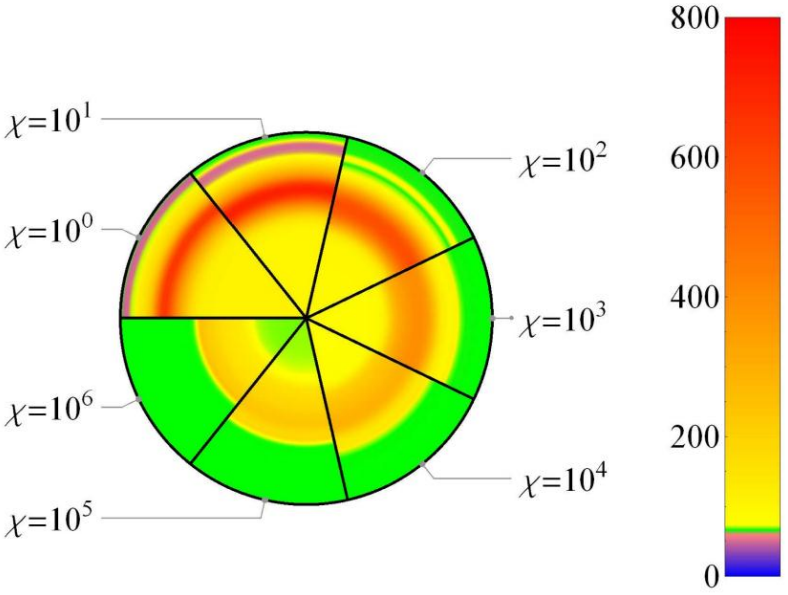
$n=10^5$ cm^{-3}, M=1 $M_\odot$

Carbon Chemistry – Fractionation in PDRs



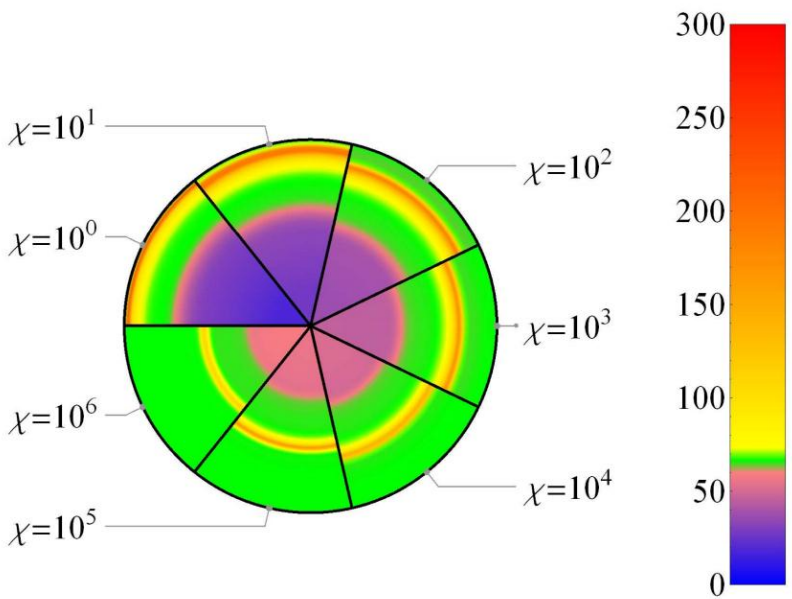
Standard behavior of carbon isotopologues in PDRs:

- C and HCO^+ show mixed behavior



$n=10^3$ cm^{-3}, M=1 $M_\odot$

$HCO^+/H^{13}CO^+$



$n=10^5$ cm^{-3}, M=1 $M_\odot$

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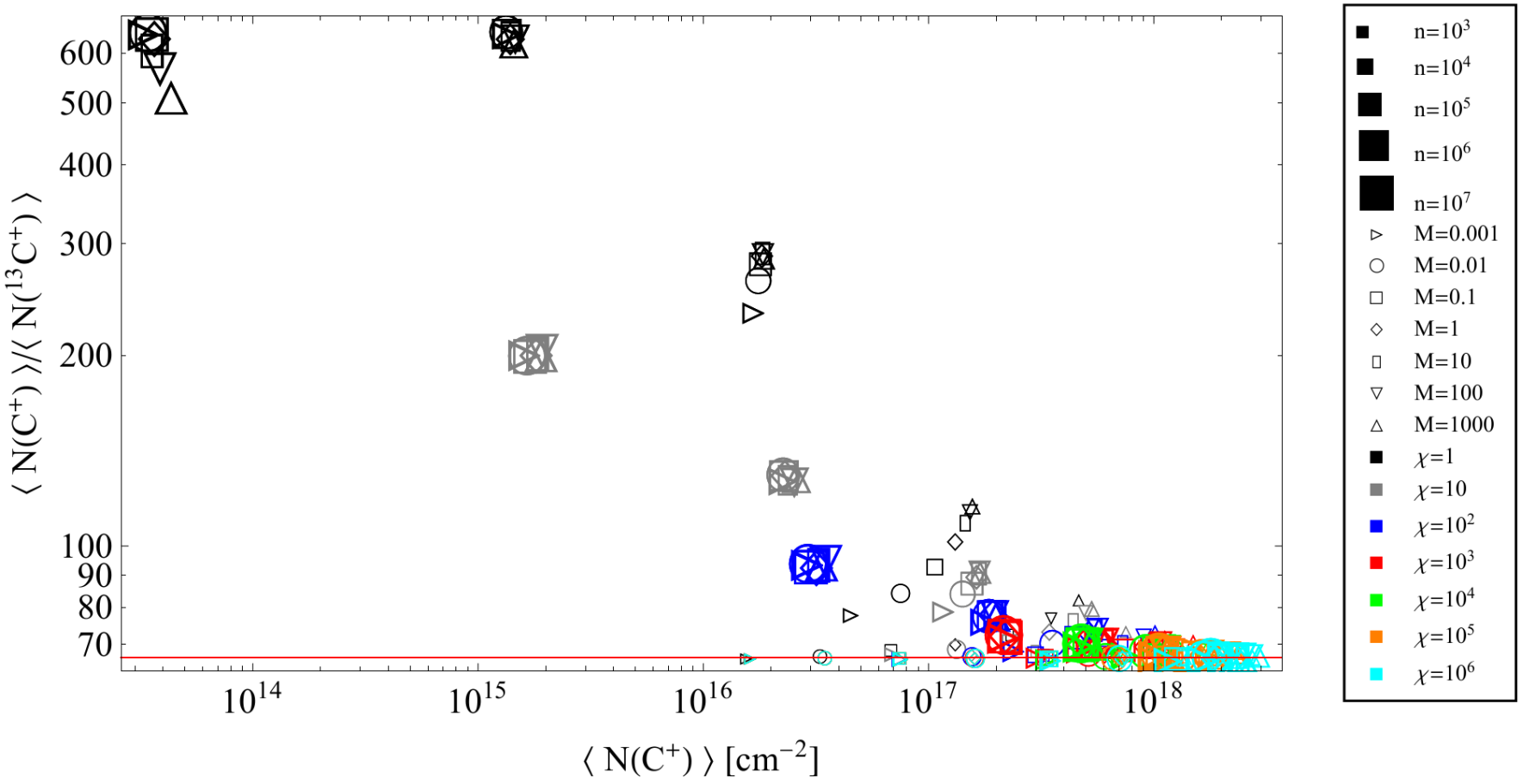
Standard behavior of carbon isotopologues in PDRs:

Column density ratio

C^+ fractionation needs cool, shielded C^+ gas (weak column density effect)



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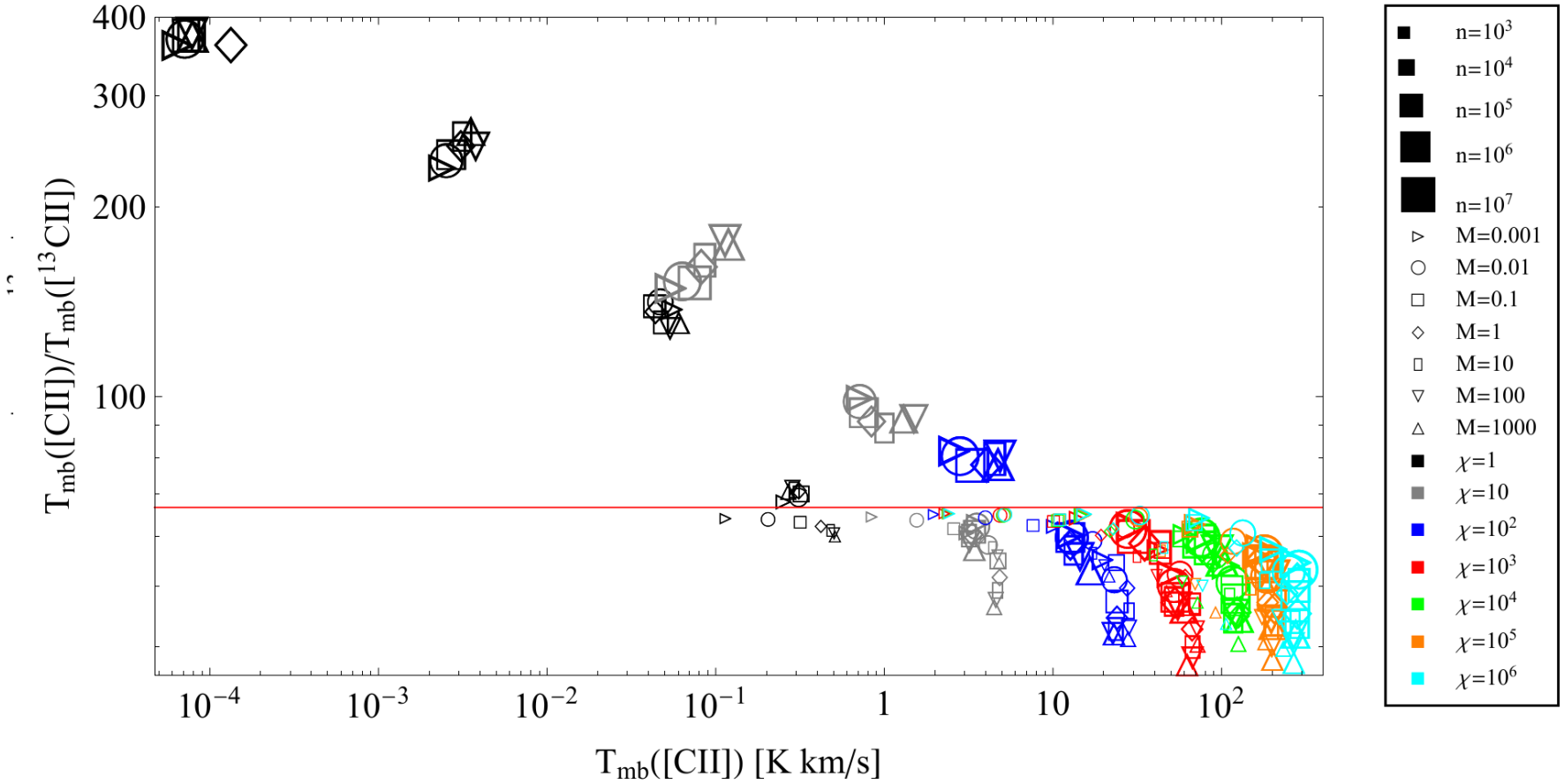
Standard behavior of carbon isotopologues in PDRs:

C^+ is also subject to optical depth effects

Intensity ratio

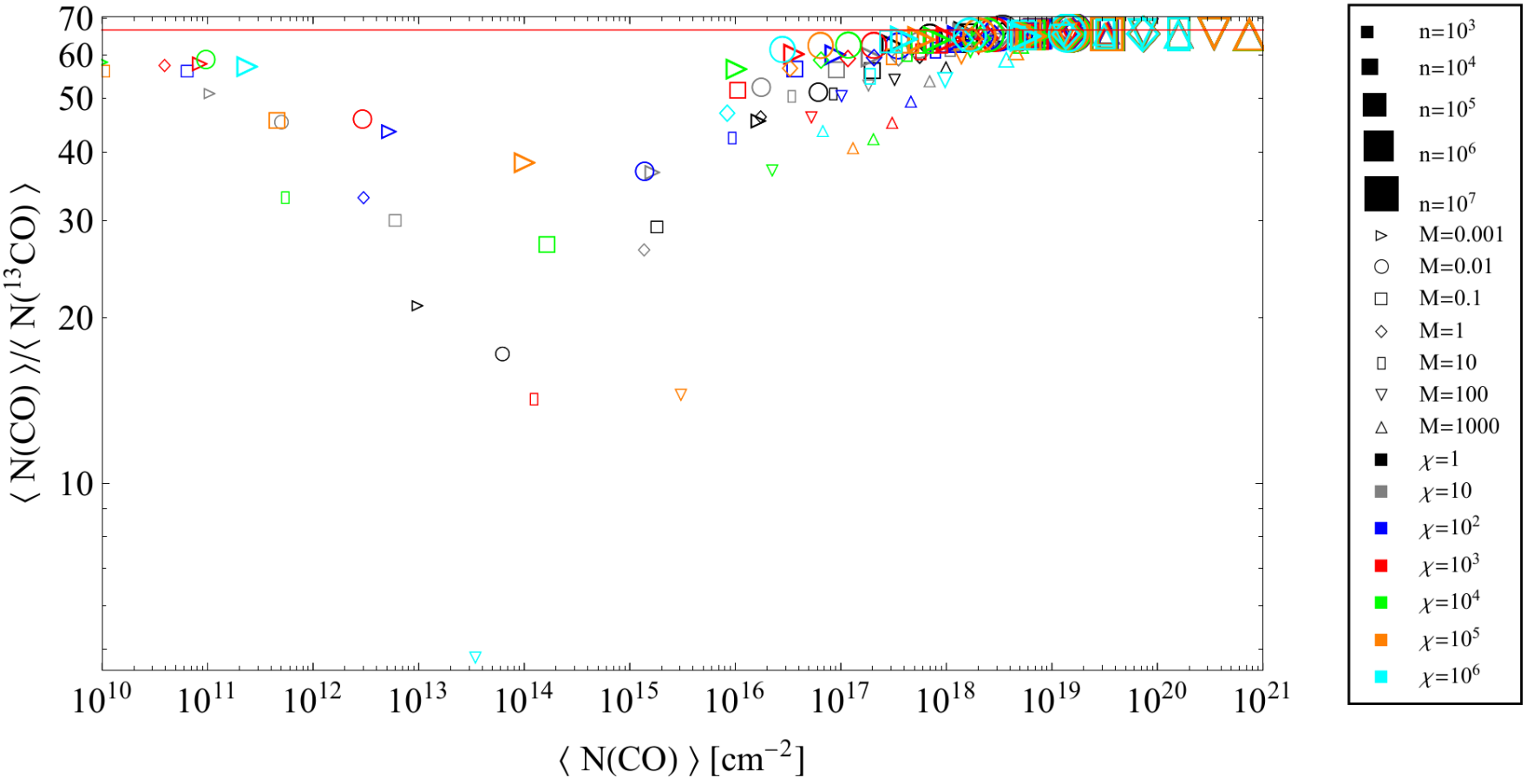


Carbon Chemistry – Fractionation in PDRs

Standard behavior of carbon isotopologues in PDRs:

Column density ratio

CO fractionation needs hot, unshielded CO gas (weak column density effect)



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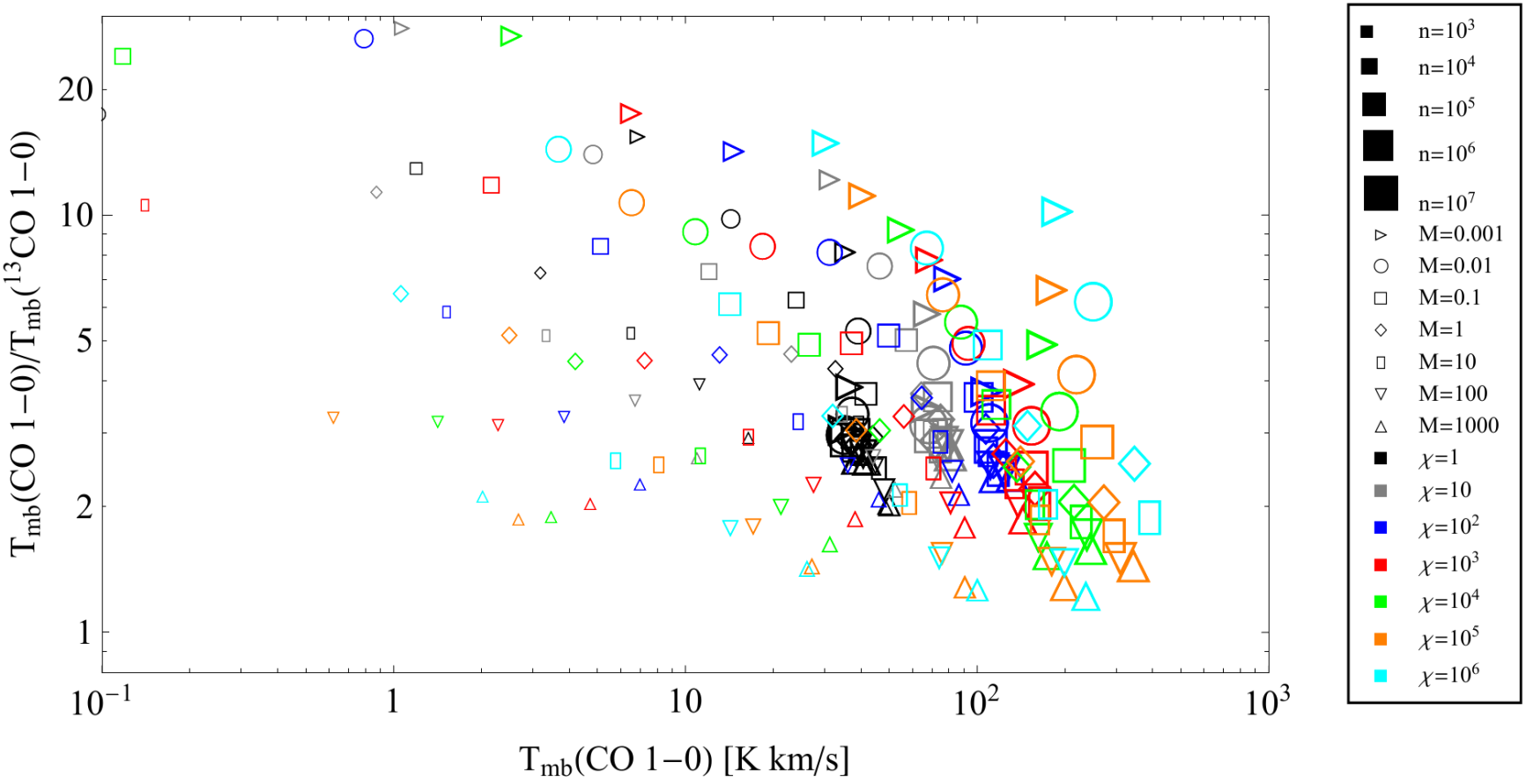
Standard behavior of carbon isotopologues in PDRs:

CO lines are optically thick

Intensity ratio



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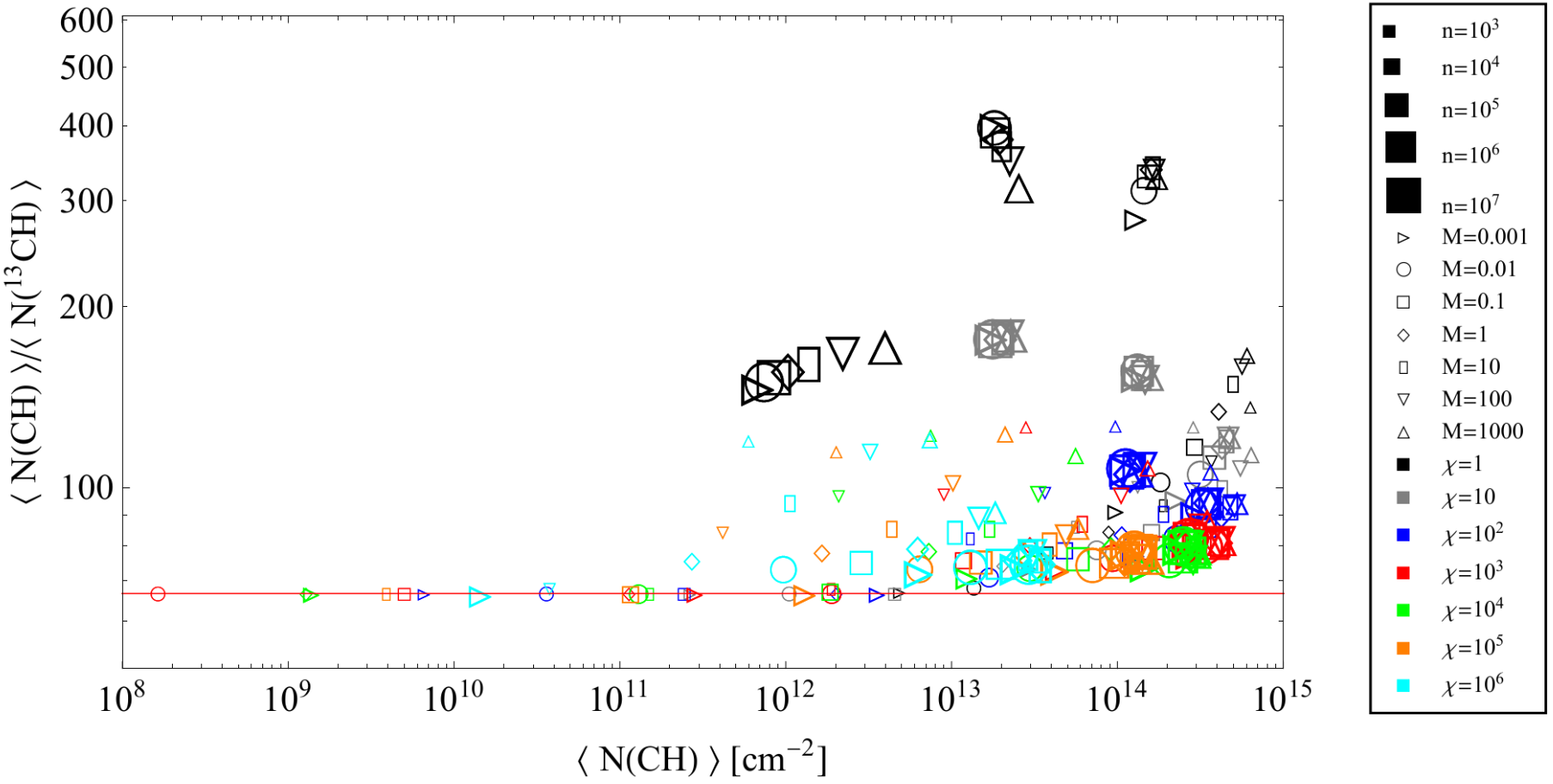
Standard behavior of carbon isotopologues in PDRs:

CH appears to be strongly fractionated across a larger parameter range



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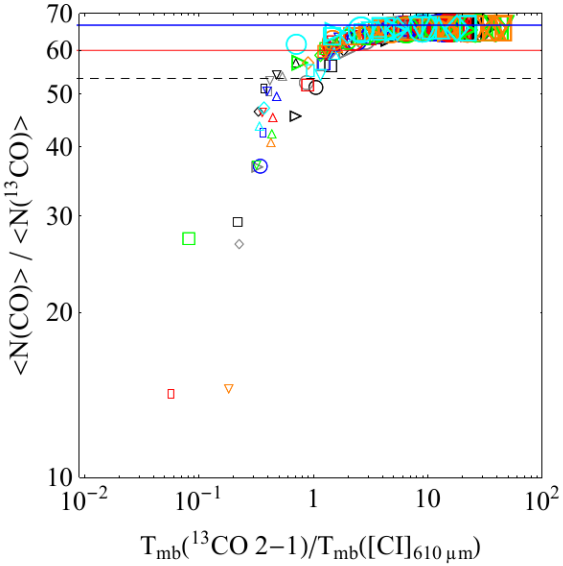
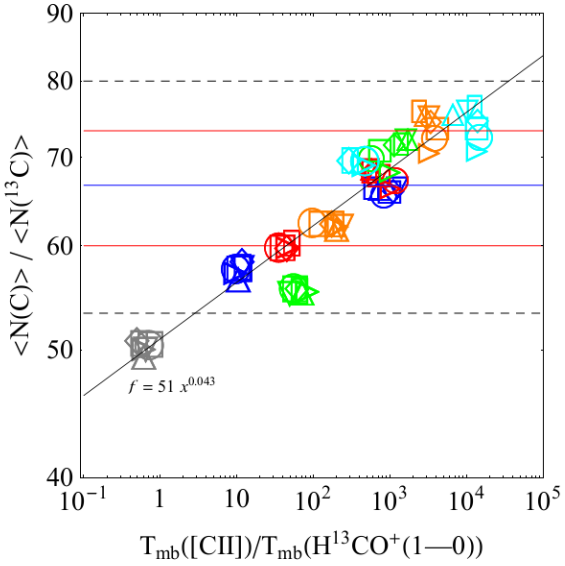
Diagnostic line ratios to detect column density fractionation of C^+, C, and CO.

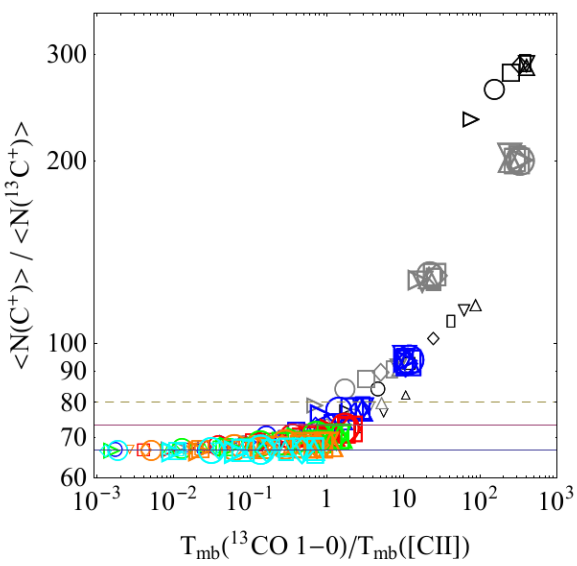
CO



C



C^+



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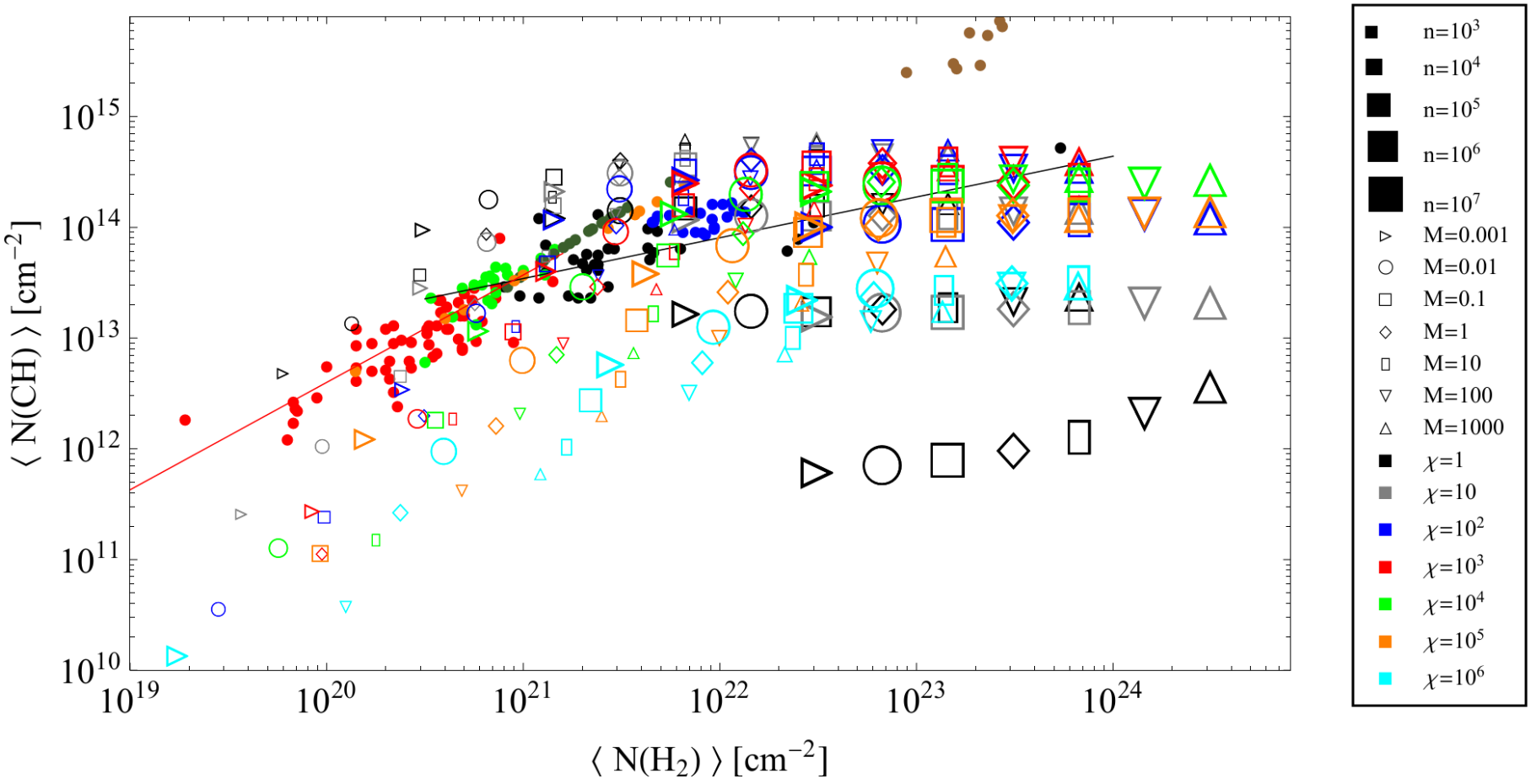
Many problems unresolved yet.

CH column densities are still difficult to reproduce in the models

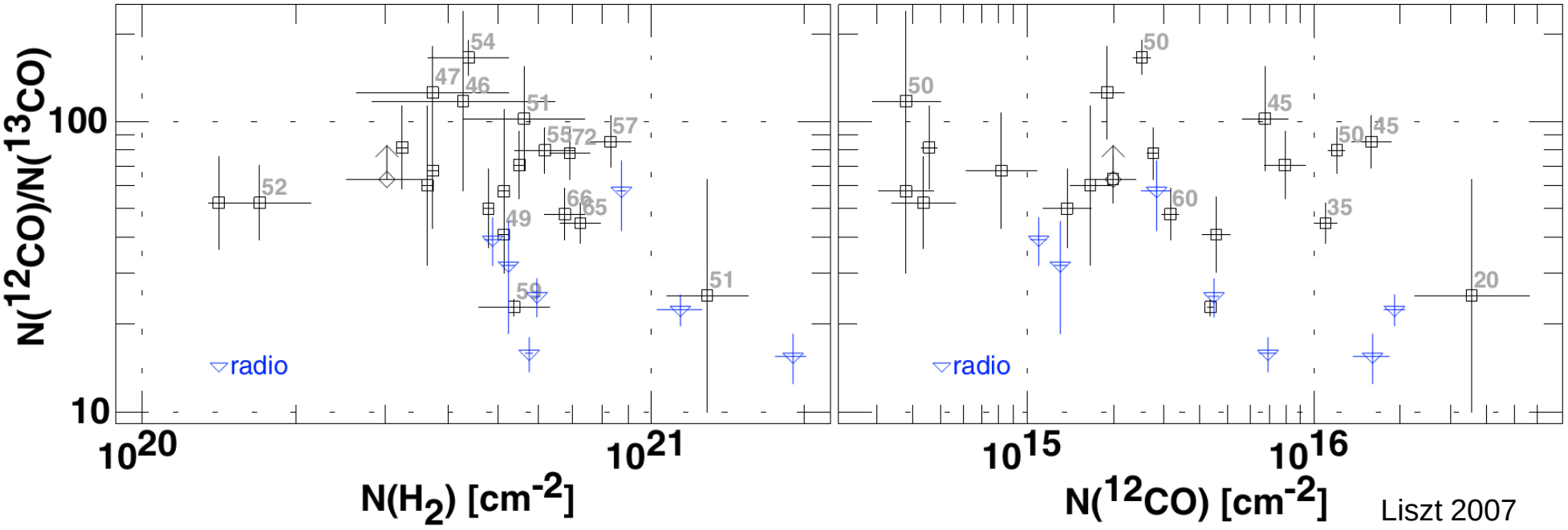


Carbon Chemistry – Fractionation in PDRs

Many problems unresolved yet.

CO fractionation is observed in both directions (in the diffuse gas)

still unreproducable in PDR codes



Liszt 2007

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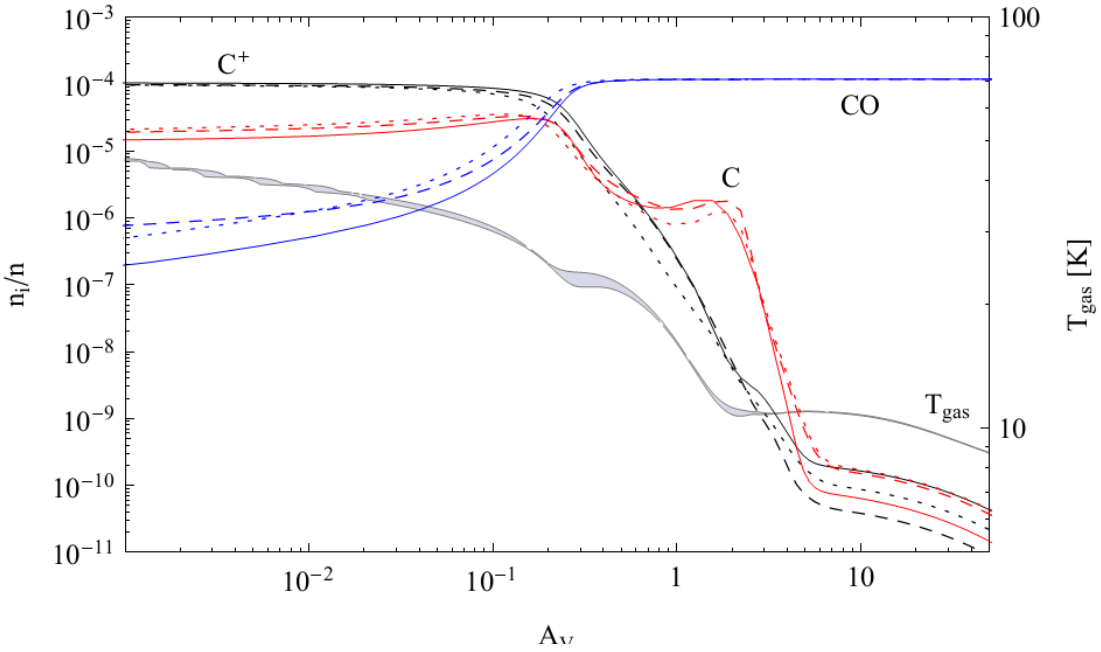

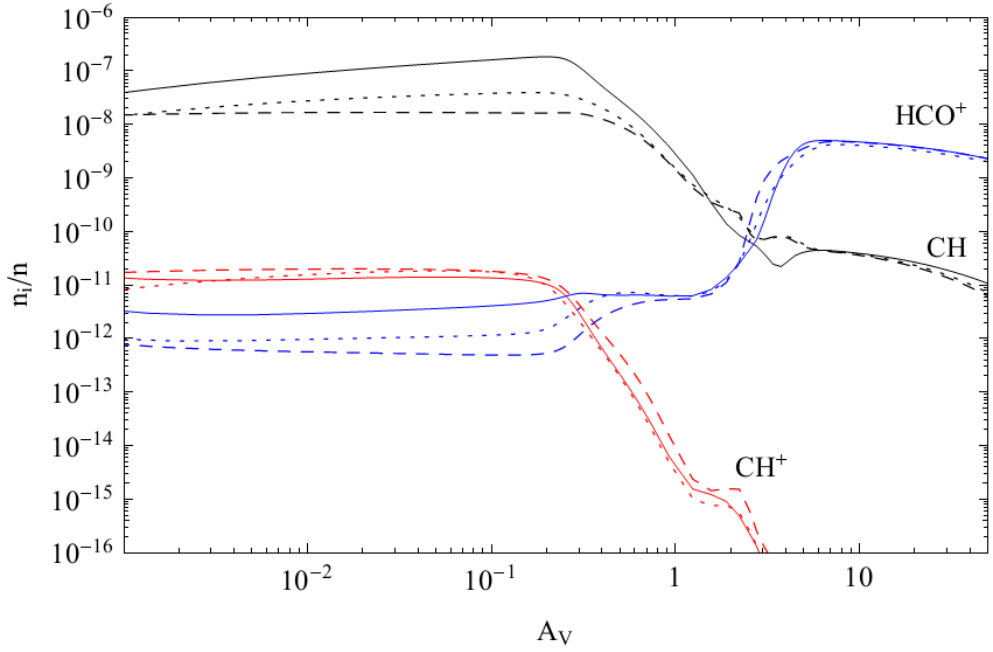

Loose ends:

Influence of different chemical databases
(UDfA, OSU, KIDA)

- In the models, CO is always fractionated with FR≤ER
- Observations also show show FR=ER, which can not be reproduced in PDR models
- CH is expected to be fractionated under most conditions (no collision rates, no observations,…)