The effects of the initial gas conditions on the properties of the dense gas in GMCs

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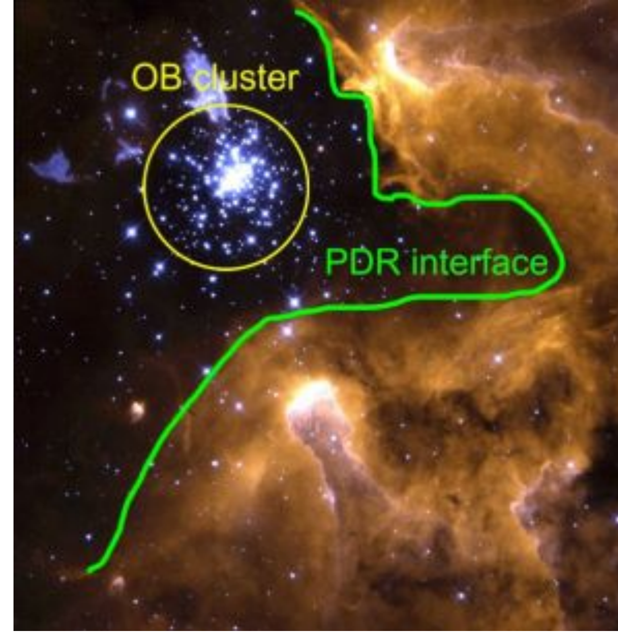
Key question(s)

- How do the initial physical and chemical conditions affect the chemistry of the gas that is/will be forming stars?
- How important *for the chemistry* is the mode of collapse of dense gas?

Many papers investigating the transition from atomic to molecular hydrogen (H→H_2) and from ionized to atomic to molecular carbon (C+ →C→CO) [Glover & McLow (2011); Offner et al. (2013);, Bisbas et al. (2015) ; Bialy & Sternberg 2016 etc – see Bolatto et al. 2013 review].

→ These transitions occurs at very low Avs (depending on several parameters (e.g. Bell et al. 2006)

→ **let's look deeper into the gas at higher Av (>3 mags).**



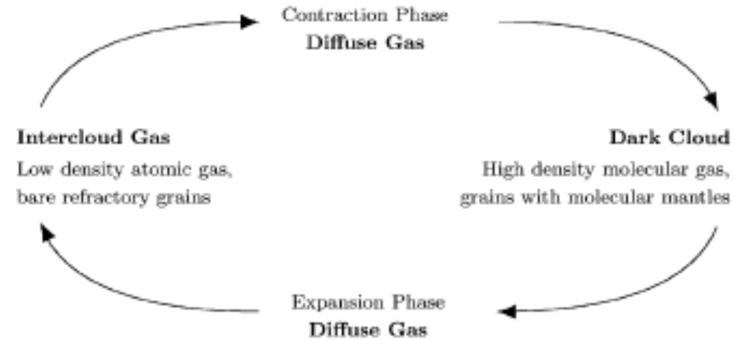
Credit: Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington), You-Hua Chu (Univ. Illinois Urbana-Champaign), and NASA

Some of the influencing factors:

- The H/H_2
- Initial elemental abundances
- "Dynamics"
- Time
- Flux(es)

Caveat: these are **not** independent parameters → we shall however look at them individually first but see later.

1. “Dynamics” (e.g. Price et al. 2003)



Contraction Phase

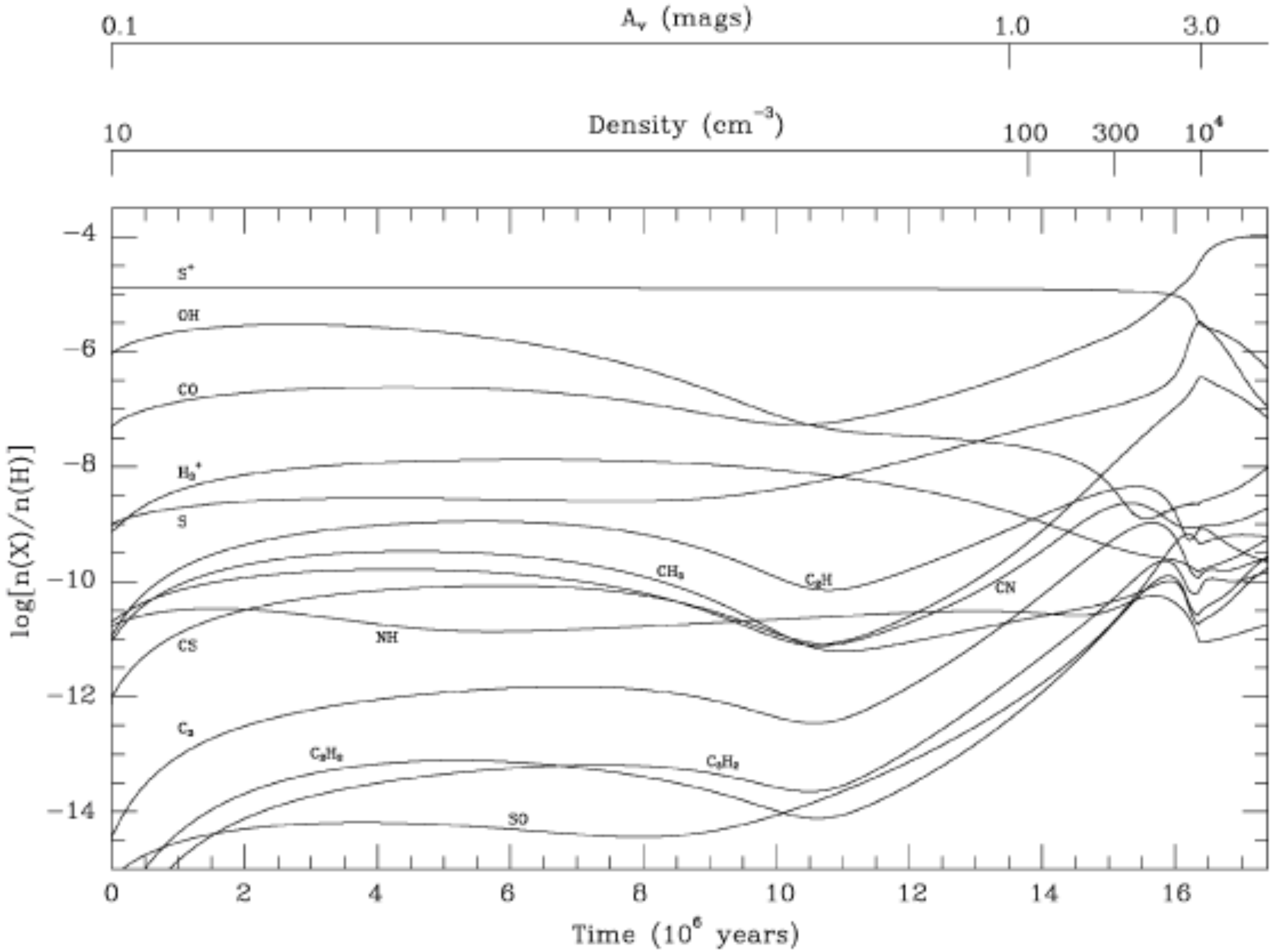
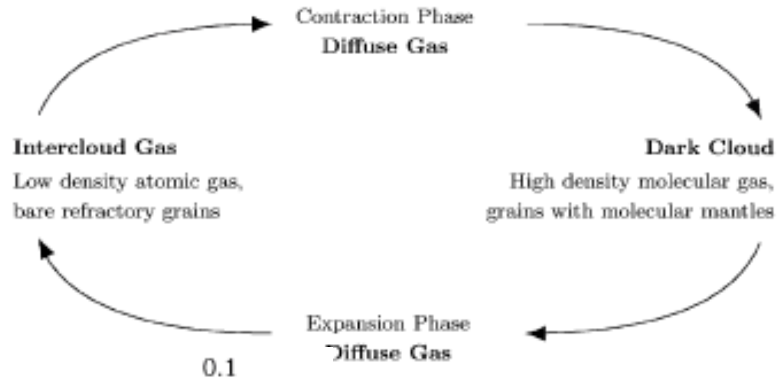


Figure 2. The fractional abundance of a selection of species relative to hydrogen over time, during the collapse phase.

1. “Dynamics” (e.g. Price et al. 2003)

Expansion Phase



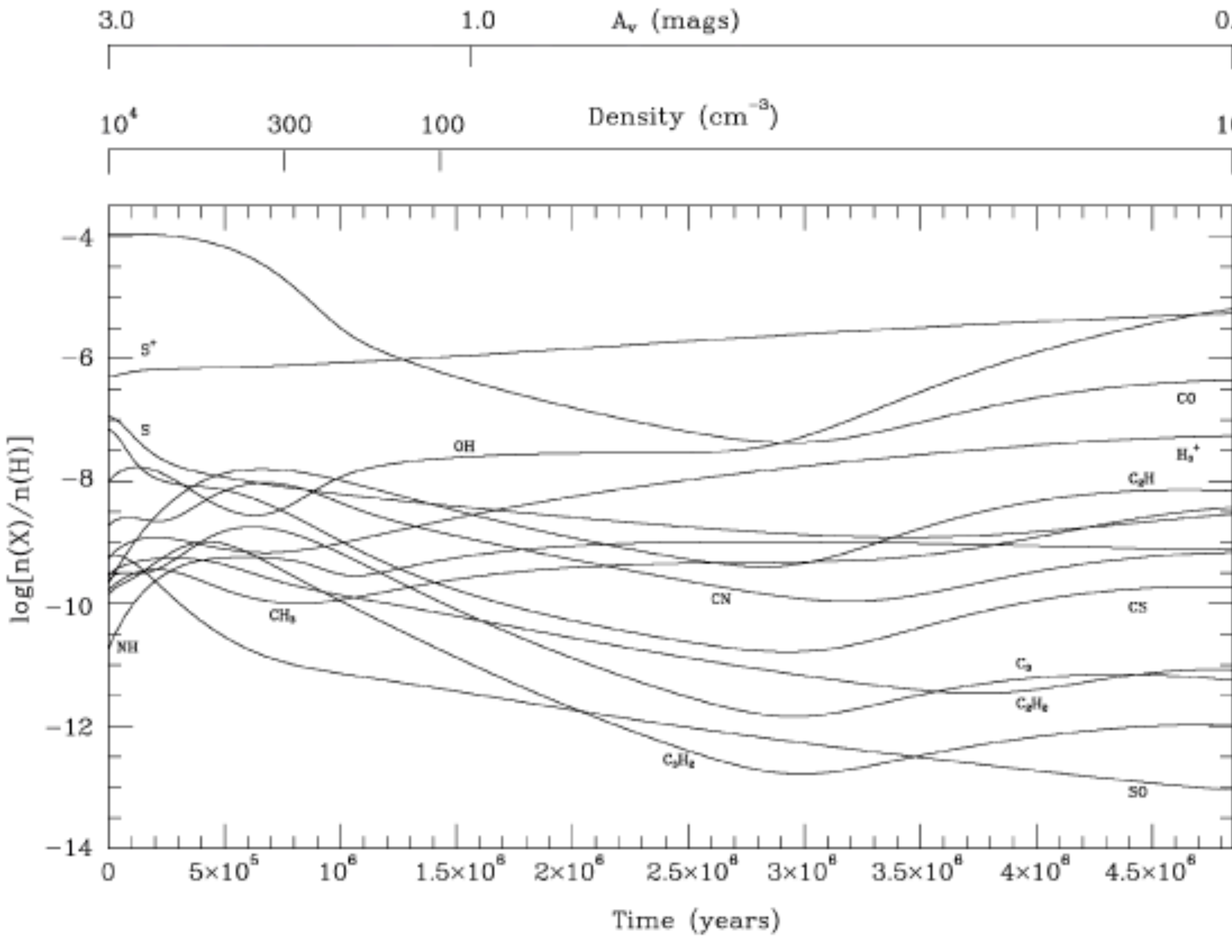


Figure 3. The fractional abundance of a selection of species relative to hydrogen over time, during the expansion phase.

Are there observational evidence of either 'direction' in the diffuse clouds?

Table 2. Column densities of species at a spatial density of 100 cm^{-3}. Observed column densities for ζ Per have been taken from the literature, where available. Observed column densities enclosed in brackets represent observations made in other lines of sight; some are discussed in the text. The notation a(b) represents a × 10^b.

Species	Observed	Collapse	Expansion
H_2	3.2(20)–7.1(20)[a]	8.2(+20)	8.5(+20)
S	1.8(13)[b]	8.1(+13)	7.1(+12)
O	–	7.4(+17)	5.3(+17)
C	–	1.7(+16)	8.2(+15)
S^+	1.6(16)[c]	2.1(+16)	1.8(+15)
CS	[0.5(12)–2(12)][d]	8.2(+11)	3.5(+11)
SO	[1.0(12)–1.0(13)][d]	2.0(+09)	7.0(+09)
CO	6.1(14)[b]	8.7(+14)	1.0(+15)
C_2H	[7.0(12)][e]	1.9(+12)	6.7(+12)
C_3H_2	[4.8(12)][e]	5.5(+09)	3.1(+10)
NH	1.0(12)[f]	5.0(+10)	8.6(+11)
CN	3.0(12)[g]	4.0(+11)	2.5(+12)
OH	4.0(13)[g]	3.6(+13)	4.0(+13)
H^+_3	8.0(14)[h]	2.2(+12)	3.8(+12)
C_3	–	6.4(+10)	1.8(+11)
HCO^+	–	1.5(+11)	2.2(+11)
HCN	–	3.7(+09)	6.0(+10)

[a]Savage et al. (1977), [b]Snow (1977), [c]Snow, Lamers & Joseph (1987), [d]Lucas & Liszt (2002), [e]Lucas & Liszt (2000), [f]Meyer & Roth (1991), [g]Felenbok & Roueff (1996), [h]McCall et al. (2003).

Table 3. Column densities of species at a spatial density of 300 cm^{-3}. Observed column densities for ζ Oph have been taken from the literature, where available. Observed column densities enclosed in brackets represent observations made in other lines of sight; some are discussed in the text. The notation a(b) represents a × 10^b.

Species	Observed	Collapse	Expansion
H_2	4.6(20)[a]	1.2(+21)	1.2(+21)
S	8.5(13)[b]	2.7(+14)	2.0(+13)
S^+	1.2(16)[b]	2.9(+16)	1.9(+15)
O	5.0(17)[c]	1.0(+18)	7.0(+17)
C	2.2(17)[c]	1.9(+17)	9.4(+16)
SO	[1.0(12)–1.0(13)][e]	4.7(+10)	2.7(+10)
CO	2.2(15)[a]	4.8(+15)	4.9(+16)
C_2H	[7.0(12)][f]	9.8(+12)	3.7(+13)
C_3H_2	[4.8(12)][f]	1.2(+11)	8.3(+11)
NH	8.8(11)[g]	8.0(+10)	1.3(+12)
CN	2.5(12)[a]	5.0(+12)	2.2(+13)
OH	4.6(13)[a]	1.0(+13)	8.9(+12)
H^+_3	[3.8(14)][h]	9.8(+11)	1.7(+12)
C_3	1.6(12)[i]	1.3(+12)	3.7(+12)
HCO^+	9.1(11)[a]	2.2(+10)	4.0(+10)
HCN	3.6(11))[a]	1.2(+10)	1.5(+11)
CH	2.5(13)[a]	9.1(+13)	2.4(+14)

[a]Liszt & Lucas (2001), [b]Morton (1975), [c]van Dishoeck (1998), [e]Lucas & Liszt (1997), [f]Lucas & Liszt (2000), [g]Crawford & Williams (1997), [h]McCall et al. (1999), [i]Maier et al. (2001).

2. "Dynamics"

1. Collapse from constant density (CD, Larson 1969), 2. the collapse of an unstable (BES1, Foster & Chevalier 1993) or 3. highly unstable (BES4, Ogino et al. 1999) Bonnor-Ebert sphere, 4. collapse against magnetic support (MS, Nakamura et al. 1995) and 5. collapse resulting from ambipolar diffusion (AD, Fiedler & Mouschiavas 1993). The evolution under free-fall collapse (FF) was also included as a comparison.

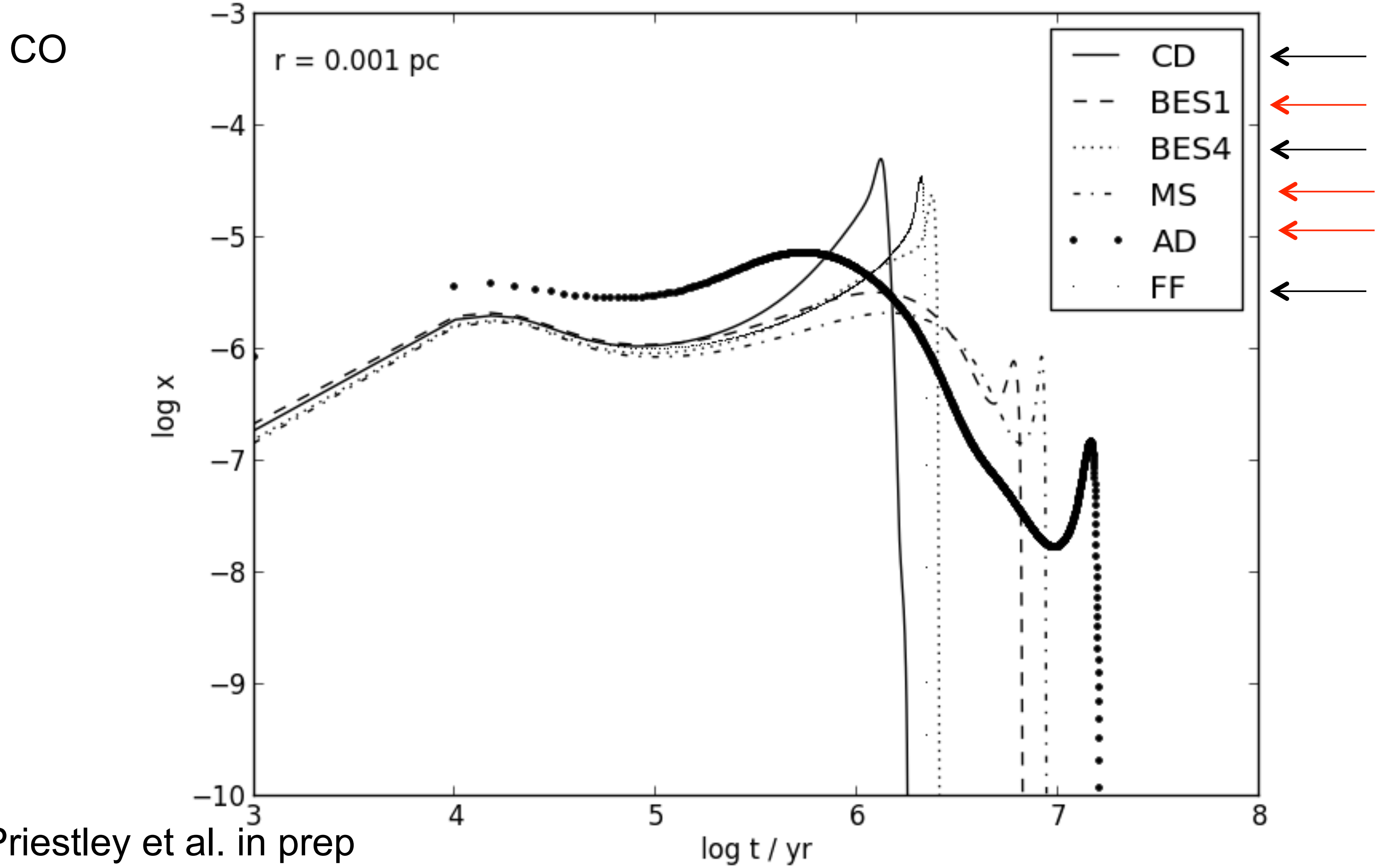
→ *Then for each 'dynamical' model one can run a grid…..*

Table 1. Values of parameters selected for the models.

Model	n_f/cm^{-3}	t_{eq}/yr	$\zeta/1.3\times10^{-17}\,\mathrm{s}^{-1}$	ε	ϕ	$Y_U V$
A	10^8	0	1	0.01	10^5	0.1
B1	10^7	0	1	0.01	10^5	0.1
B2	10^9	0	1	0.01	10^5	0.1
C1	10^8	10^4	1	0.01	10^5	0.1
C2	10^8	10^6	1	0.01	10^5	0.1
D1	10^8	0	5	0.01	10^5	0.1
D2	10^8	0	10	0.01	10^5	0.1
E1	10^8	0	1	0.01	10^5	0.1
E2	10^8	0	1	0.01	10^5	0.1
F1	10^8	0	1	0.1	10^5	0.1
F2	10^8	0	1	1.0	10^5	0.1
G1	10^8	0	1	0.01	10^4	0.1
G2	10^8	0	1	0.01	10^6	0.1
H1	10^8	0	1	0.01	10^5	0.001
H2	10^8	0	1	0.01	10^5	1.0

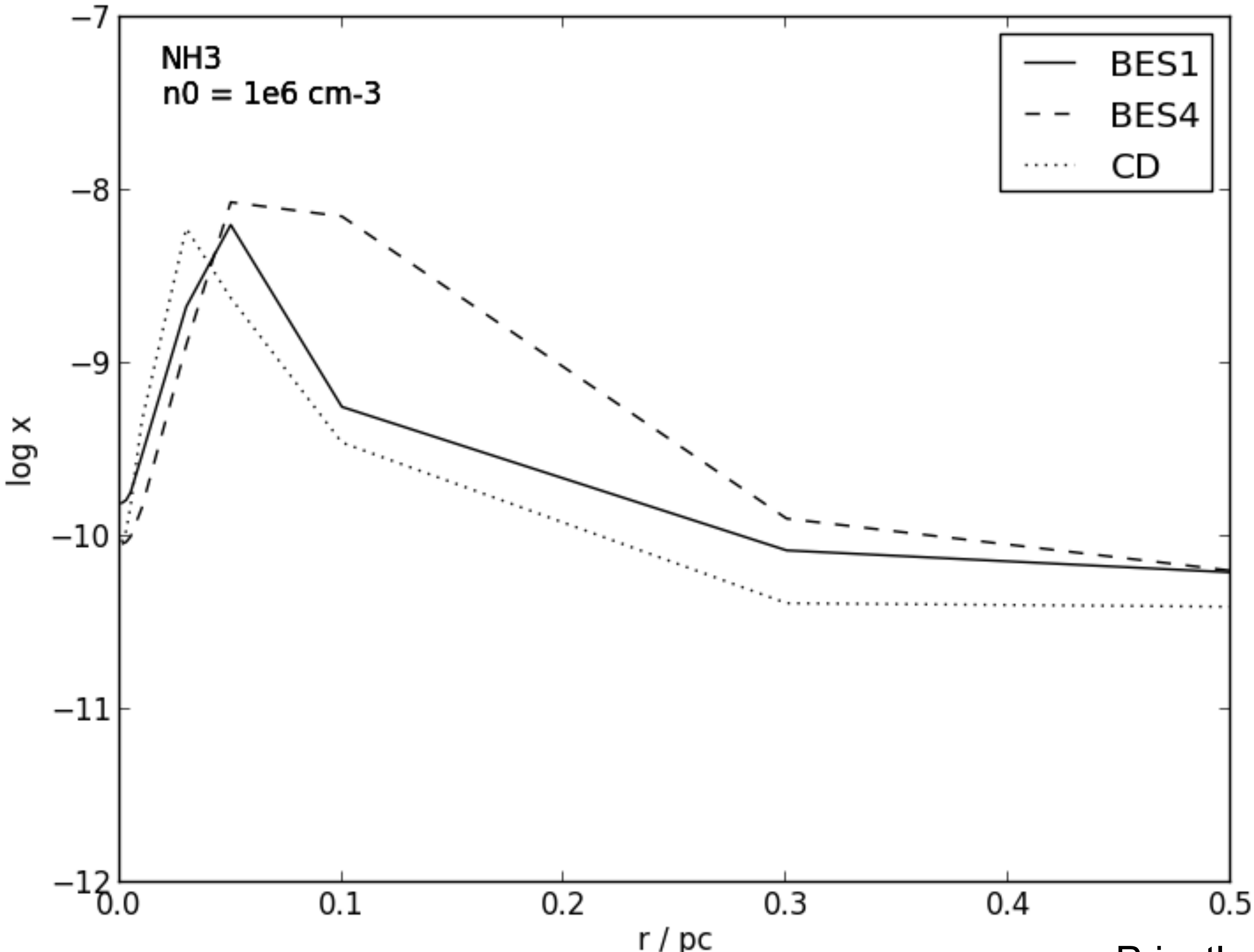
Priestley et al. in prep

1. Collapse from constant density (CD) 2. Collapse of an unstable (BES1) or 3. highly unstable (BES4) Bonnor-Ebert sphere, 4. collapse against magnetic support (MS) and 5. collapse resulting from ambipolar diffusion (AD) cf free-fall collapse (FF)



Priestley et al. in prep

Effects of ‘speed’ of collapse (BES1=collapse of an unstable BE; BES4=collapse of an highly unstable BE; CD=collapse form constant density)



Priestley et al. in prep

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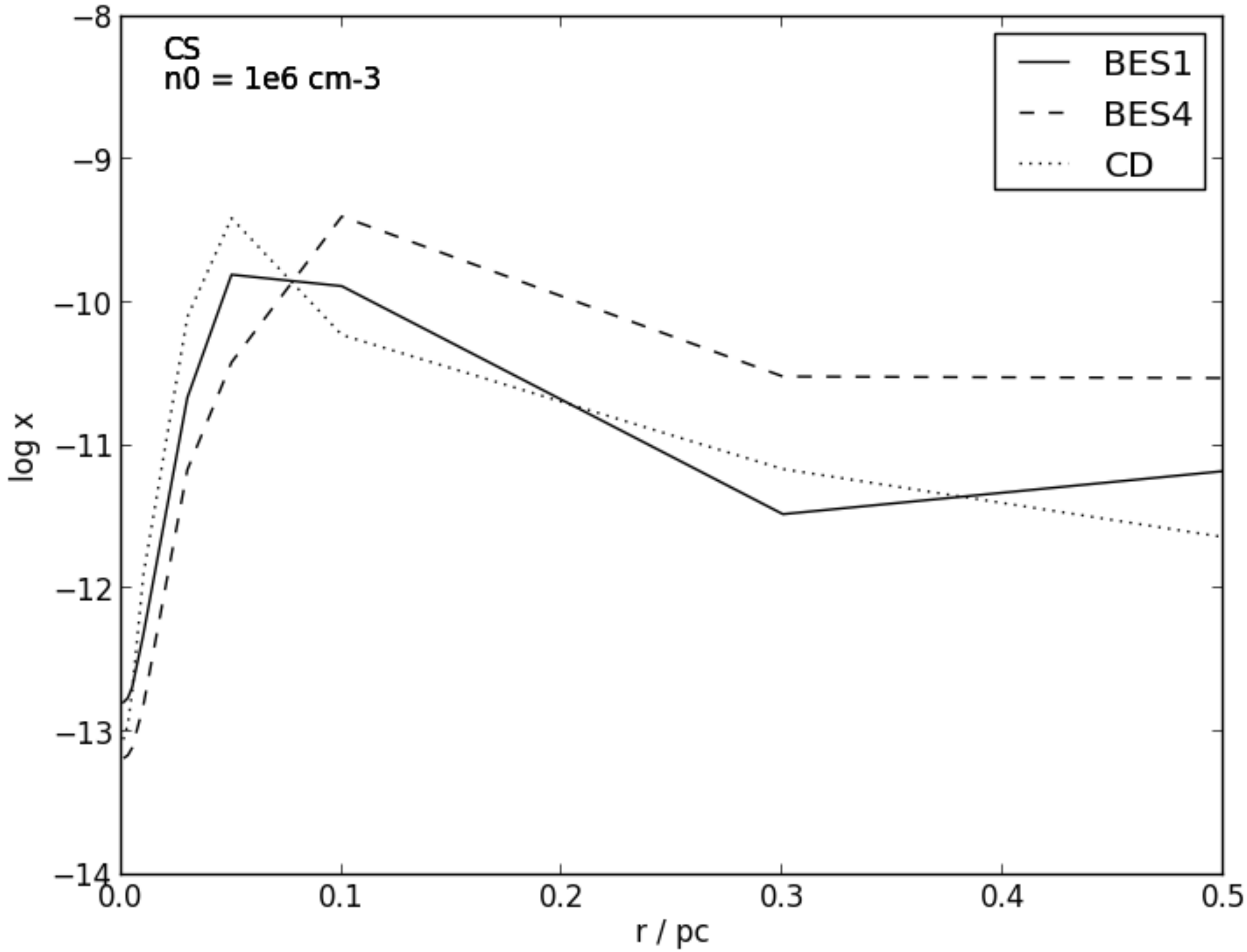

Priestley et al. in prep

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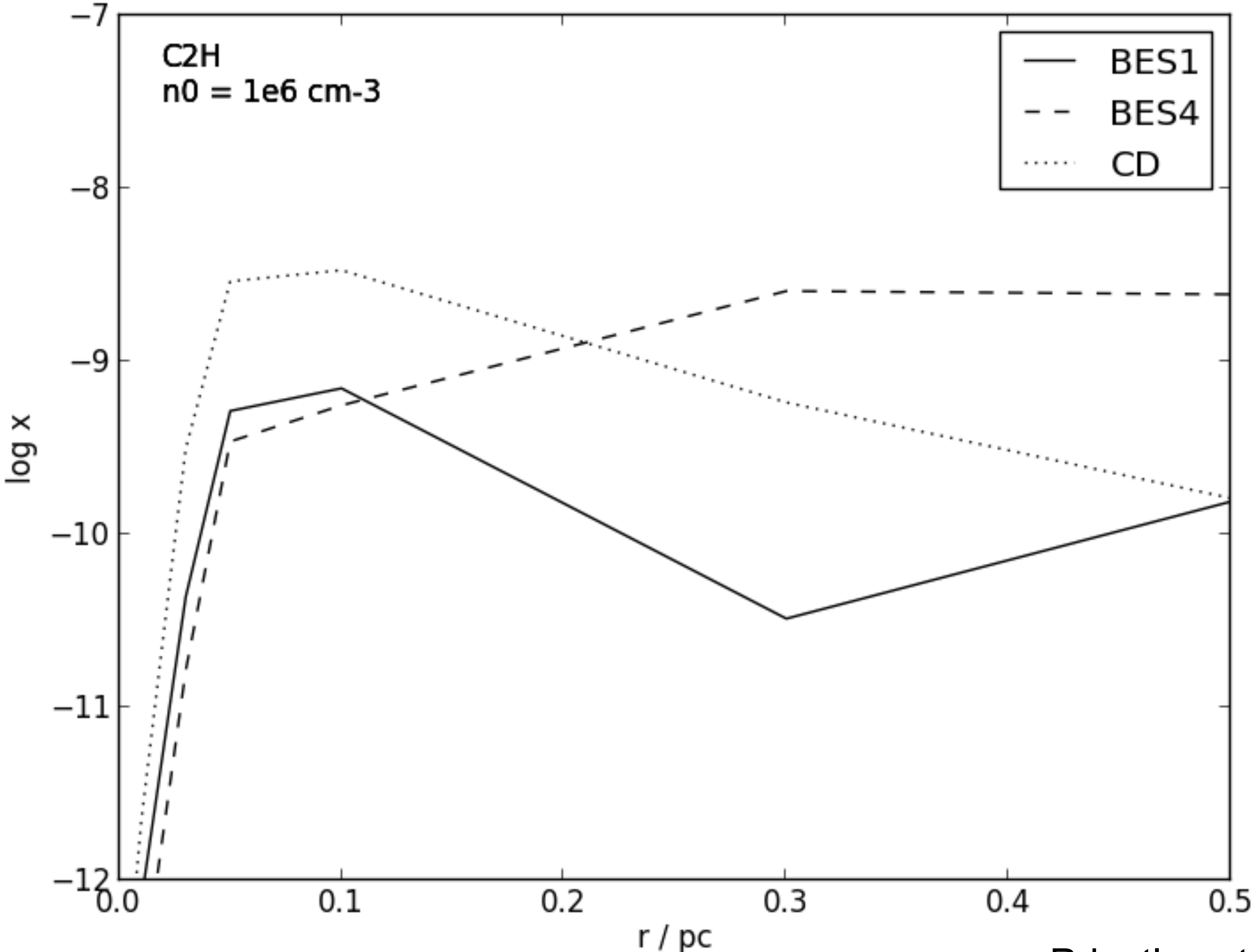

Priestley et al. in prep

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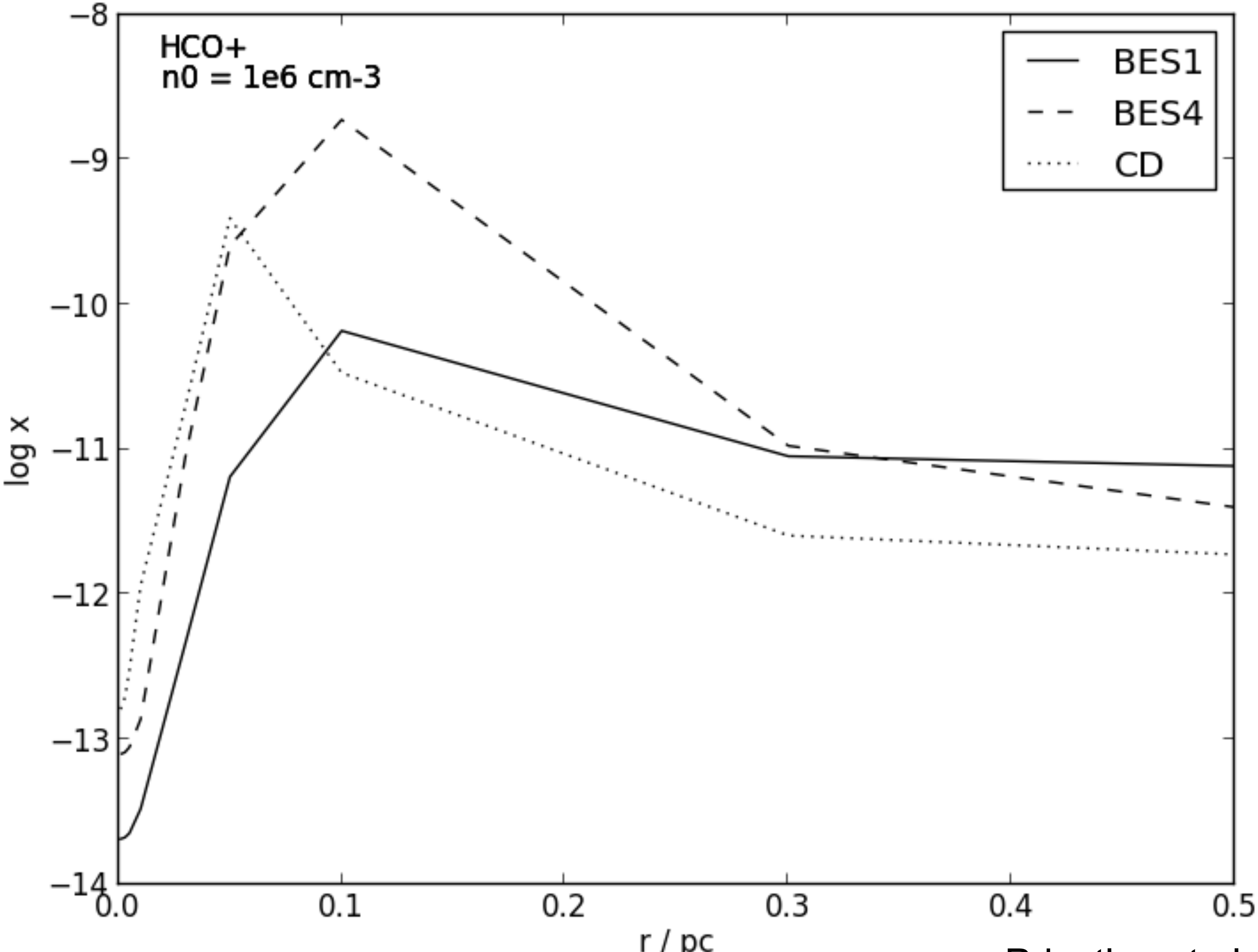

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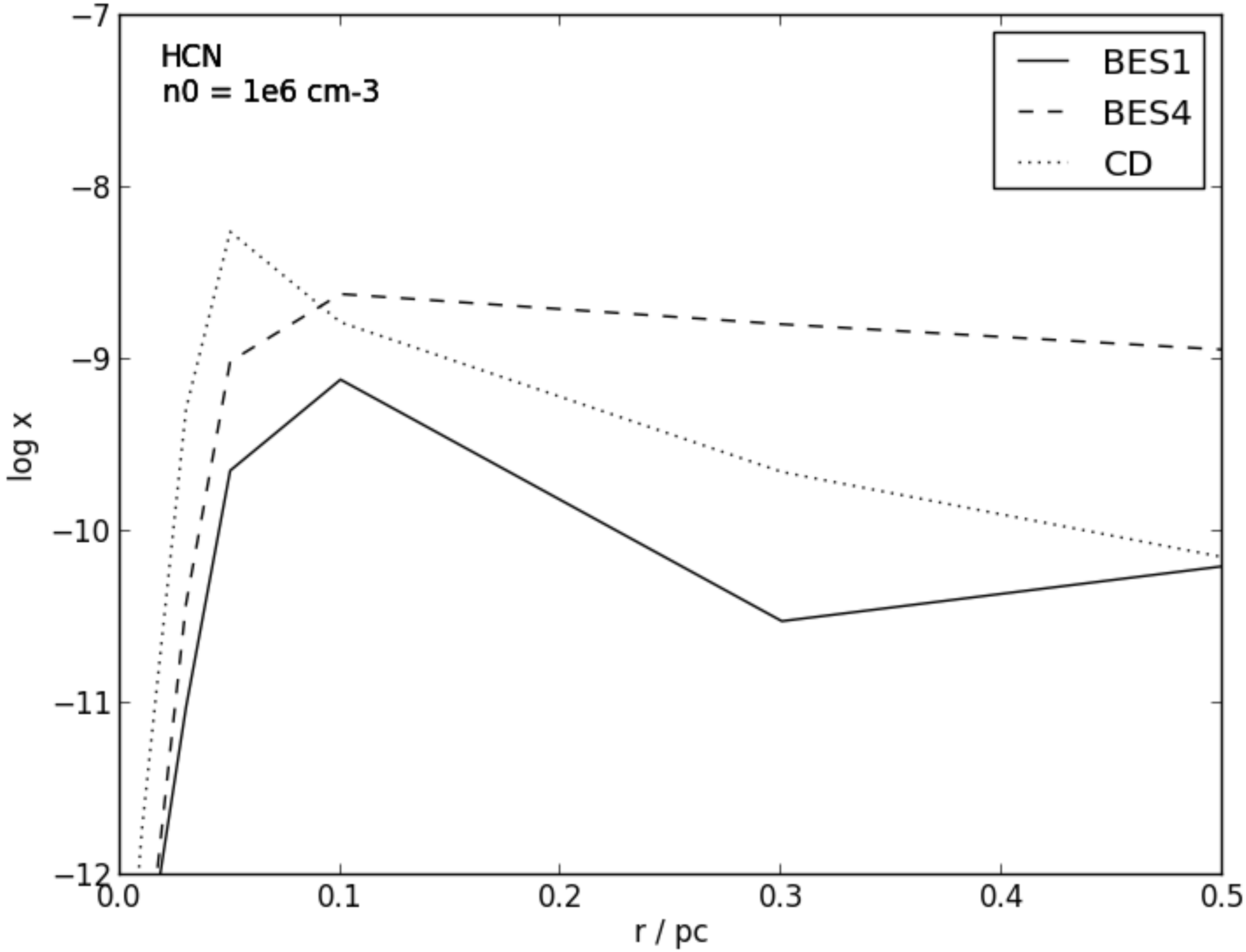
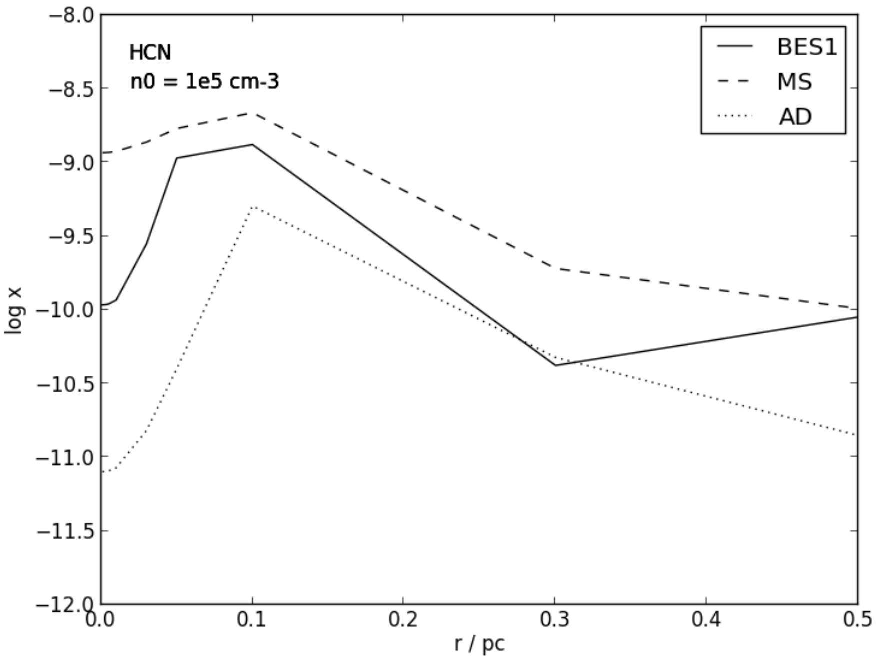
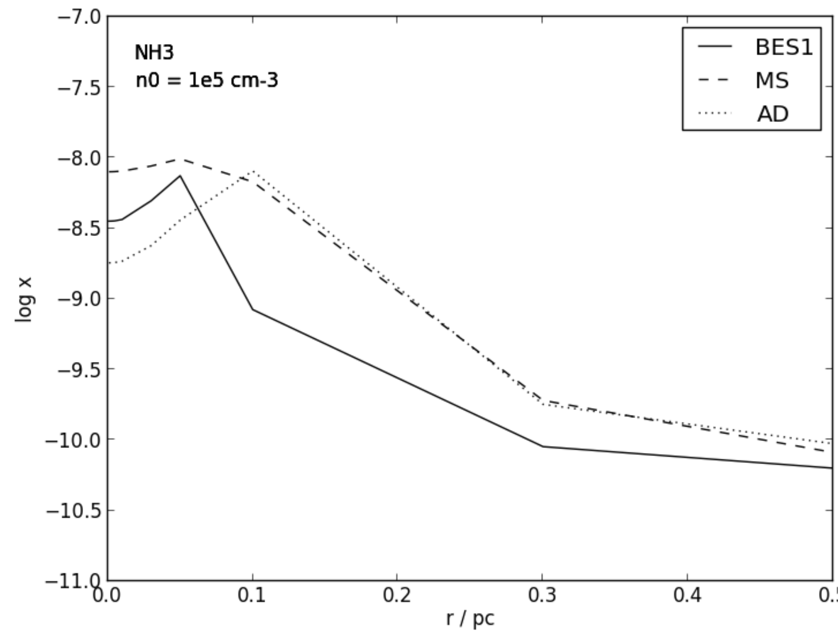
Effects of ‘speed’ of collapse (BES1=collapse of an unstable BE; BES4=collapse of an highly unstable BE; CD=collapse form constant density)

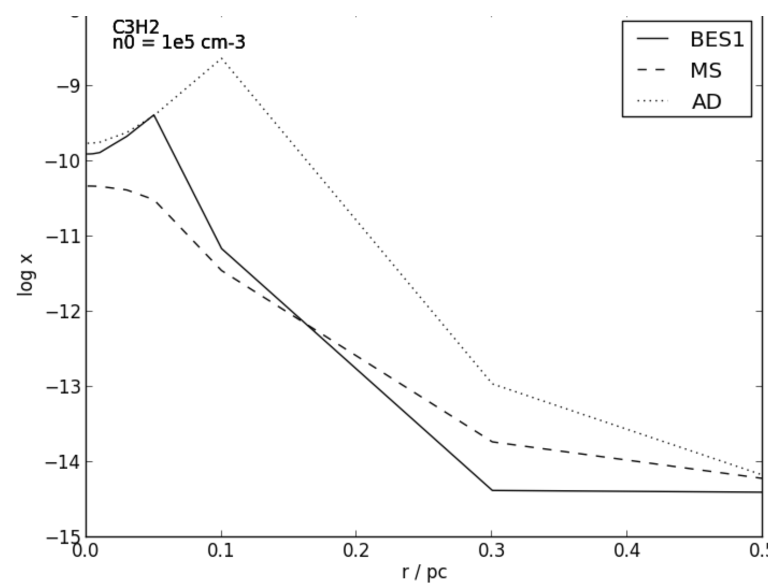


Priestley et al. in prep

The presence of magnetic fields: (BES1 = Collapse of an unstable BE; MS = collapse against magnetic support ; AD = collapse resulting from ambipolar diffusion)







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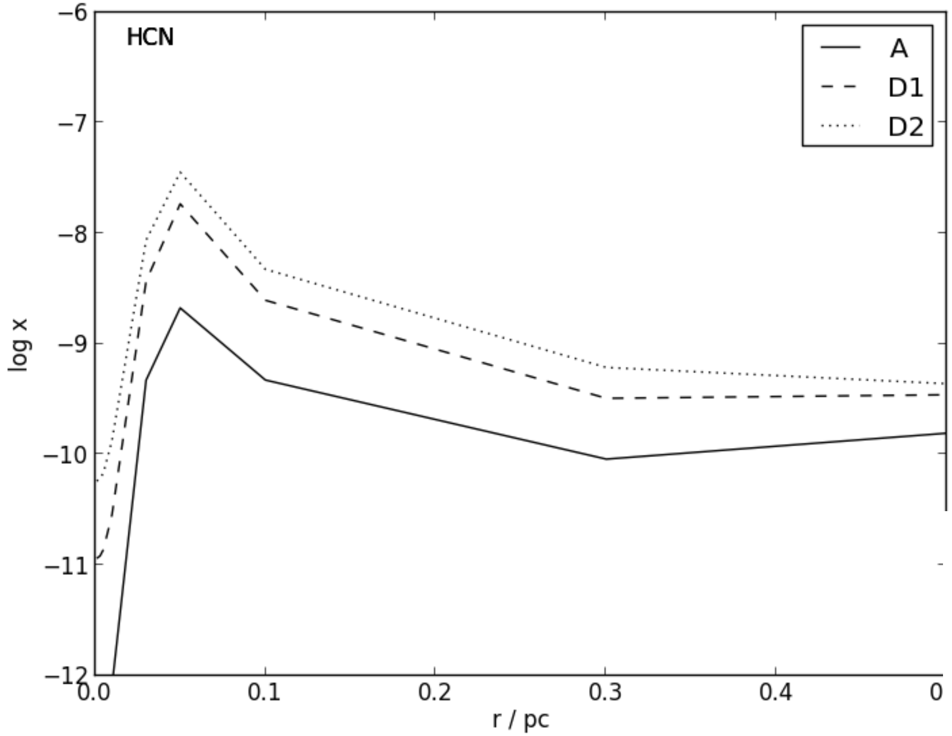
Dynamics + fluxes: the effects of cosmic rays → more important for models where collapse results from ambipolar diffusion

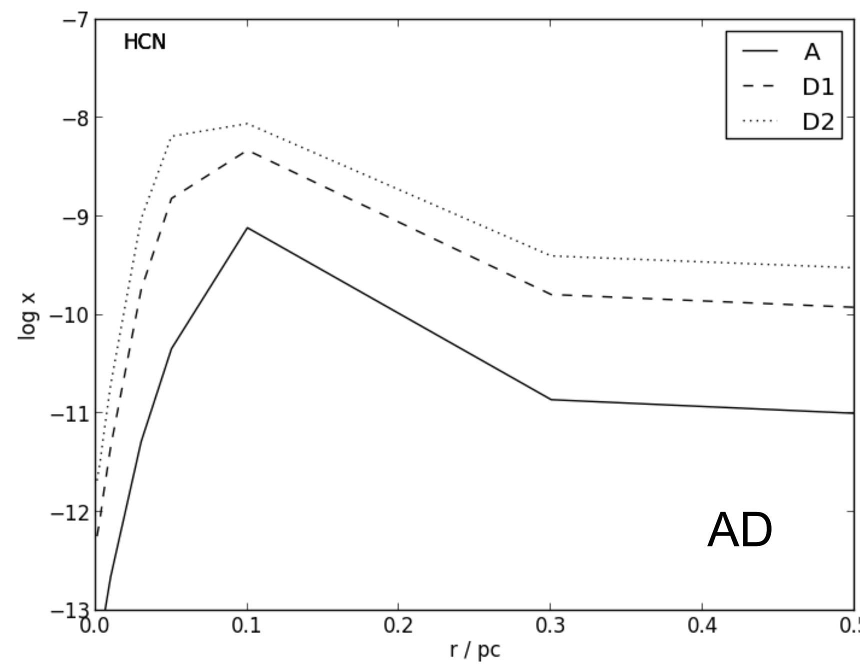
Table 1. Values of parameters selected for the models.

Model	n_f/cm^{-3}	t_{eq}/yr	$\zeta/1.3\times10^{-17}\,\mathrm{s}^{-1}$	ε	ϕ	Y_UV
A	10^8	0	1	0.01	10^5	0.1
B1	10^7	0	1	0.01	10^5	0.1
B2	10^9	0	1	0.01	10^5	0.1
C1	10^8	10^4	1	0.01	10^5	0.1
C2	10^8	10^6	1	0.01	10^5	0.1
D1	10^8	0	5	0.01	10^5	0.1
D2	10^8	0	10	0.01	10^5	0.1
E1	10^8	0	1	0.01	10^5	0.1
E2	10^8	0	1	0.01	10^5	0.1
F1	10^8	0	1	0.1	10^5	0.1
F2	10^8	0	1	1.0	10^5	0.1
G1	10^8	0	1	0.01	10^4	0.1
G2	10^8	0	1	0.01	10^6	0.1
H1	10^8	0	1	0.01	10^5	0.001
H2	10^8	0	1	0.01	10^5	1.0



BES1

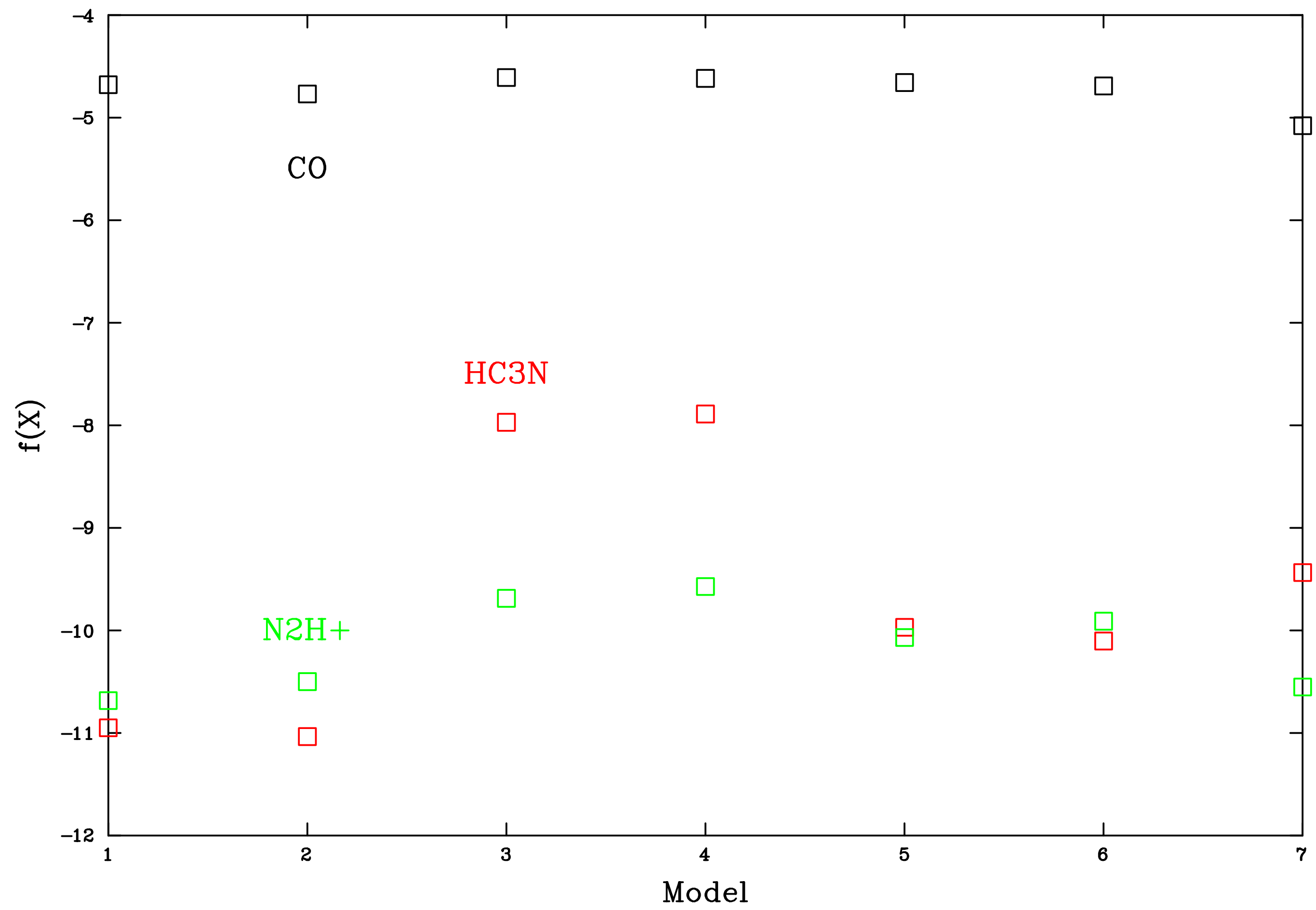
Priestley et al. in prep



AD

"Density-Time"

$n\_f = 10^4$ cm^{-3}

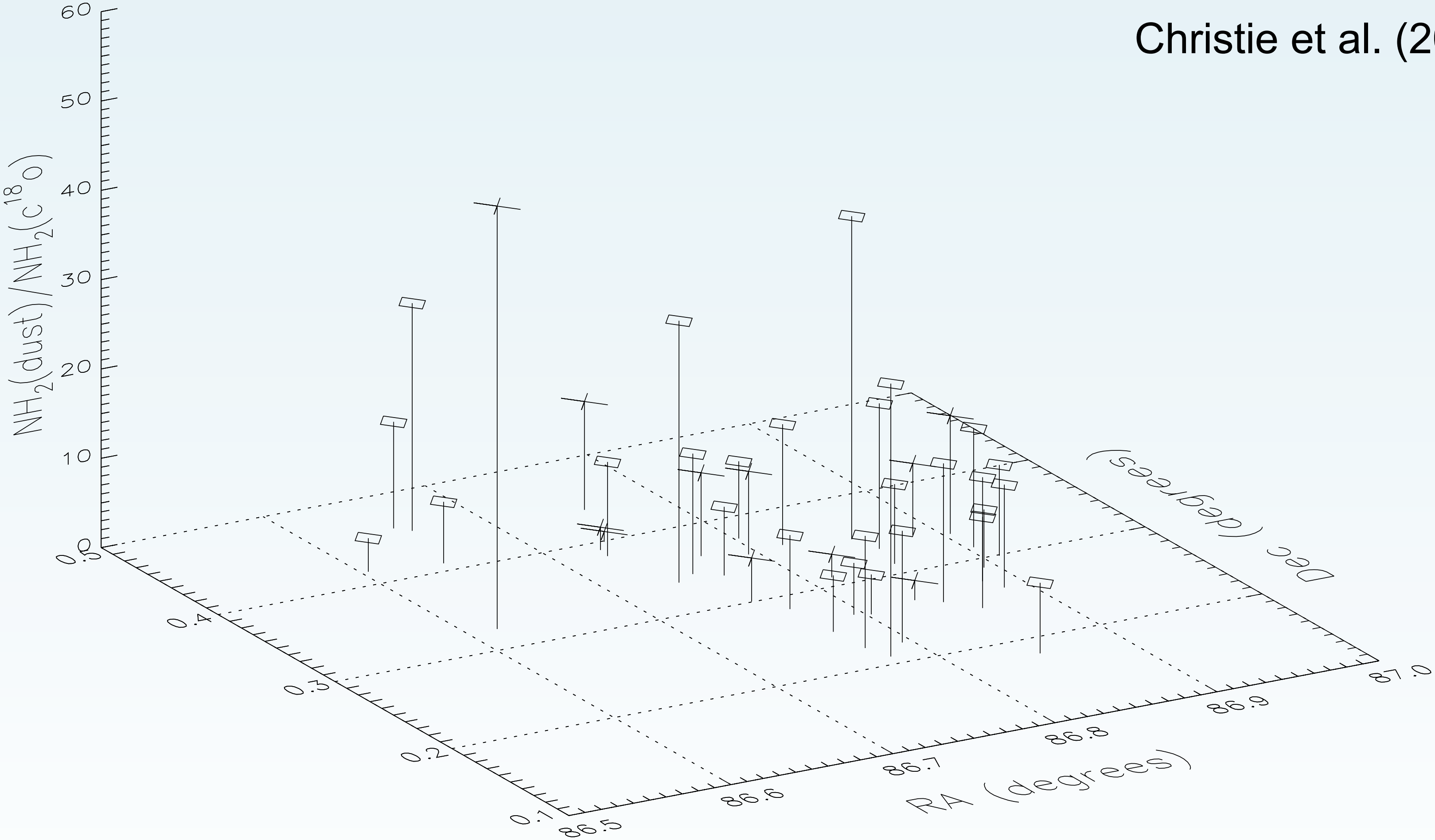


Note that HC_3N/N_2H^+ ratio is used as an age indicator for pre-stellar cores! (e.g. Hohashi et al. 2015)

Model 1: n_{H_i} = 10 cm^{-3}, solar; Model 2: n_{H_i} = 100 cm^{-3}; solar
Model 3: n_{H_i} = 10 cm^{-3}, TMC-1; Model 4: n_{H_i} = 100 cm^{-3}; TMC-1
Model 5: n_{H_i} = 10 cm^{-3}, L134N; Model 6: n_{H_i} = 100 cm^{-3}; L134N
Model 7: n_{H_i} = 100 cm^{-3}; solar; long lived

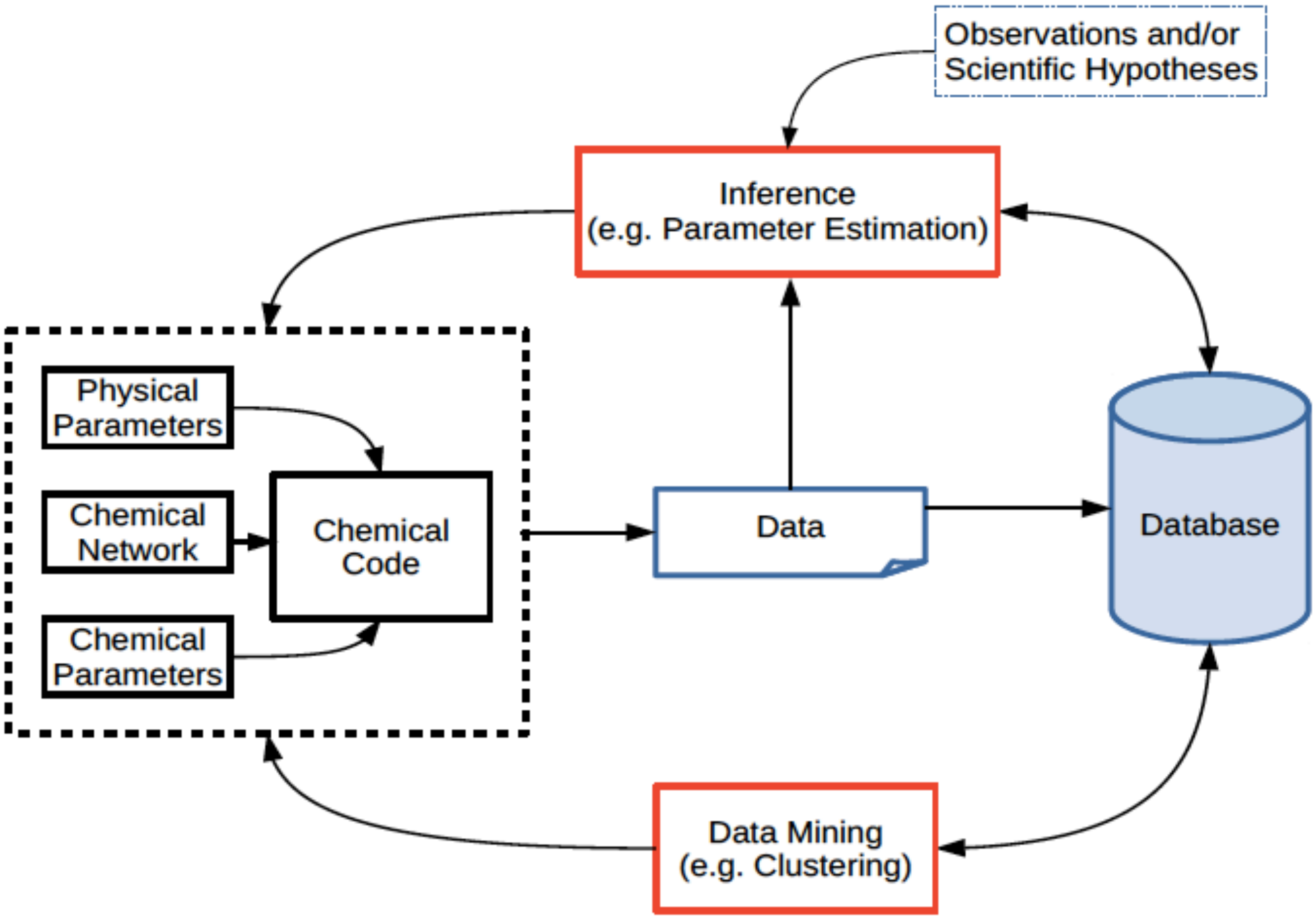
NGC 2071: squares are starless cores; crosses protostellar cores → small variations in CO abundances

Christie et al. (2012)



Small variations in the abundance of **abundant** molecules → **large** variations in the abundance of **tracer** molecules

Probing effects of initial conditions on the chemistry: a statistical approach



Makrymallis & Viti, 2014, 2016

Hierarchical clustering

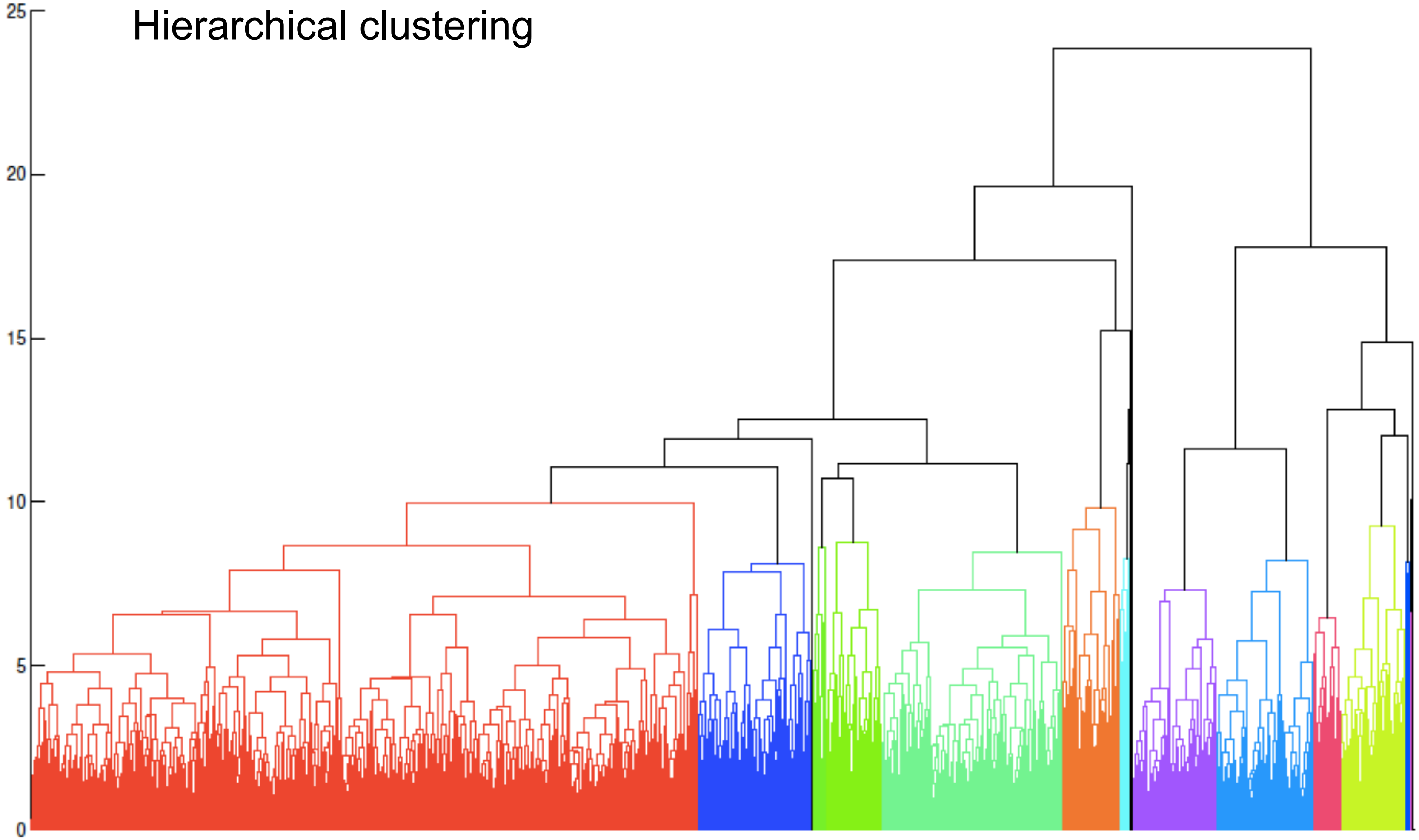


Figure 2.6: Full dendrogram for the bottom-up agglomerative hierarchical clustering on our data. Different clusters are indicated by different color according to a user defined level of pruning the tree. Each of the leaves in the dendrogram represents a model. The x-axis labeling though has been deactivated due to the large number of leaves.

Probabilistic hierarchical clustering

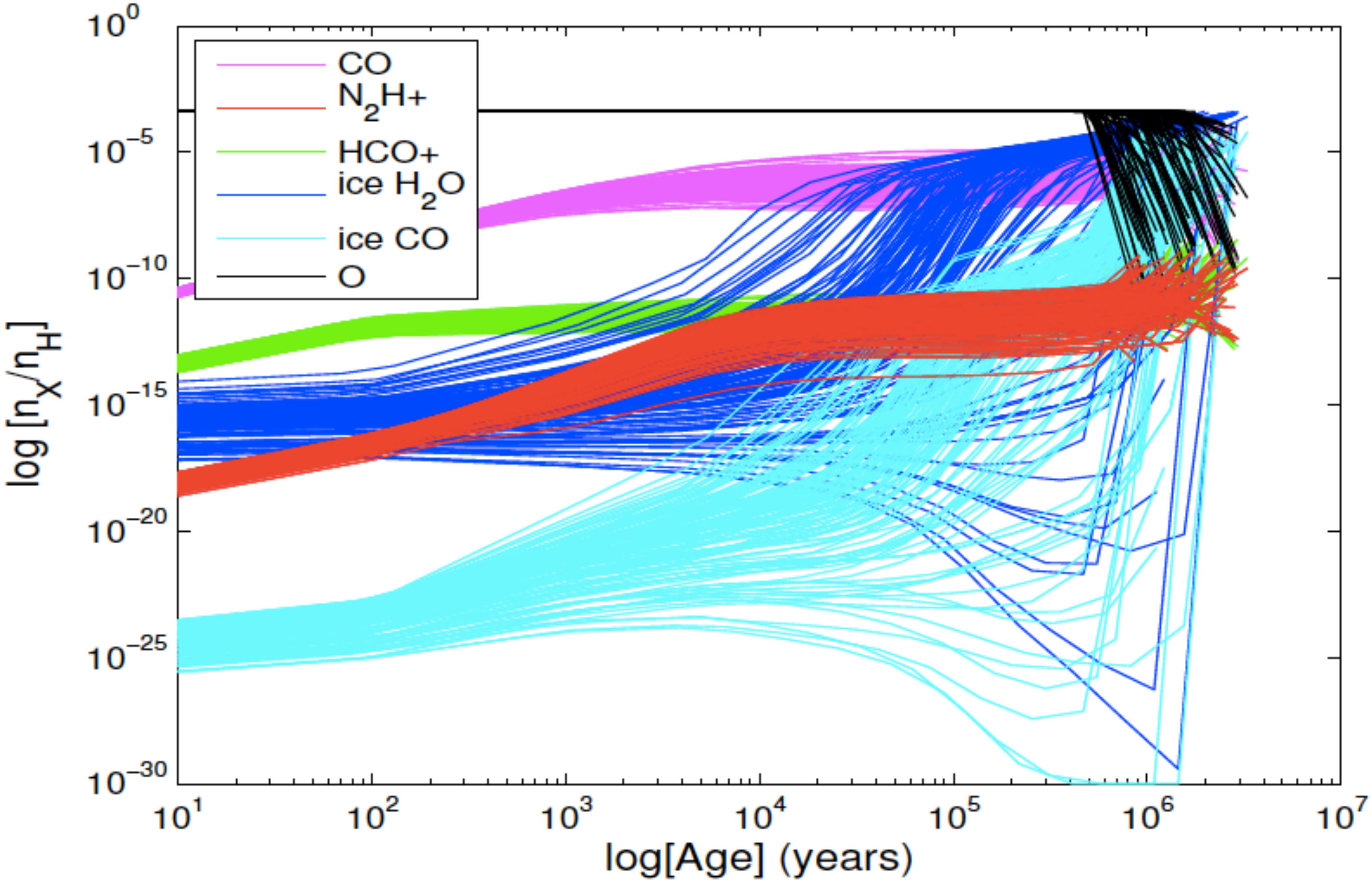


Figure 2.11: Probabilistic hierarchical clustering of our toy example application. Each color represents a distinct cluster and coincides with a distinct species as well.

Example: water icy mantle 'fits'

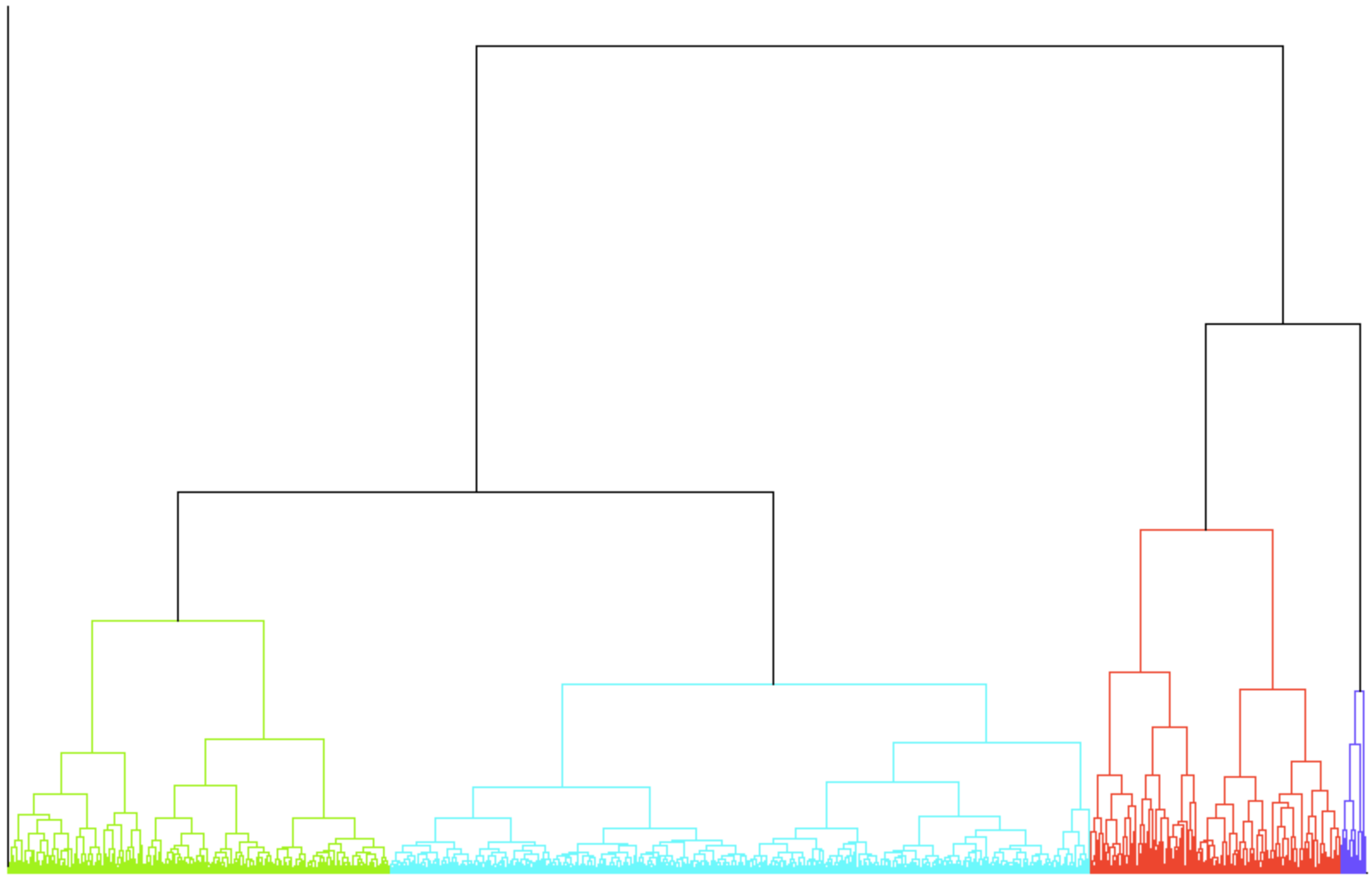


Figure 2.12: Dendrogram for the probabilistic hierarchical clustering on ice water data. Different clusters are indicated by different color according to the algorithm's suggested number of clusters. The tree is pruned for practical visualization reasons.

Accelerated Bayesian inference applied to the 'problem' of ices

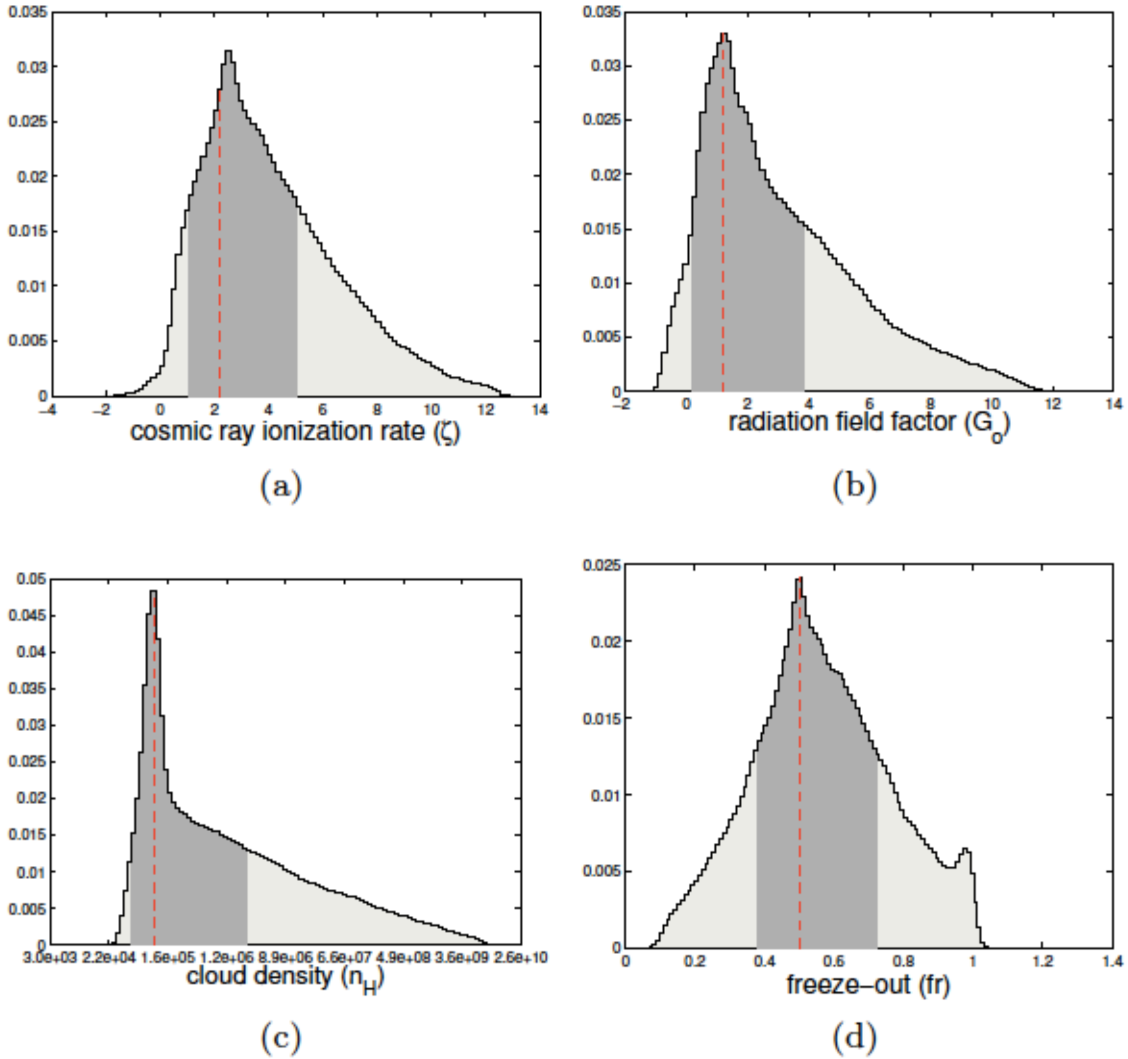


Figure 4.3: 1D Marginalized Posterior Probability Distribution for each of the four parameters using accelerated Bayesian inference with ANNs. The plots show the Gaussian kernel density estimator of each Probability Density Function. Dark gray area indicate 68% highest density region, while dashed red lines indicate the pre-defined parameter values.

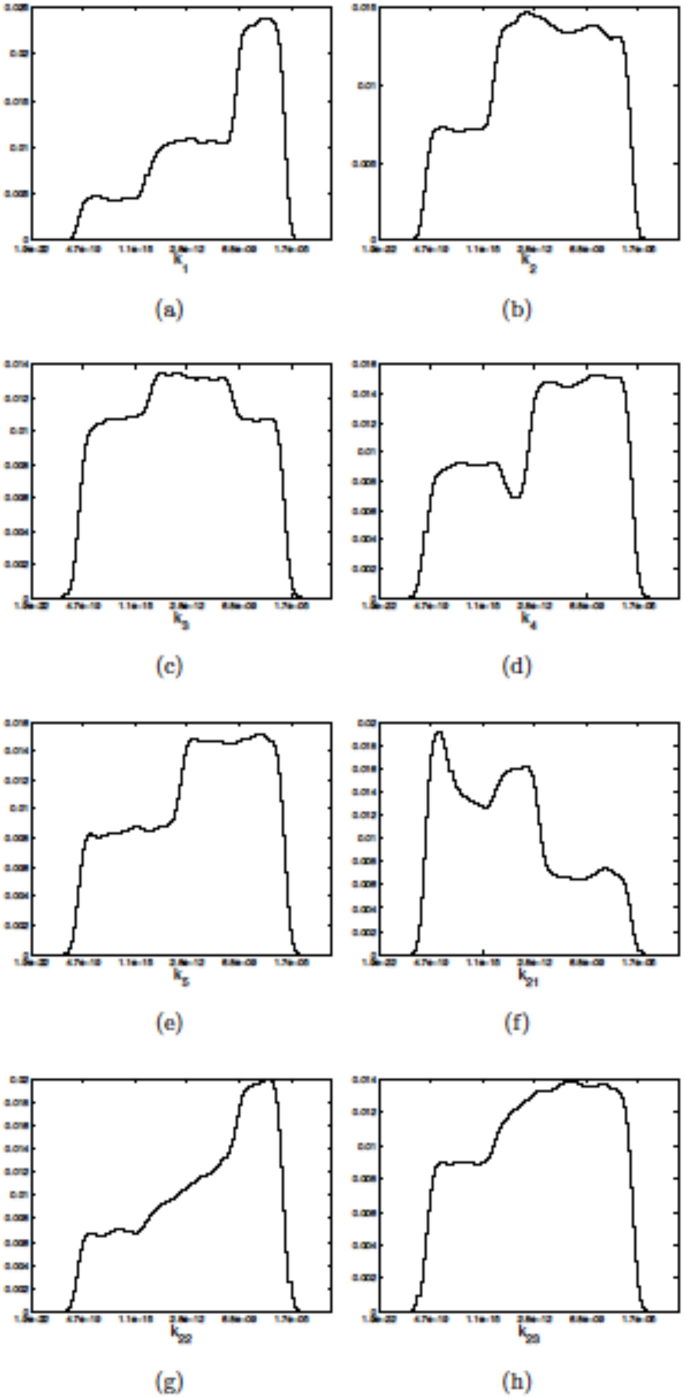
Bayesian Uncertainty Analysis of Surface Reactions in Icy Mantles (Makrymallis & Viti, 2016, submitted)

Can we prioritize specific experiments under specific conditions by the use of probabilistic inference?

Advantage of this method: we do not need to worry about how surface reaction rates are calculated

$$O_{int} = [10^{-8}, 10^{-4}] = \{x \in \mathbb{R} | 10^{-8} \leq x \leq 10^{-4}\}.$$

No.	Reactions				
1.	O	+	H	→	OH
2.	OH	+	H	→	H_2O
3.	CO	+	OH	→	CO_2
4.	S	+	H	→	HS
5.	HS	+	H	→	H_2S
6.	H_2S	+	S	→	H_2S_2
7.	CS	+	H	→	HCS
8.	HCS	+	H	→	H_2CS
9.	CO	+	S	→	OCS
10.	OCS	+	H	→	HOCS
11.	H_2S	+	CO	→	OCS
12.	H_2S	+	H_2S	→	H_2S_2
13.	H_2S_2	+	CO	→	CS2 + O
14.	H_2S	+	O	→	SO_2
15.	CS_2	+	O	→	OCS + S
16.	CO	+	HS	→	OCS
17.	S	+	O	→	SO
18.	SO	+	O	→	SO_2
19.	SO	+	H	→	HSO
20.	HSO	+	H	→	SO
21.	CO	+	H	→	HCO
22.	HCO	+	H	→	H_2CO
23.	H_2CO	+	H	→	CH_3OH



(a) (b) (c) (d) (e) (f) (g) (h)

Over a million chemical models

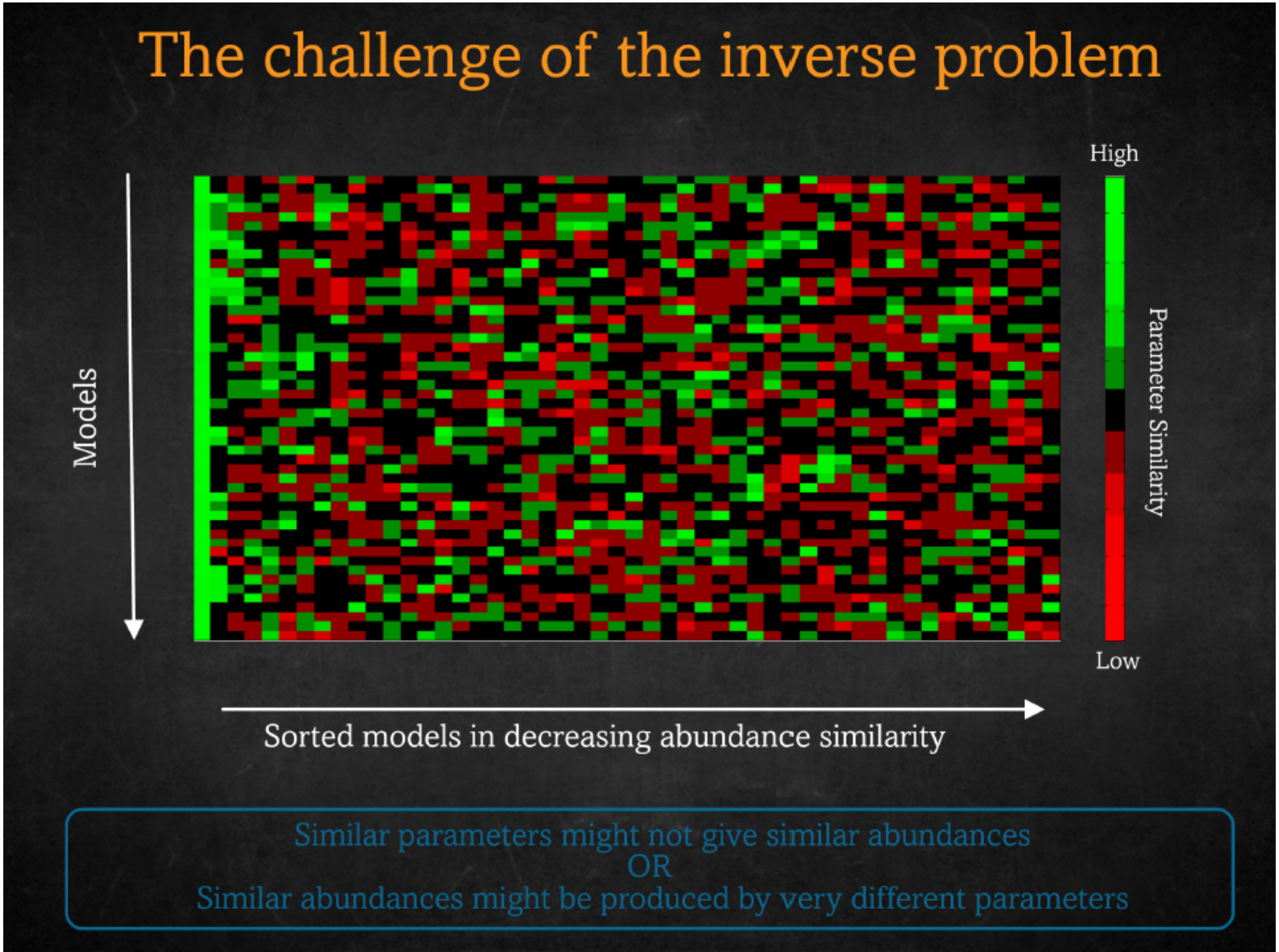
↓

Only 8 out of 23 reactions show variability
e.g. 15 out of 23 reactions may not be needed

i.e reactions of rates with uniform distribution do not impact on the outcome

No.	Reactions				
1.	O	+	H	→	OH
2.	OH	+	H	→	H_2O
3.	CO	+	OH	→	CO_2
4.	S	+	H	→	HS
5.	HS	+	H	→	H_2S
6.	H_2S	+	S	→	H_2S_2
7.	CS	+	H	→	HCS
8.	HCS	+	H	→	H_2CS
9.	CO	+	S	→	OCS
10.	OCS	+	H	→	HOCS
11.	H_2S	+	CO	→	OCS
12.	H_2S	+	H_2S	→	H_2S_2
13.	H_2S_2	+	CO	→	CS2 + O
14.	H_2S	+	O	→	SO_2
15.	CS_2	+	O	→	OCS + S
16.	CO	+	HS	→	OCS
17.	S	+	O	→	SO
18.	SO	+	O	→	SO_2
19.	SO	+	H	→	HSO
20.	HSO	+	H	→	SO
21.	CO	+	H	→	HCO
22.	HCO	+	H	→	H_2CO
23.	H_2CO	+	H	→	CH_3OH

Small variations in the abundance of **abundant** molecules → **large** variations in the abundance of **tracer** molecules
The complexity of the chemical models is unavoidable: new approaches to disentangling simple conclusions are necessary



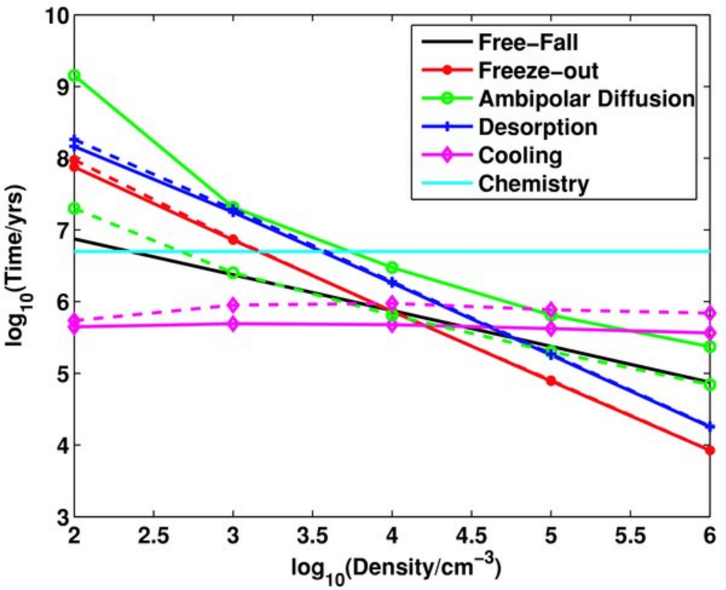
Star formation timescales

Low-mass star formation is relatively well-studied for Milky Way conditions and controlled by several critical timescales

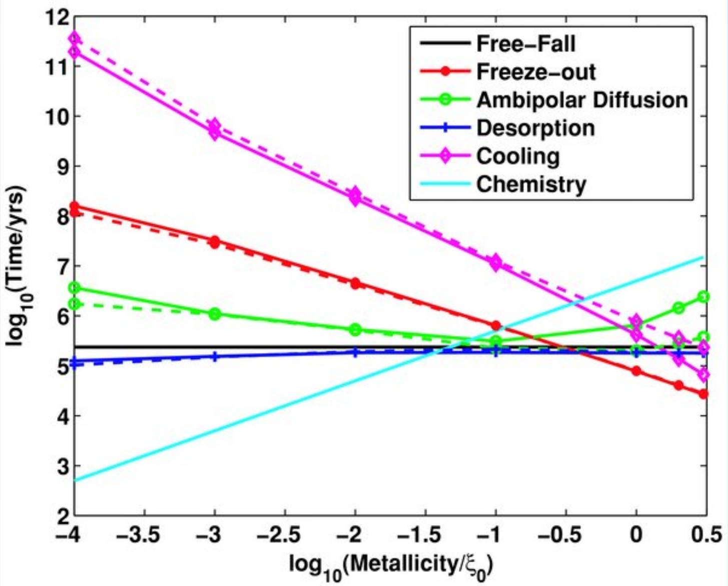
1. Collapse under gravity
2. Cooling by molecules and dust
3. Freeze-out of molecules on to dust
4. Desorption
5. Ambipolar diffusion
6. Chemistry

Timescales in galaxies: dependence on density

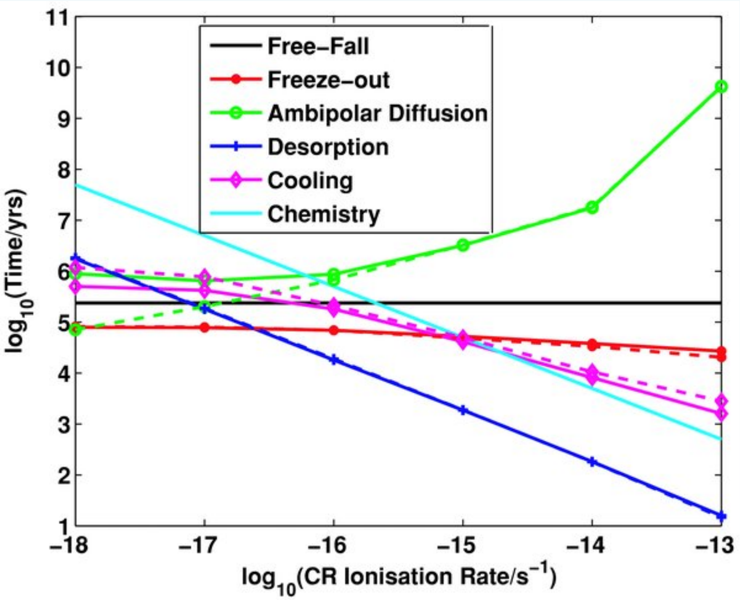
Banerji et al. 2009



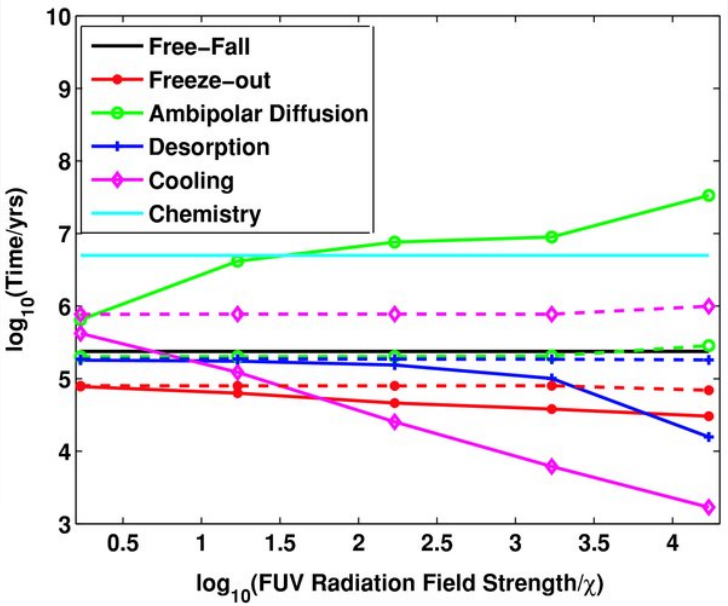
Timescales in galaxies: dependence on metallicity

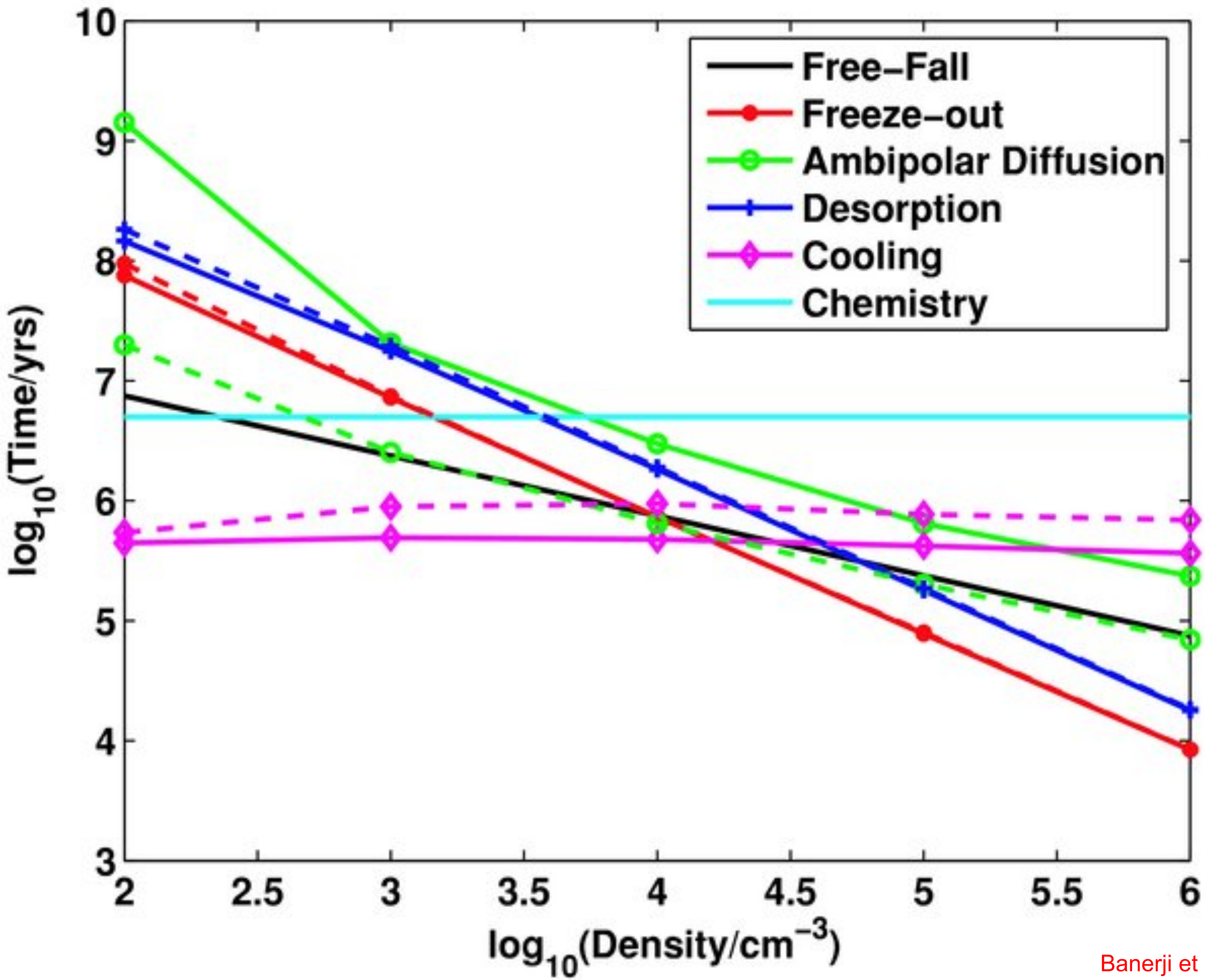


Timescales in galaxies: dependence on cosmic rays

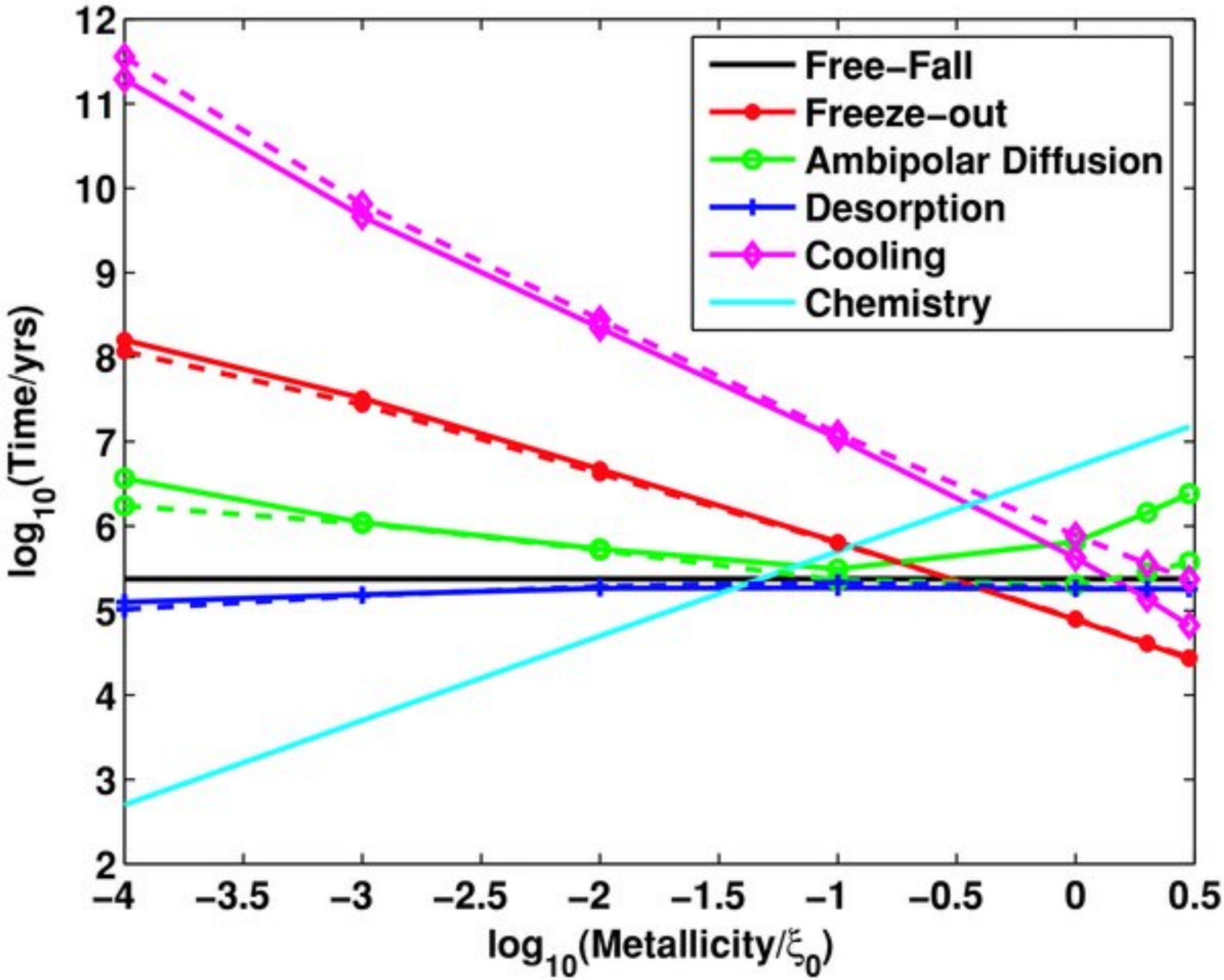


Timescales in galaxies: dependence on FUV intensity

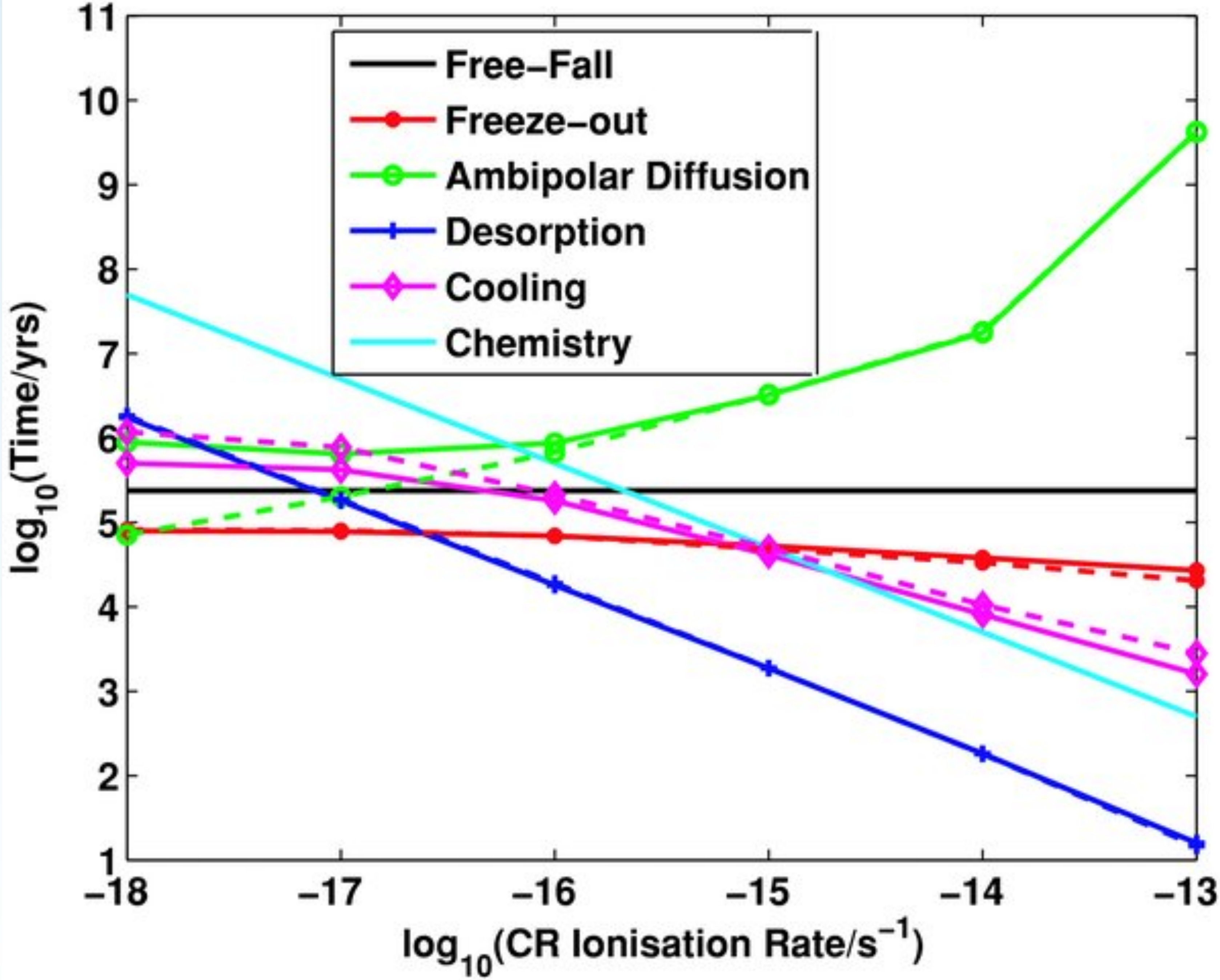




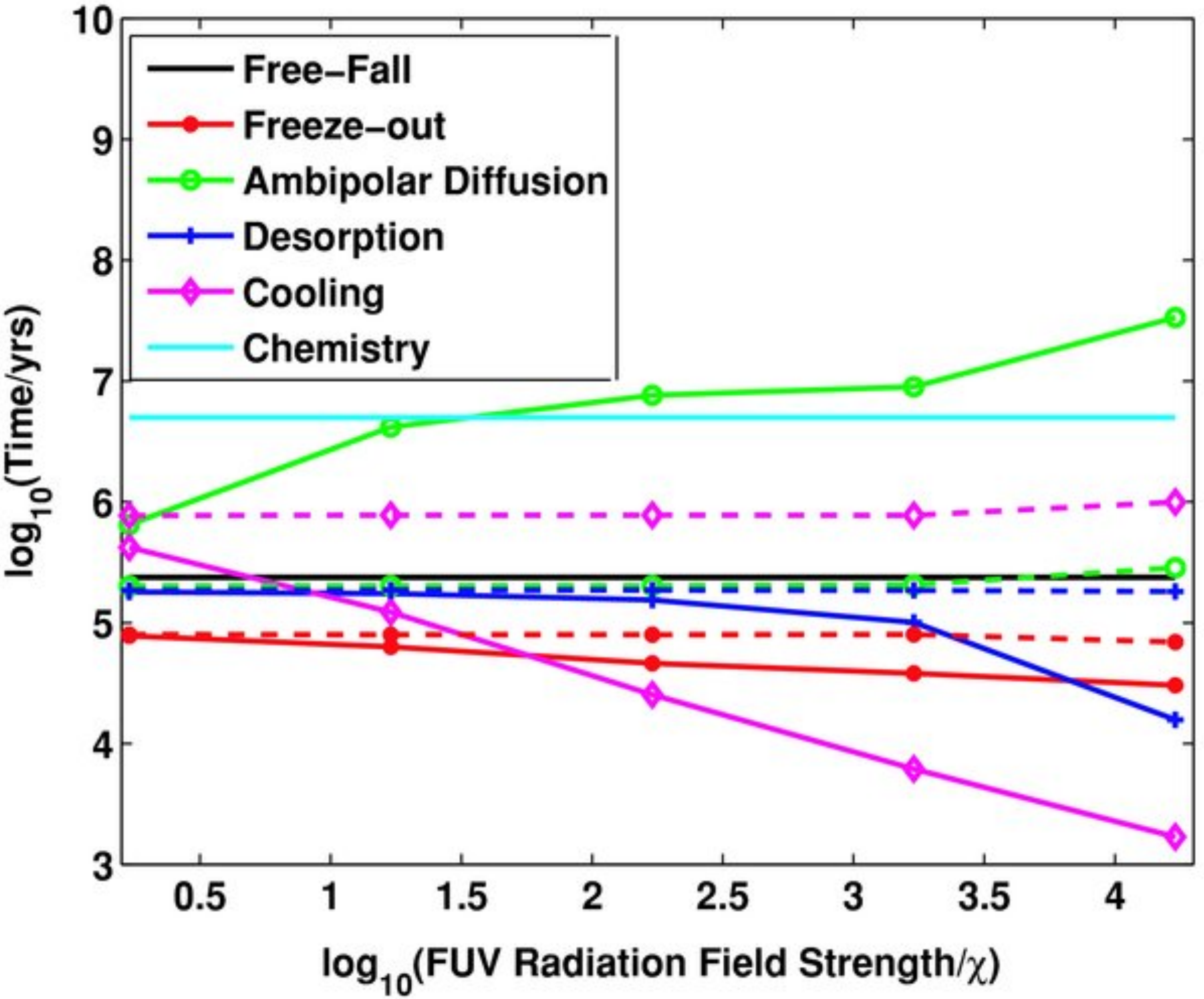
Banerji et al. 2009



Banerji et al. 2009



Banerji et al. 2009



Banerji et al. 2009

Timescales in external galaxies: some considerations

If low mass star formation inhibited → "top-heavy" IMF??

This may be true in:

(i) Low metallicity systems

(ii) Active galaxies (very high FUV and cosmic rays) with solar metallicity (collapse likely impeded by magnetic pressure)

High-redshift Models: Inputs to the Model as well as the Form of the IMF Associated with These Physical Conditio

Model	Density (cm^{-3})	Metallicity ($\xi_\odot$)	CR Ionization Rate (s^{-1})	FUV Flux (Draine)
I	10^4	0.05	10^{-13}	1.7×10^4
II	10^5	0.05	10^{-14}	1.7×10^3
III	10^5	1.00	10^{-14}	1.7×10^3

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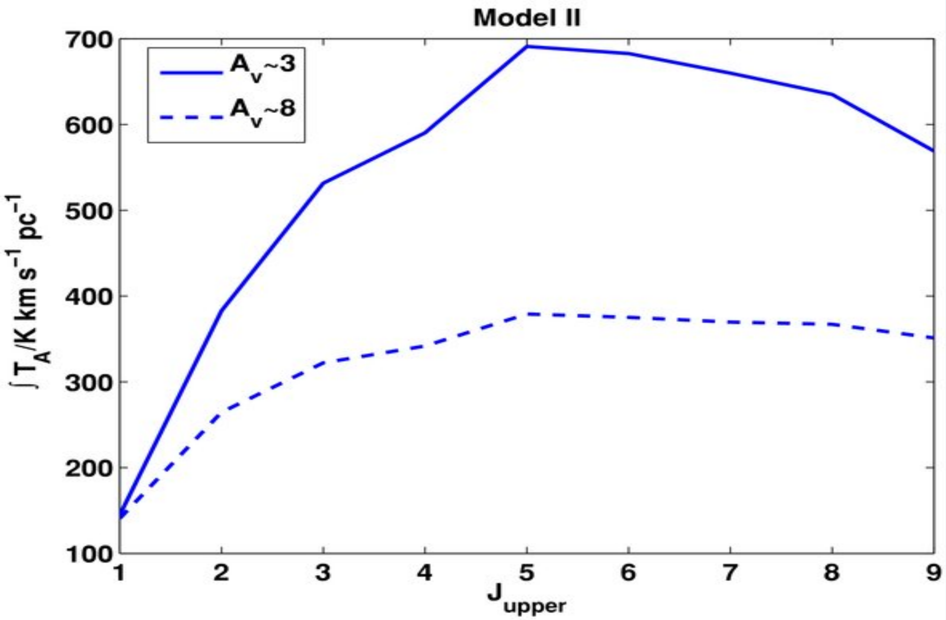

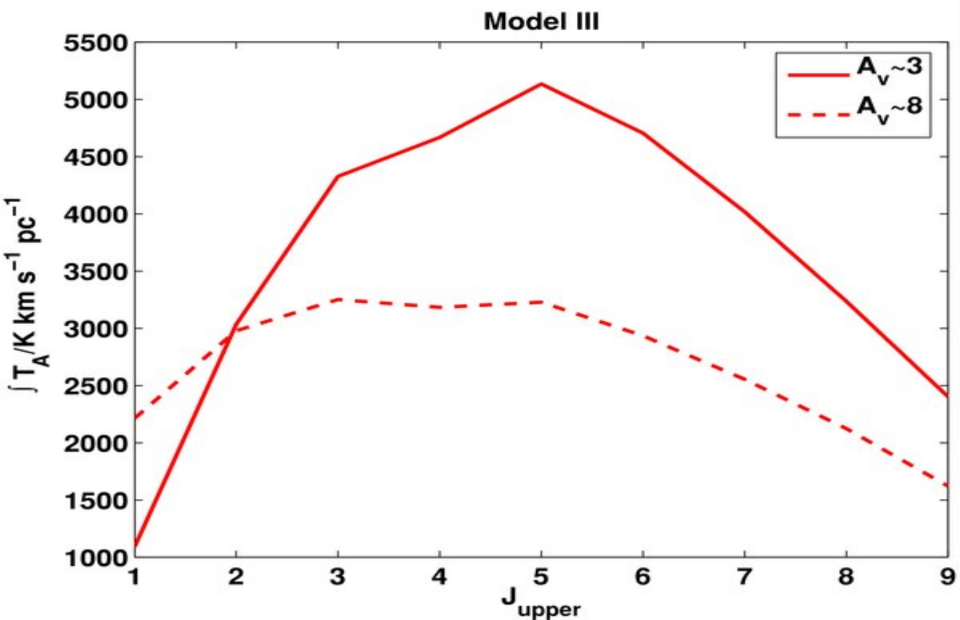

similar CO rotational spectra

But:

Distribution flatter model II

Shape of spectrum indicates IMF?

High J CO observations coupled with dynamical and chemical models → clues about the IMF?