VENTSPILS AUGSTSKOLA

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(VIRAC)

Cosmic-ray induced diffusion, reactions and destruction of molecules in interstellar ices

Valsts izglītības attīstības aģentūra

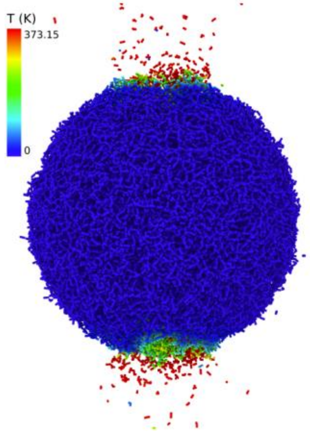
NACIONĀLAIS ATTĪSTĪBAS PLĀNS 2020

EIROPAS SAVIENĪBA
Eiropas Reģionālās attīstības fonds

IEGULDĪJUMS TAVĀ NĀKOTNĒ

Micro- to **macroscopic** perspective

Cosmic ray particles impact icy interstellar grains



Mainitz *et al.* 2016, A&A 592

Composition of interstellar gas and ices

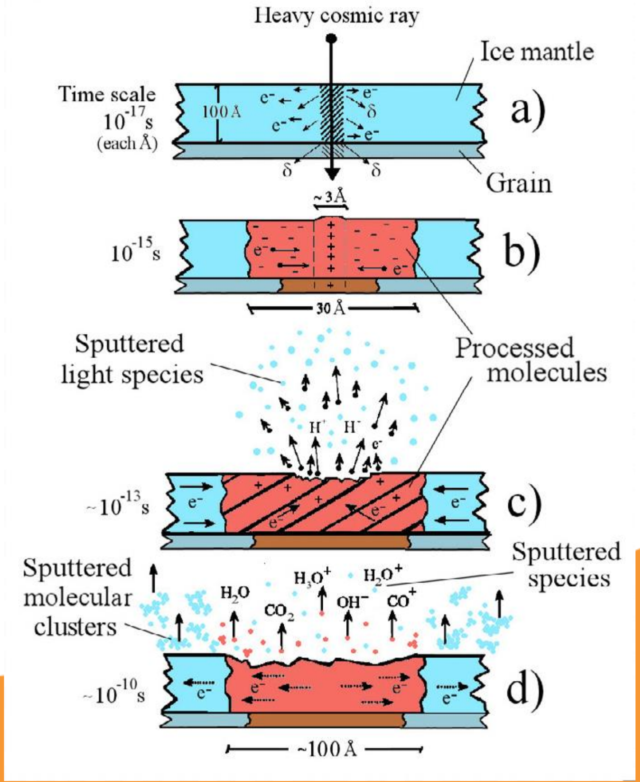
ESO and Igor Chekalin

Cosmic-ray (CR) impact

- Excitation and ionization
- Heating along the CR track
- Destruction of molecules
- Sputtering

- Time-scale ≤ 10^{-10} s

Pilling *et al.* 2010, A&A 509



Relaxation

- Heat expands to the whole grain, reaching a temperature of 70 K for 10^{-5} s
- Molecule diffusion and evaporation
- Cooling via evaporation or radiation

CR-induced processing of icy species

- Sputtering
- Dissociation
- Local heating
  - diffusion
  - evaporation
  - reactions
- Whole-grain heating
  - diffusion
  - evaporation
  - reactions
- Ice explosions

Image credits: ESO and Igor Chekalin

In astrochemical models

- Sputtering – ineffective
- Dissociation – not investigated
- Local heating
  - diffusion – not investigated
  - evaporation – ineffective
  - reactions – not investigated
- Whole-grain heating
  - diffusion – important for complex molecules
  - **evaporation** – important
  - reactions – not investigated
- Ice explosions – do they occur?

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Image credits: ESO and Igor Chekalin

To be modelled

- Sputtering
- Dissociation
- Local heating
  - diffusion
  - evaporation
  - reactions
- Whole-grain heating
  - diffusion
  - evaporation
  - reactions
- Ice explosions

Sequence of CR-induced grain surface processes

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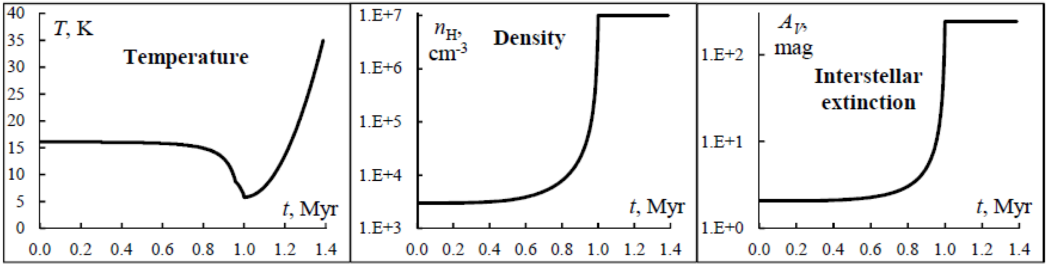
Image credits: ESO and Igor Chekalin

Sequence for surface molecules

- Dissociation, high-temperature reactions
- Local-heating grain surface chemistry
- Whole-grain heating surface chemistry
- Cooling via CO evaporation

The models

- Kinetic rate-equation astrochemical simulations
- **#1:** starless cloud core; t = 1 Myr
  n_{H} = 2×10^{4} cm^{-3}; T_{dust} = 10 K
- **#2:** Collapsing prestellar core; t = 1+0.4 Myr
  n_{H} = 3×10^{3} ... 10^{7} cm^{-3}; T$_{\mathrm{dust}}$ = 6 ... 35 K



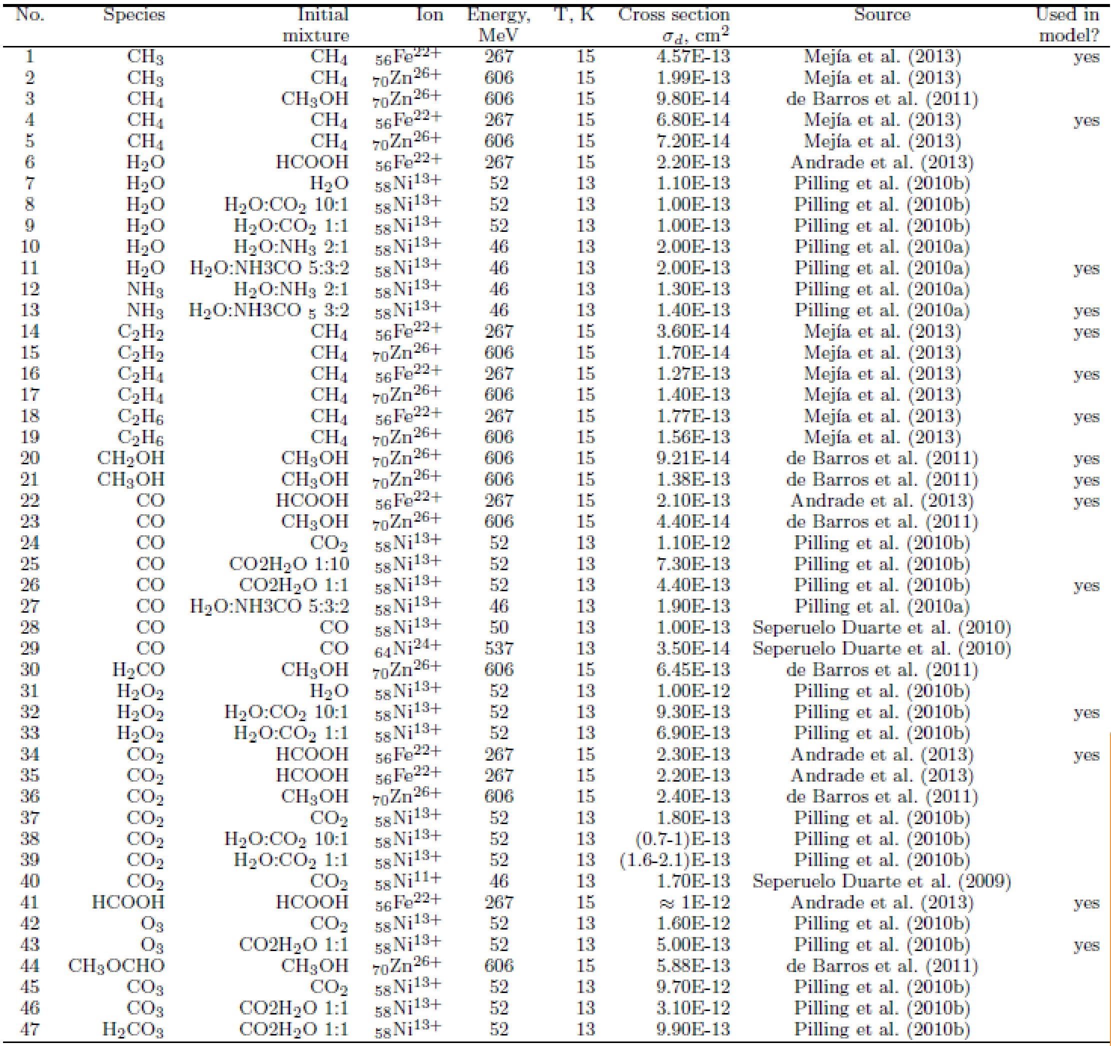
(Kalvāns 2015, A&A 573)

Macroscopic effects of CR-induced processes in interstellar ices

CR-induced dissociation

- Dissociation rates derived from experiments
- Produces radicals in ices
- Subsequent reactions in icy mantles affect ice composition

Selected experimental results of interstellar ice analog irradiation by heavy ions.

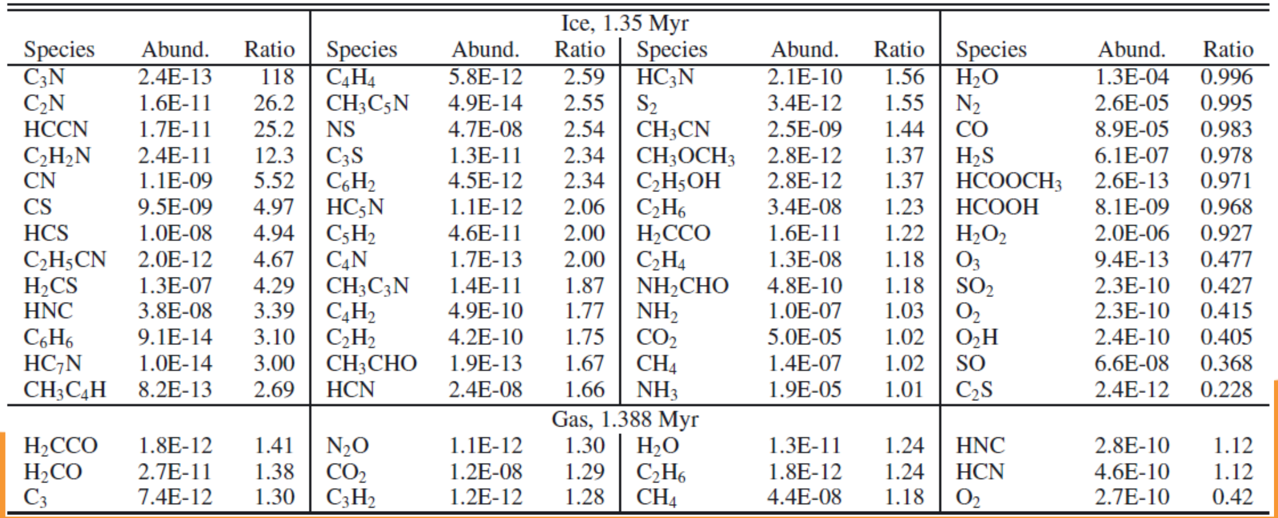


No.	Species	Initial mixture	Ion	Energy, MeV	T, K	Cross section σ_d, cm^2	Source	Used in model?
1	CH_3	CH_4	$_{56}Fe^{22+}$	267	15	4.57E-13	Mejía et al. (2013)	yes
2	CH_3	CH_4	$_{70}Zn^{26+}$	606	15	1.99E-13	Mejía et al. (2013)	
3	CH_4	CH_3OH	$_{70}Zn^{26+}$	606	15	9.80E-14	de Barros et al. (2011)	
4	CH_4	CH_4	$_{56}Fe^{22+}$	267	15	6.80E-14	Mejía et al. (2013)	yes
5	CH_4	CH_4	$_{70}Zn^{26+}$	606	15	7.20E-14	Mejía et al. (2013)	
6	H_2O	HCOOH	$_{56}Fe^{22+}$	267	15	2.20E-13	Andrade et al. (2013)	
7	H_2O	H_2O	$_{58}Ni^{13+}$	52	13	1.10E-13	Pilling et al. (2010b)	
8	H_2O	$H_2O:CO_2$ 10:1	$_{58}Ni^{13+}$	52	13	1.00E-13	Pilling et al. (2010b)	
9	H_2O	$H_2O:CO_2$ 1:1	$_{58}Ni^{13+}$	52	13	1.00E-13	Pilling et al. (2010b)	
10	H_2O	$H_2O:NH_3$ 2:1	$_{58}Ni^{13+}$	46	13	2.00E-13	Pilling et al. (2010a)	
11	H_2O	H_2O:NH3CO 5:3:2	$_{58}Ni^{13+}$	46	13	2.00E-13	Pilling et al. (2010a)	yes
12	NH_3	$H_2O:NH_3$ 2:1	$_{58}Ni^{13+}$	46	13	1.30E-13	Pilling et al. (2010a)	
13	NH_3	H_2O:NH3CO $_5$ 3:2	$_{58}Ni^{13+}$	46	13	1.40E-13	Pilling et al. (2010a)	yes
14	C_2H_2	CH_4	$_{56}Fe^{22+}$	267	15	3.60E-14	Mejía et al. (2013)	yes
15	C_2H_2	CH_4	$_{70}Zn^{26+}$	606	15	1.70E-14	Mejía et al. (2013)	
16	C_2H_4	CH_4	$_{56}Fe^{22+}$	267	15	1.27E-13	Mejía et al. (2013)	yes
17	C_2H_4	CH_4	$_{70}Zn^{26+}$	606	15	1.40E-13	Mejía et al. (2013)	
18	C_2H_6	CH_4	$_{56}Fe^{22+}$	267	15	1.77E-13	Mejía et al. (2013)	yes
19	C_2H_6	CH_4	$_{70}Zn^{26+}$	606	15	1.56E-13	Mejía et al. (2013)	
20	CH_2OH	CH_3OH	$_{70}Zn^{26+}$	606	15	9.21E-14	de Barros et al. (2011)	yes
21	CH_3OH	CH_3OH	$_{70}Zn^{26+}$	606	15	1.38E-13	de Barros et al. (2011)	yes
22	CO	HCOOH	$_{56}Fe^{22+}$	267	15	2.10E-13	Andrade et al. (2013)	yes
23	CO	CH_3OH	$_{70}Zn^{26+}$	606	15	4.40E-14	de Barros et al. (2011)	
24	CO	CO_2	$_{58}Ni^{13+}$	52	13	1.10E-12	Pilling et al. (2010b)	
25	CO	CO2H_2O 1:10	$_{58}Ni^{13+}$	52	13	7.30E-13	Pilling et al. (2010b)	
26	CO	CO2H_2O 1:1	$_{58}Ni^{13+}$	52	13	4.40E-13	Pilling et al. (2010b)	yes
27	CO	H_2O:NH3CO 5:3:2	$_{58}Ni^{13+}$	46	13	1.90E-13	Pilling et al. (2010a)	
28	CO	CO	$_{58}Ni^{13+}$	50	13	1.00E-13	Seperuelo Duarte et al. (2010)	
29	CO	CO	$_{64}Ni^{24+}$	537	13	3.50E-14	Seperuelo Duarte et al. (2010)	
30	H_2CO	CH_3OH	$_{70}Zn^{26+}$	606	15	6.45E-13	de Barros et al. (2011)	
31	H_2O_2	H_2O	$_{58}Ni^{13+}$	52	13	1.00E-12	Pilling et al. (2010b)	
32	H_2O_2	$H_2O:CO_2$ 10:1	$_{58}Ni^{13+}$	52	13	9.30E-13	Pilling et al. (2010b)	yes
33	H_2O_2	$H_2O:CO_2$ 1:1	$_{58}Ni^{13+}$	52	13	6.90E-13	Pilling et al. (2010b)	
34	CO_2	HCOOH	$_{56}Fe^{22+}$	267	15	2.30E-13	Andrade et al. (2013)	yes
35	CO_2	HCOOH	$_{56}Fe^{22+}$	267	15	2.20E-13	Andrade et al. (2013)	
36	CO_2	CH_3OH	$_{70}Zn^{26+}$	606	15	2.40E-13	de Barros et al. (2011)	
37	CO_2	CO_2	$_{58}Ni^{13+}$	52	13	1.80E-13	Pilling et al. (2010b)	
38	CO_2	$H_2O:CO_2$ 10:1	$_{58}Ni^{13+}$	52	13	(0.7-1)E-13	Pilling et al. (2010b)	
39	CO_2	$H_2O:CO_2$ 1:1	$_{58}Ni^{13+}$	52	13	(1.6-2.1)E-13	Pilling et al. (2010b)	
40	CO_2	CO_2	$_{58}Ni^{11+}$	46	13	1.70E-13	Seperuelo Duarte et al. (2009)	
41	HCOOH	HCOOH	$_{56}Fe^{22+}$	267	15	$\approx$ 1E-12	Andrade et al. (2013)	yes
42	O_3	CO_2	$_{58}Ni^{13+}$	52	13	1.60E-12	Pilling et al. (2010b)	
43	O_3	CO2H_2O 1:1	$_{58}Ni^{13+}$	52	13	5.00E-13	Pilling et al. (2010b)	yes
44	CH_3OCHO	CH_3OH	$_{70}Zn^{26+}$	606	15	5.88E-13	de Barros et al. (2011)	
45	CO_3	CO_2	$_{58}Ni^{13+}$	52	13	9.70E-12	Pilling et al. (2010b)	
46	CO_3	CO2H_2O 1:1	$_{58}Ni^{13+}$	52	13	3.10E-12	Pilling et al. (2010b)	
47	H_2CO_3	CO2H_2O 1:1	$_{58}Ni^{13+}$	52	13	9.90E-13	Pilling et al. (2010b)	

CR induced dissociation: results

- Induces abundance changes within 10 % for abundant icy species (H_2O, CO, CO_2)
- Favors carbon chains (C_8, C_3N, etc.), with abundance increases by up to a factor of 100

Results of Model #2, (pre)stellar core



					Ice, 1.35 Myr						
Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio
C_3N	2.4E-13	118	C_4H_4	5.8E-12	2.59	HC_3N	2.1E-10	1.56	H_2O	1.3E-04	0.996
C_2N	1.6E-11	26.2	CH_3C_5N	4.9E-14	2.55	S_2	3.4E-12	1.55	N_2	2.6E-05	0.995
HCCN	1.7E-11	25.2	NS	4.7E-08	2.54	CH_3CN	2.5E-09	1.44	CO	8.9E-05	0.983
C_2H_2N	2.4E-11	12.3	C_3S	1.3E-11	2.34	CH_3OCH_3	2.8E-12	1.37	H_2S	6.1E-07	0.978
CN	1.1E-09	5.52	C_6H_2	4.5E-12	2.34	C_2H_5OH	2.8E-12	1.37	$HCOOCH_3$	2.6E-13	0.971
CS	9.5E-09	4.97	HC_5N	1.1E-12	2.06	C_2H_6	3.4E-08	1.23	HCOOH	8.1E-09	0.968
HCS	1.0E-08	4.94	C_5H_2	4.6E-11	2.00	H_2CCO	1.6E-11	1.22	H_2O_2	2.0E-06	0.927
C_2H_5CN	2.0E-12	4.67	C_4N	1.7E-13	2.00	C_2H_4	1.3E-08	1.18	O_3	9.4E-13	0.477
H_2CS	1.3E-07	4.29	CH_3C_3N	1.4E-11	1.87	NH_2CHO	4.8E-10	1.18	SO_2	2.3E-10	0.427
HNC	3.8E-08	3.39	C_4H_2	4.9E-10	1.77	NH_2	1.0E-07	1.03	O_2	2.3E-10	0.415
C_6H_6	9.1E-14	3.10	C_2H_2	4.2E-10	1.75	CO_2	5.0E-05	1.02	O_2H	2.4E-10	0.405
HC_7N	1.0E-14	3.00	CH_3CHO	1.9E-13	1.67	CH_4	1.4E-07	1.02	SO	6.6E-08	0.368
CH_3C_4H	8.2E-13	2.69	HCN	2.4E-08	1.66	NH_3	1.9E-05	1.01	C_2S	2.4E-12	0.228
					Gas, 1.388 Myr						
H_2CCO	1.8E-12	1.41	N_2O	1.1E-12	1.30	H_2O	1.3E-11	1.24	HNC	2.8E-10	1.12
H_2CO	2.7E-11	1.38	CO_2	1.2E-08	1.29	C_2H_6	1.8E-12	1.24	HCN	4.6E-10	1.12
C_3	7.4E-12	1.30	C_3H_2	1.2E-12	1.28	CH_4	4.4E-08	1.18	O_2	2.7E-10	0.42

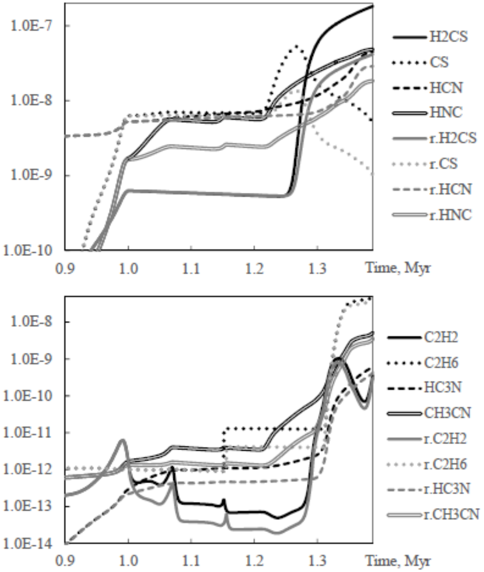
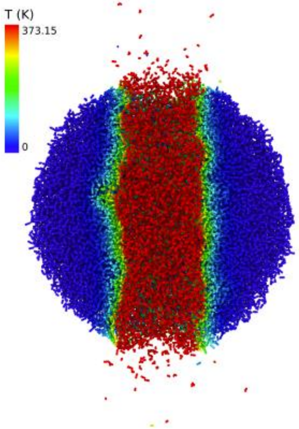


Fig. 5. Abundance, relative to hydrogen, of selected ice molecules in model with CR-induced dissociation. The respective abundances from the reference model are shown for comparison.

Local heating: chemistry in ‘ice fluid’

- A high-temperature fluid is formed in the icy mantle along the CR track for ~10^{-10} s

(Mainitz *et al.* 2016)



- The dissociation products first appear in this fluid
- No chemical signature found from modelled reactions in the fluid with T = 300 K

Whole grain heating: surface diffusion

- CR-induced diffusion of surface species at 70 K promotes formation of complex organic molecules
- Observable effect primarily at low extinctions ($A_V \approx 3^m$)
- Reference: Reboussin *et al.* 2014, MNRAS 440

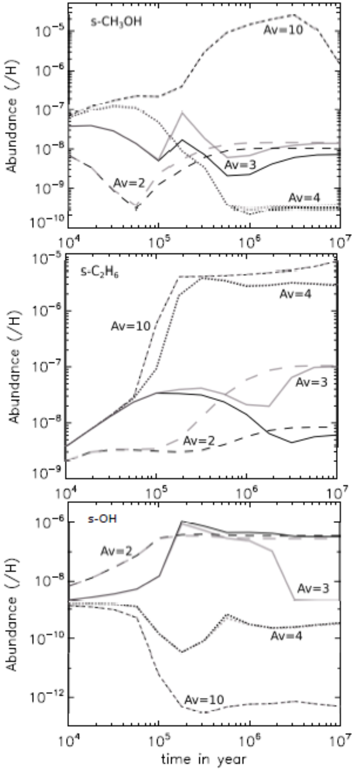


Figure 5. Surface species abundances of a selection of molecules as a function of time computed for different visual extinctions. The results obtained with Model A are represented by black lines and grey lines represent those obtained with Model C. For $A_V=10$, the curves are superimposed.

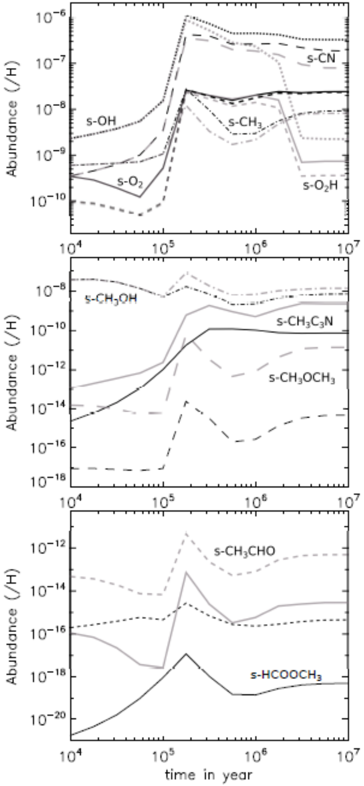
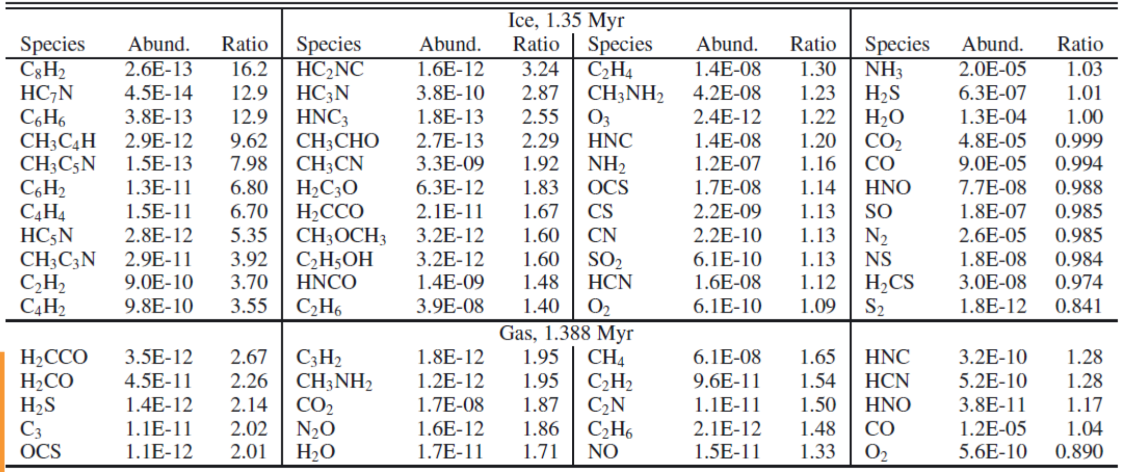


Figure 6. Grain-surface abundances of simple (top) and complex molecules (bottom) as a function of time for $A_V=3$. Black lines are the results obtained with Model A and grey lines the results obtained with Model C.

Whole-grain heating: exchange between surface and bulk-ice

- Thermal diffusion enables diffusion of molecules between different layers of ice
- Effects:
  - removal of H_2 from the icy mantle → less efficient hydrogenation; more oxidized molecules
  - mixing of CO and H_2O:NH_3 ice layers promotes organic chemistry
  - more carbon chains thanks to enhanced mobility of C atoms (CO photodissociation product)
  - abundances of major species affected by no more than a few per cent

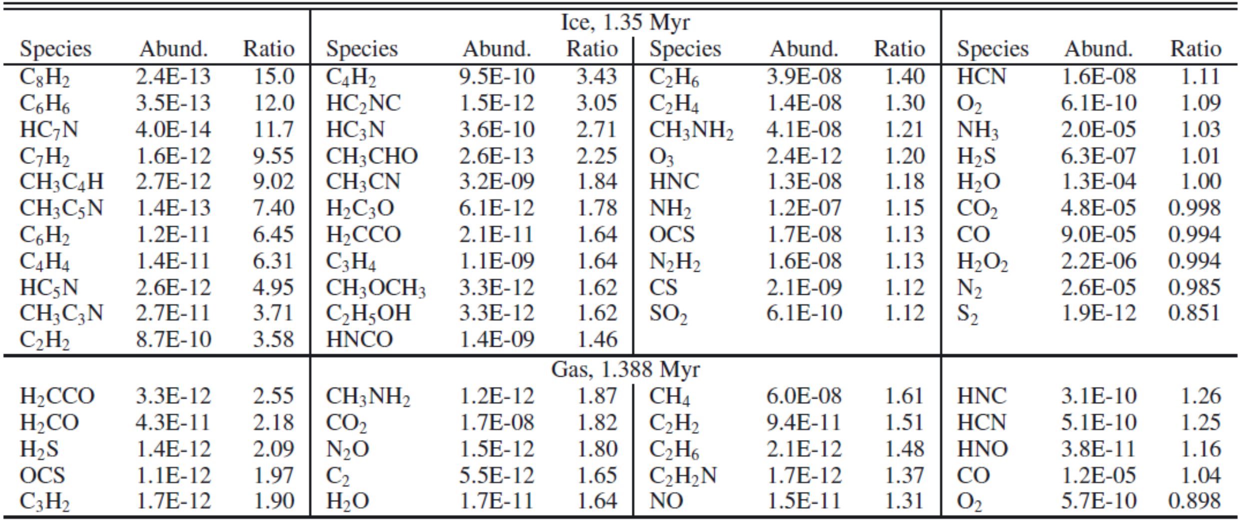


Ice, 1.35 Myr											
Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio
C_8H_2	2.6E-13	16.2	HC_2NC	1.6E-12	3.24	C_2H_4	1.4E-08	1.30	NH_3	2.0E-05	1.03
HC_7N	4.5E-14	12.9	HC_3N	3.8E-10	2.87	CH_3NH_2	4.2E-08	1.23	H_2S	6.3E-07	1.01
C_6H_6	3.8E-13	12.9	HNC_3	1.8E-13	2.55	O_3	2.4E-12	1.22	H_2O	1.3E-04	1.00
CH_3C_4H	2.9E-12	9.62	CH_3CHO	2.7E-13	2.29	HNC	1.4E-08	1.20	CO_2	4.8E-05	0.999
CH_3C_5N	1.5E-13	7.98	CH_3CN	3.3E-09	1.92	NH_2	1.2E-07	1.16	CO	9.0E-05	0.994
C_6H_2	1.3E-11	6.80	H_2C_3O	6.3E-12	1.83	OCS	1.7E-08	1.14	HNO	7.7E-08	0.988
C_4H_4	1.5E-11	6.70	H_2CCO	2.1E-11	1.67	CS	2.2E-09	1.13	SO	1.8E-07	0.985
HC_5N	2.8E-12	5.35	CH_3OCH_3	3.2E-12	1.60	CN	2.2E-10	1.13	N_2	2.6E-05	0.985
CH_3C_3N	2.9E-11	3.92	C_2H_5OH	3.2E-12	1.60	SO_2	6.1E-10	1.13	NS	1.8E-08	0.984
C_2H_2	9.0E-10	3.70	HNCO	1.4E-09	1.48	HCN	1.6E-08	1.12	H_2CS	3.0E-08	0.974
C_4H_2	9.8E-10	3.55	C_2H_6	3.9E-08	1.40	O_2	6.1E-10	1.09	S_2	1.8E-12	0.841
Gas, 1.388 Myr											
H_2CCO	3.5E-12	2.67	C_3H_2	1.8E-12	1.95	CH_4	6.1E-08	1.65	HNC	3.2E-10	1.28
H_2CO	4.5E-11	2.26	CH_3NH_2	1.2E-12	1.95	C_2H_2	9.6E-11	1.54	HCN	5.2E-10	1.28
H_2S	1.4E-12	2.14	CO_2	1.7E-08	1.87	C_2N	1.1E-11	1.50	HNO	3.8E-11	1.17
C_3	1.1E-11	2.02	N_2O	1.6E-12	1.86	C_2H_6	2.1E-12	1.48	CO	1.2E-05	1.04
OCS	1.1E-12	2.01	H_2O	1.7E-11	1.71	NO	1.5E-11	1.33	O_2	5.6E-10	0.890

Results of Model #2, (pre)stellar core

Whole-grain heating: reactions in ice

- Facilitates overcoming of diffusion and reaction barriers for molecules on the surface and in bulk ice
- Results similar to those for diffusion on warm grains (carbon chains and complex organics promoted)



Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio	Species	Abund.	Ratio
						Ice, 1.35 Myr					
C_8H_2	2.4E-13	15.0	C_4H_2	9.5E-10	3.43	C_2H_6	3.9E-08	1.40	HCN	1.6E-08	1.11
C_6H_6	3.5E-13	12.0	HC_2NC	1.5E-12	3.05	C_2H_4	1.4E-08	1.30	O_2	6.1E-10	1.09
HC_7N	4.0E-14	11.7	HC_3N	3.6E-10	2.71	CH_3NH_2	4.1E-08	1.21	NH_3	2.0E-05	1.03
C_7H_2	1.6E-12	9.55	CH_3CHO	2.6E-13	2.25	O_3	2.4E-12	1.20	H_2S	6.3E-07	1.01
CH_3C_4H	2.7E-12	9.02	CH_3CN	3.2E-09	1.84	HNC	1.3E-08	1.18	H_2O	1.3E-04	1.00
CH_3C_5N	1.4E-13	7.40	H_2C_3O	6.1E-12	1.78	NH_2	1.2E-07	1.15	CO_2	4.8E-05	0.998
C_6H_2	1.2E-11	6.45	H_2CCO	2.1E-11	1.64	OCS	1.7E-08	1.13	CO	9.0E-05	0.994
C_4H_4	1.4E-11	6.31	C_3H_4	1.1E-09	1.64	N_2H_2	1.6E-08	1.13	H_2O_2	2.2E-06	0.994
HC_5N	2.6E-12	4.95	CH_3OCH_3	3.3E-12	1.62	CS	2.1E-09	1.12	N_2	2.6E-05	0.985
CH_3C_3N	2.7E-11	3.71	C_2H_5OH	3.3E-12	1.62	SO_2	6.1E-10	1.12	S_2	1.9E-12	0.851
C_2H_2	8.7E-10	3.58	HNCO	1.4E-09	1.46						
						Gas, 1.388 Myr					
H_2CCO	3.3E-12	2.55	CH_3NH_2	1.2E-12	1.87	CH_4	6.0E-08	1.61	HNC	3.1E-10	1.26
H_2CO	4.3E-11	2.18	CO_2	1.7E-08	1.82	C_2H_2	9.4E-11	1.51	HCN	5.1E-10	1.25
H_2S	1.4E-12	2.09	N_2O	1.5E-12	1.80	C_2H_6	2.1E-12	1.48	HNO	3.8E-11	1.16
OCS	1.1E-12	1.97	C_2	5.5E-12	1.65	C_2H_2N	1.7E-12	1.37	CO	1.2E-05	1.04
C_3H_2	1.7E-12	1.90	H_2O	1.7E-11	1.64	NO	1.5E-11	1.31	O_2	5.7E-10	0.898

The complete model

- Combined CR-induced dissociation and chemistry induced by whole-grain heating
- Dissociation dominates but the produced radicals tend to combine into smaller molecules on the warm grains
- This partially cancels the effects of dissociation

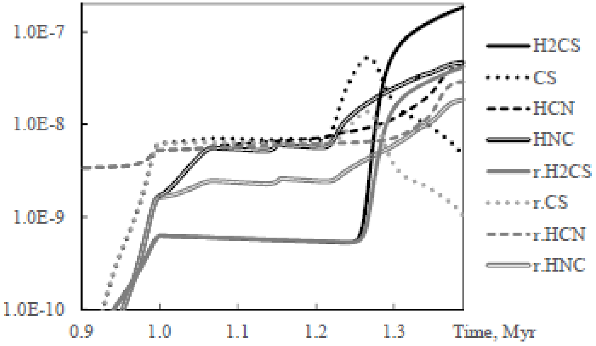
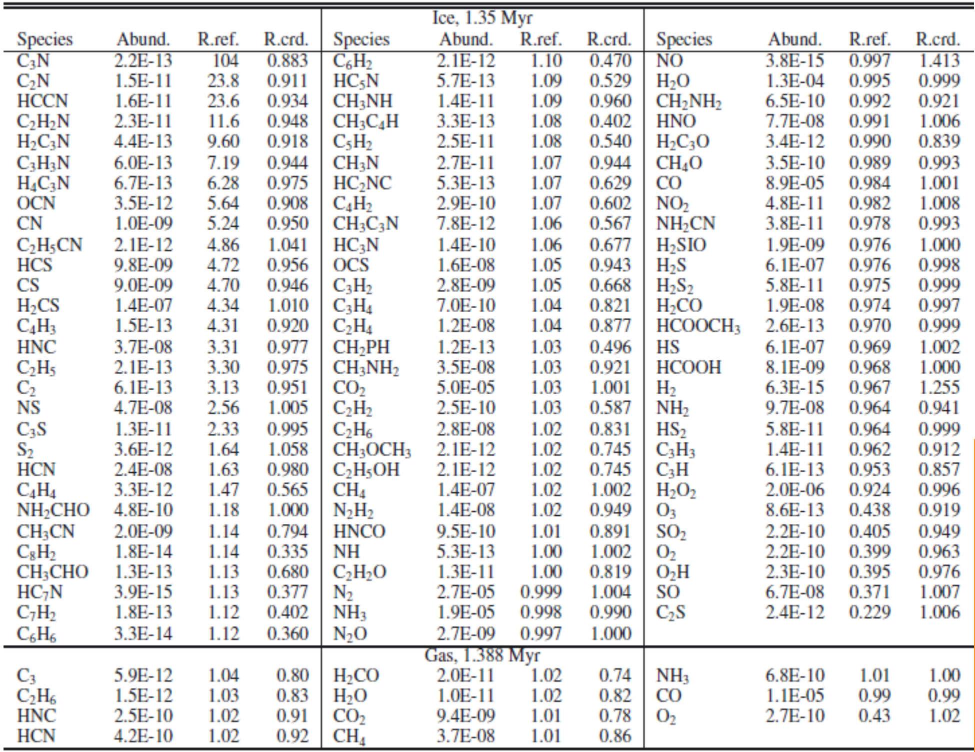


Fig. 6. Abundance, relative to hydrogen, of selected ice molecules in the combined model. The respective abundances from the reference model are shown for comparison.



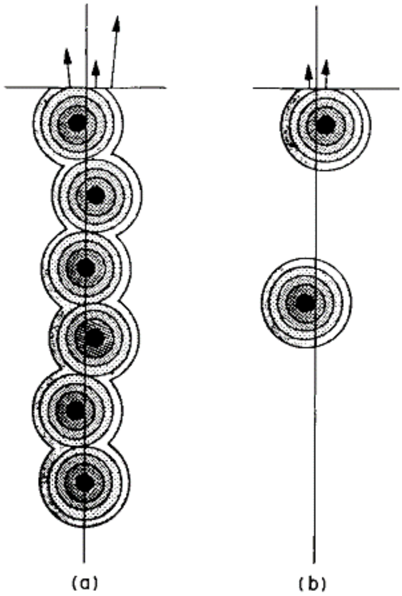
Ice, 1.35 Myr											
Species	Abund.	R.ref.	R.crd.	Species	Abund.	R.ref.	R.crd.	Species	Abund.	R.ref.	R.crd.
C_3N	2.2E-13	104	0.883	C_6H_2	2.1E-12	1.10	0.470	NO	3.8E-15	0.997	1.413
C_2N	1.5E-11	23.8	0.911	HC_5N	5.7E-13	1.09	0.529	H_2O	1.3E-04	0.995	0.999
HCCN	1.6E-11	23.6	0.934	CH_3NH	1.4E-11	1.09	0.960	CH_2NH_2	6.5E-10	0.992	0.921
C_2H_2N	2.3E-11	11.6	0.948	CH_3C_4H	3.3E-13	1.08	0.402	HNO	7.7E-08	0.991	1.006
H_2C_3N	4.4E-13	9.60	0.918	C_5H_2	2.5E-11	1.08	0.540	H_2C_3O	3.4E-12	0.990	0.839
C_3H_3N	6.0E-13	7.19	0.944	CH_3N	2.7E-11	1.07	0.944	CH_4O	3.5E-10	0.989	0.993
H_4C_3N	6.7E-13	6.28	0.975	HC_2NC	5.3E-13	1.07	0.629	CO	8.9E-05	0.984	1.001
OCN	3.5E-12	5.64	0.908	C_4H_2	2.9E-10	1.07	0.602	NO_2	4.8E-11	0.982	1.008
CN	1.0E-09	5.24	0.950	CH_3C_3N	7.8E-12	1.06	0.567	NH_2CN	3.8E-11	0.978	0.993
C_2H_5CN	2.1E-12	4.86	1.041	HC_3N	1.4E-10	1.06	0.677	H_2SIO	1.9E-09	0.976	1.000
HCS	9.8E-09	4.72	0.956	OCS	1.6E-08	1.05	0.943	H_2S	6.1E-07	0.976	0.998
CS	9.0E-09	4.70	0.946	C_3H_2	2.8E-09	1.05	0.668	H_2S_2	5.8E-11	0.975	0.999
H_2CS	1.4E-07	4.34	1.010	C_3H_4	7.0E-10	1.04	0.821	H_2CO	1.9E-08	0.974	0.997
C_4H_3	1.5E-13	4.31	0.920	C_2H_4	1.2E-08	1.04	0.877	$HCOOCH_3$	2.6E-13	0.970	0.999
HNC	3.7E-08	3.31	0.977	CH_2PH	1.2E-13	1.03	0.496	HS	6.1E-07	0.969	1.002
C_2H_5	2.1E-13	3.30	0.975	CH_3NH_2	3.5E-08	1.03	0.921	HCOOH	8.1E-09	0.968	1.000
C_2	6.1E-13	3.13	0.951	CO_2	5.0E-05	1.03	1.001	H_2	6.3E-15	0.967	1.255
NS	4.7E-08	2.56	1.005	C_2H_2	2.5E-10	1.03	0.587	NH_2	9.7E-08	0.964	0.941
C_3S	1.3E-11	2.33	0.995	C_2H_6	2.8E-08	1.02	0.831	HS_2	5.8E-11	0.964	0.999
S_2	3.6E-12	1.64	1.058	CH_3OCH_3	2.1E-12	1.02	0.745	C_3H_3	1.4E-11	0.962	0.912
HCN	2.4E-08	1.63	0.980	C_2H_5OH	2.1E-12	1.02	0.745	C_3H	6.1E-13	0.953	0.857
C_4H_4	3.3E-12	1.47	0.565	CH_4	1.4E-07	1.02	1.002	H_2O_2	2.0E-06	0.924	0.996
NH_2CHO	4.8E-10	1.18	1.000	N_2H_2	1.4E-08	1.02	0.949	O_3	8.6E-13	0.438	0.919
CH_3CN	2.0E-09	1.14	0.794	HNCO	9.5E-10	1.01	0.891	SO_2	2.2E-10	0.405	0.949
C_8H_2	1.8E-14	1.14	0.335	NH	5.3E-13	1.00	1.002	O_2	2.2E-10	0.399	0.963
CH_3CHO	1.3E-13	1.13	0.680	C_2H_2O	1.3E-11	1.00	0.819	O_2H	2.3E-10	0.395	0.976
HC_7N	3.9E-15	1.13	0.377	N_2	2.7E-05	0.999	1.004	SO	6.7E-08	0.371	1.007
C_7H_2	1.8E-13	1.12	0.402	NH_3	1.9E-05	0.998	0.990	C_2S	2.4E-12	0.229	1.006
C_6H_6	3.3E-14	1.12	0.360	N_2O	2.7E-09	0.997	1.000				
Gas, 1.388 Myr											
C_3	5.9E-12	1.04	0.80	H_2CO	2.0E-11	1.02	0.74	NH_3	6.8E-10	1.01	1.00
C_2H_6	1.5E-12	1.03	0.83	H_2O	1.0E-11	1.02	0.82	CO	1.1E-05	0.99	0.99
HNC	2.5E-10	1.02	0.91	CO_2	9.4E-09	1.01	0.78	O_2	2.7E-10	0.43	1.02
HCN	4.2E-10	1.02	0.92	CH_4	3.7E-08	1.01	0.86				

Conclusions

- Among the CR-induced surface processes, dissociation is probably the most important, behind desorption.
- Abundances of major icy species are affected by no more than 5-10 %. This determines the amount of atoms available for the synthesis of minor species.

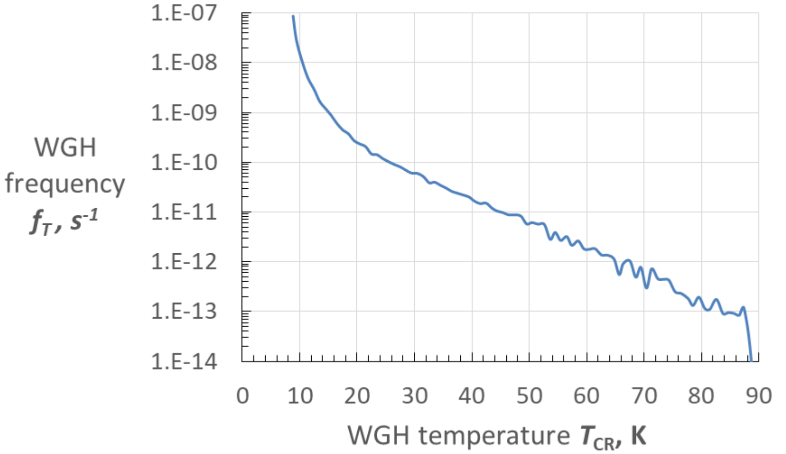
Problems, challenges, future

- This research has to be re-done with new CR spectra!
- More **experimental cross-sections** welcome for CR-induced dissociation; especially, for complex species.
- **Radiative grain cooling** must be considered: surface CO not available for grains in diffuse gas
- Grain heating by **light CR elements** to temperatures of 30-40 K occurs 100 times as often and is important!



Brown *et al.* 1984, NIMPB 2-3

- Whole-grain heating re-evaluated: 70 K is not the most efficient heating regime!



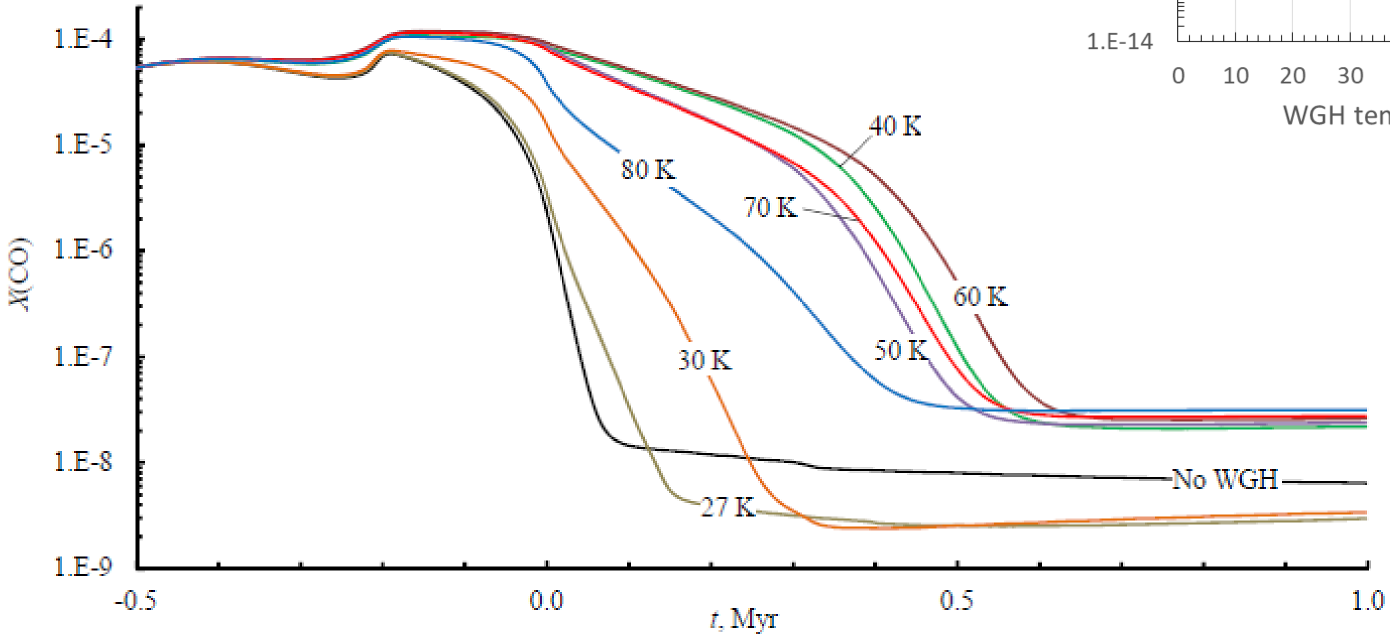


Figure 2. Calculated relative abundances of gas-phase CO for a model without CRD and models with different WGH temperatures $T_{\rm CR}$ as indicated.

Questions?

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