

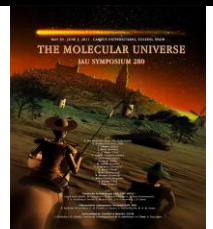
# Molecules in supernova ejecta

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# Overview

- Which supernovae ?
- Evidence for molecules from observations
- Modelling supernova ejecta: chemistry & mixing
- Results: molecules as tracers of dust synthesis?
- Conclusions

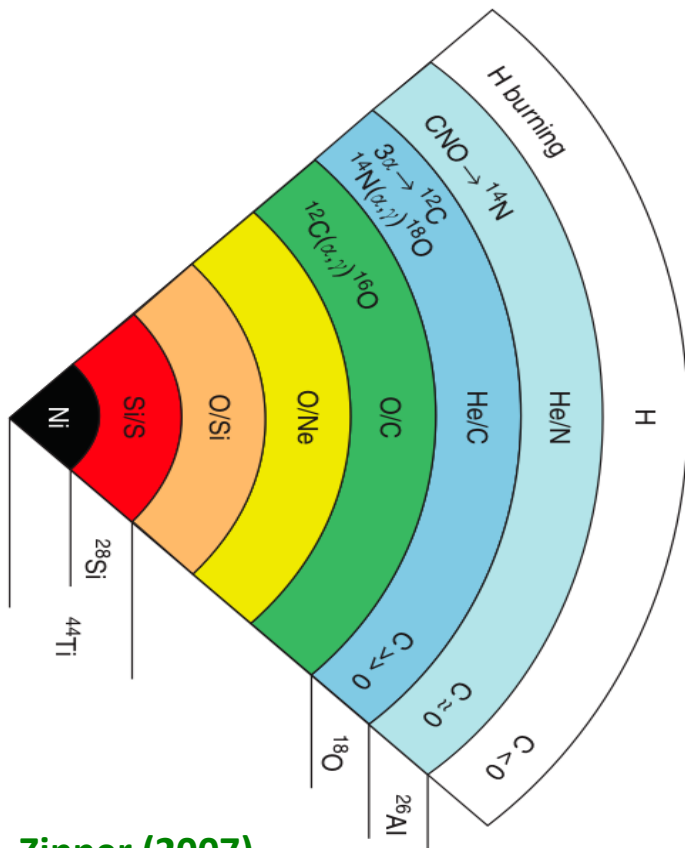
A ESF CoDustMas network collaboration – coll: ArkaprabhaSarangi  
[www.codustmas.eu](http://www.codustmas.eu)

# Which supernovae?

## Core-collapse Type II supernovae

Progenitors: blue/red supergiants – typical mass  $\sim 10 - 25 M_{\text{sun}}$

Pre-SN core



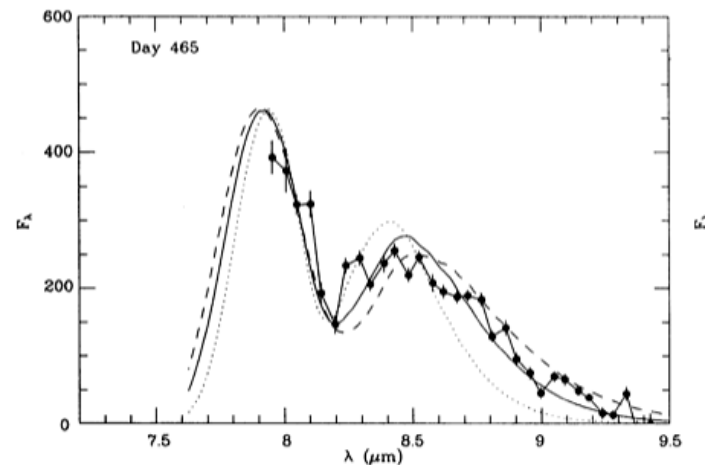
Zinner (2007)

- Few examples of type II supernovae: **SN1987A, SN2004dj, SN2005af**
- He core mass:  **$2 - 6 M_{\text{sun}}$**
- Explosion energy  $\sim$   **$1 \times 10^{51}$  ergs**
- Explosion nucleosynthesis products -  $^{56}\text{Ni}$  drives **radioactivity** in the ejecta
- Large uncertainties on the  $^{56}\text{Ni}$  mass and progenitor mass (e.g.,  $13 - 20 M_{\text{sun}}$  for SN2004et)

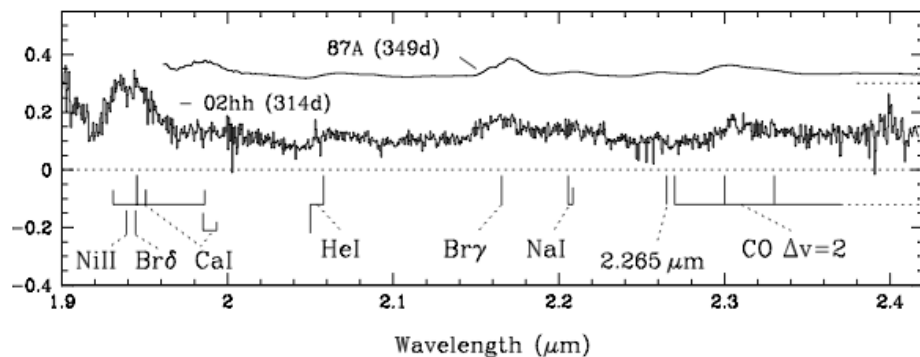
**Dust and molecule** formation observed in the infrared

# Evidence for molecules from observations

- SN1987A: IR detection of **CO**, **SiO** and dust [ $10^{-4}$  -  $10^{-3} M_{\text{sun}}$ ] from  $\sim$  **150 days** to  $\sim$  **800 days** post-explosion (Roche et al. 1991, Meikle et al. 1993, Ercolano et al. 2007)
- SN2005af: **CO** and **SiO** observed with Spitzer (Kotak et al. 2006)
- SN2004et: detection of **CO** and **SiO**, dust  $\sim 10^{-4} M_{\text{sun}}$  (Kotak et al. 2009)
- SN2003gd, SN2004dj: dust observed with Spitzer -  $10^{-2} M_{\text{sun}}$  -  $4 \cdot 10^{-5} M_{\text{sun}}$  (Sugerman et al. 2006, Meikle et al. 2007)



SN1987A: SiO fundamental  $\Delta v=1$  ro-vibrational bands from 7.5-9.5  $\mu\text{m}$  (Roche et al. 1991)



SN2002hh: CO  $\Delta v=2$  1st overtone band detection with Spitzer (Pozzo et al. 2006)

# Evidence for molecules from observations

Molecules observed in SNRs: 330 years old remnant Cas A

Observation of the CO  
2.29  $\mu\text{m}$  first overtone  
with Spitzer

(Rho et al. 2008)

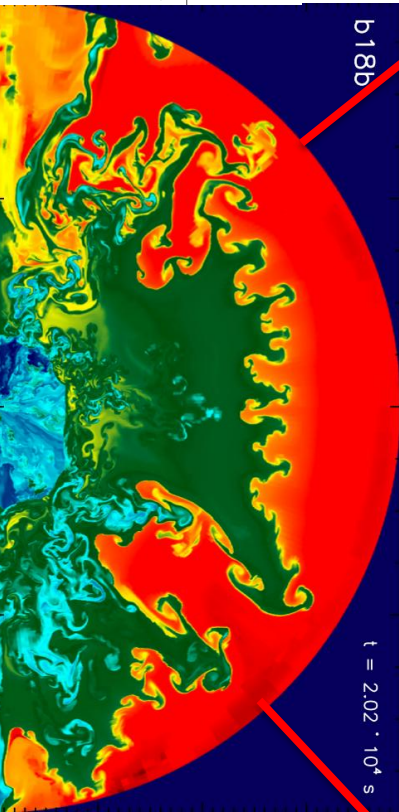
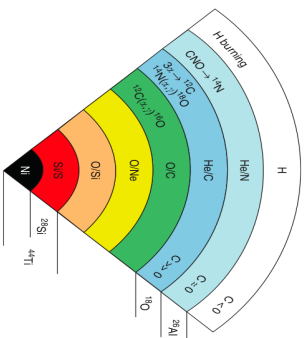
Evidence for  $\sim 0.08 M_{\text{sun}}$   
of ejecta dust with  
Herschel (Barlow et al. 2010)



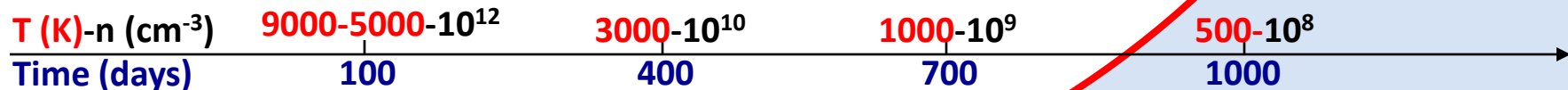
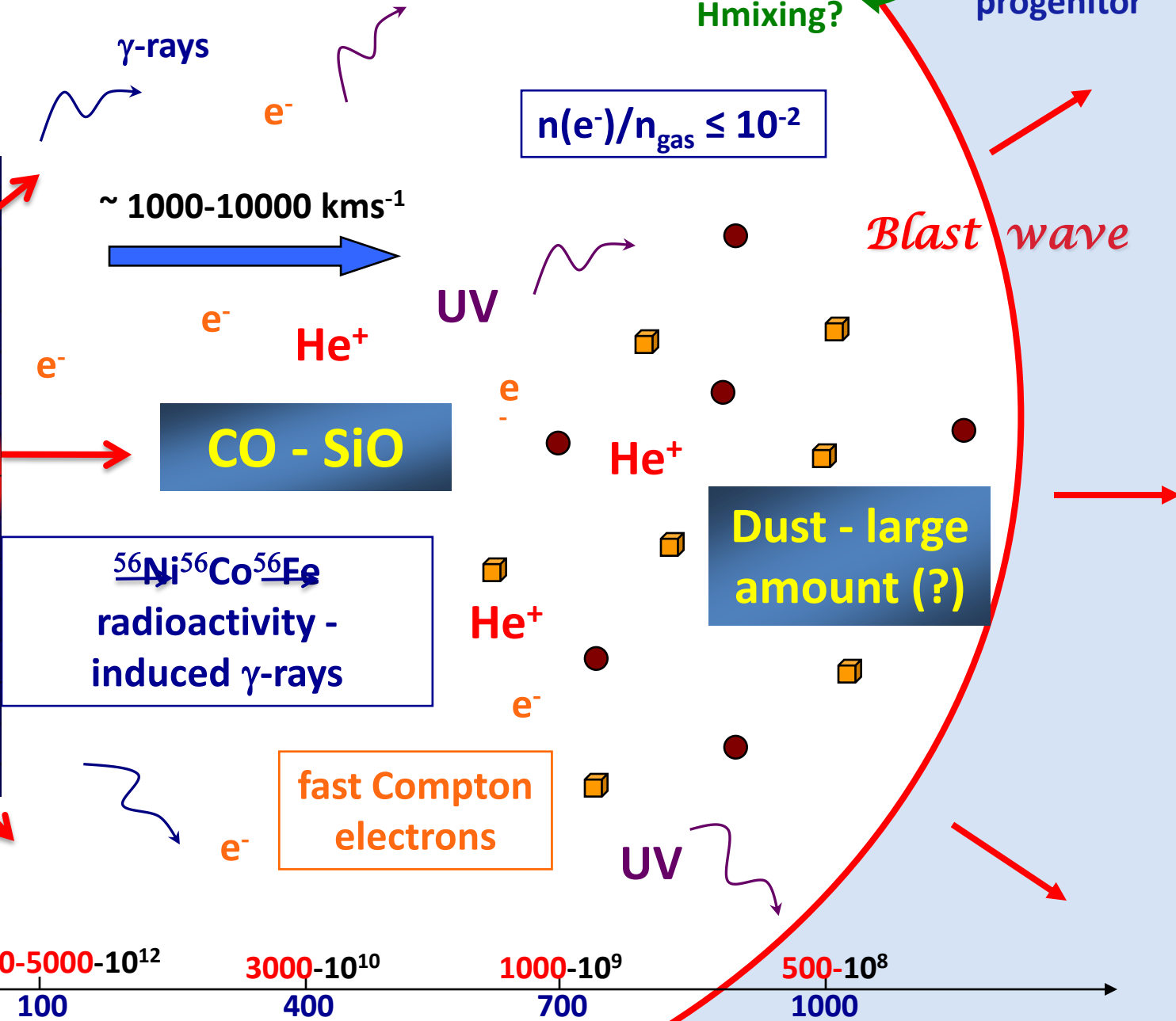
In supernova ejecta, the formation of CO and SiO (90 – 200 days)  
precedes the observation of dust (> 300 days)

**Are molecules tracers of dust formation ?**

# Supernova ejecta - 10- 25 M<sub>sun</sub>



5 h post-explosion  
Kifonidis et al. (2006)



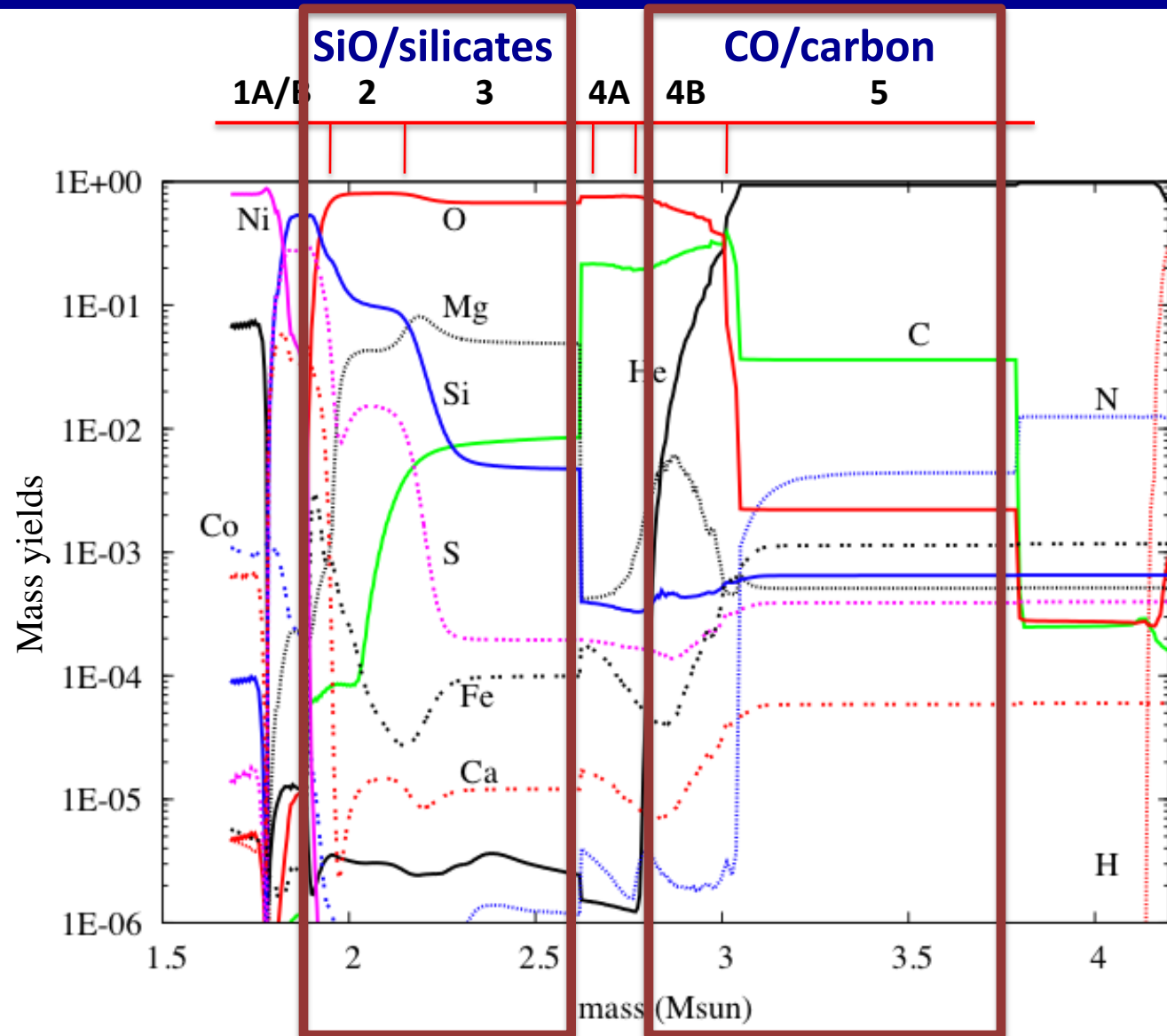
# Modelling supernova ejecta: chemistry & mixing

15  $M_{\text{sun}}$  progenitor  
He core zoning

- 1A: Fe/Si/S
- 1B: Si/S/Ca
- 2: O/Si/Mg
- 3: O/Mg/C/Si
- 4A: O/C
- 4B: O/C/He
- 5: He/C/Si

Yields can greatly vary depending on explosion models!

(Weaver & Woosley 1995, Umeda & Nomoto 2002, Heger et al. 2004)



Rauscher et al. (2002)

# Modelling supernova ejecta: chemistry & mixing

**Previous studies:** Molecule formation in SN1987A

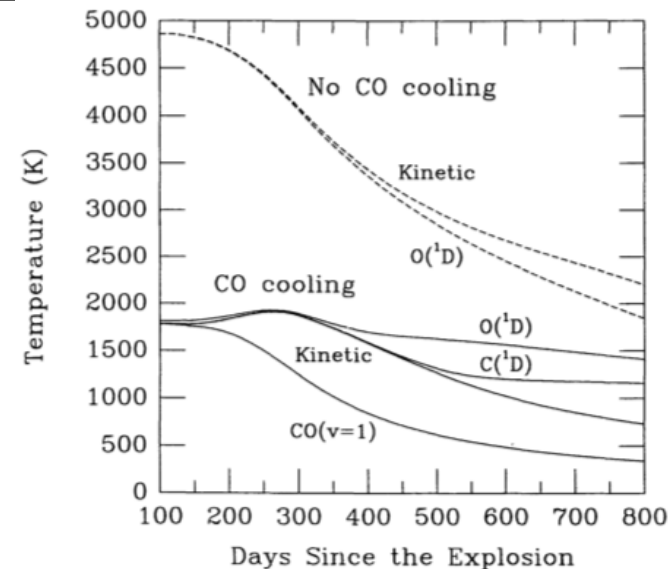
Petuchowski et al 1989 - Lepp, Dalgarno & McCray 1990 -  
Liu, Dalgarno & Lepp (1992) - Liu & Dalgarno (1994, 1995) - Gearhart  
et al. (1999)

Prevalent processes:

- radiative association reaction for formation of molecules
- dissociation/ionisation by Compton electrons as destruction

- No molecule can form when  $\text{He}^+$  is present
- Molecules are important coolants: e.g., CO

Oxygen core - Liu & Dalgarno (1995)





# Modelling supernova ejecta: chemistry & mixing

## Physics:

- 15-20  $M_{\text{sun}}$  progenitor – Explosion energy:  $\sim 10^{51}$  erg – 0.075  $M_{\text{sun}}$  of  $^{56}\text{Ni}$  (SN1987A)
- Temperature and density derived from **homogeneous** explosion models of **Nozawa et al. (2010)**:
- Compton electrons induced by  $\gamma$ -rays degradation
- UV field (10% of  $\gamma$ -rays - **Kozma&Fransson (1992)**)

## Chemistry: high temperature & high density

Formation processes: termolecular, neutral-neutral (activation barriers), radiative association, ion-molecules, charge exchange

Destruction processes: thermal fragmentation, neutral-neutral, dissociation/ionisation by Compton  $e^-$  and UV photons, charge exchange

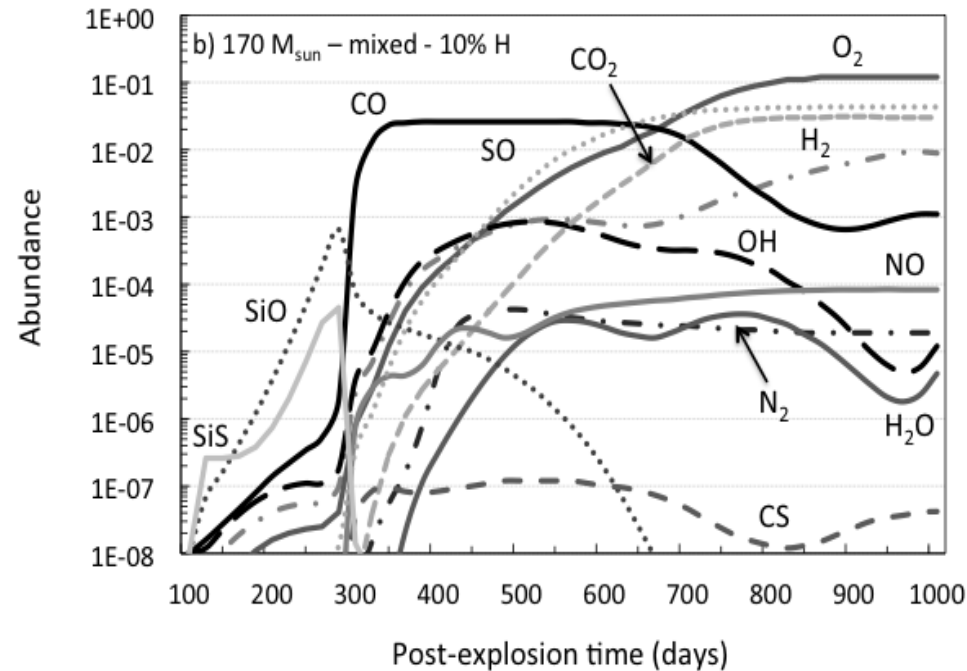
# Modelling supernova ejecta: chemistry & mixing

If hydrogen microscopically-mixed, species like **OH**, **CO<sub>2</sub>** or **H<sub>2</sub>O** should form and be observed...

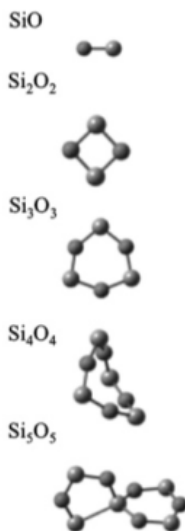
So far, only CO and SiO

**H** → free “poor” chemistry

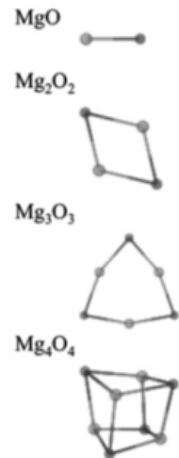
Cherchneff&Dwek (2009, 2010)



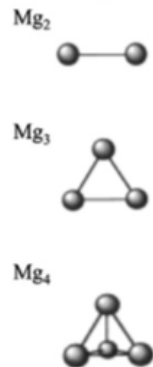
## Silicon monoxide



## Magnesium oxide



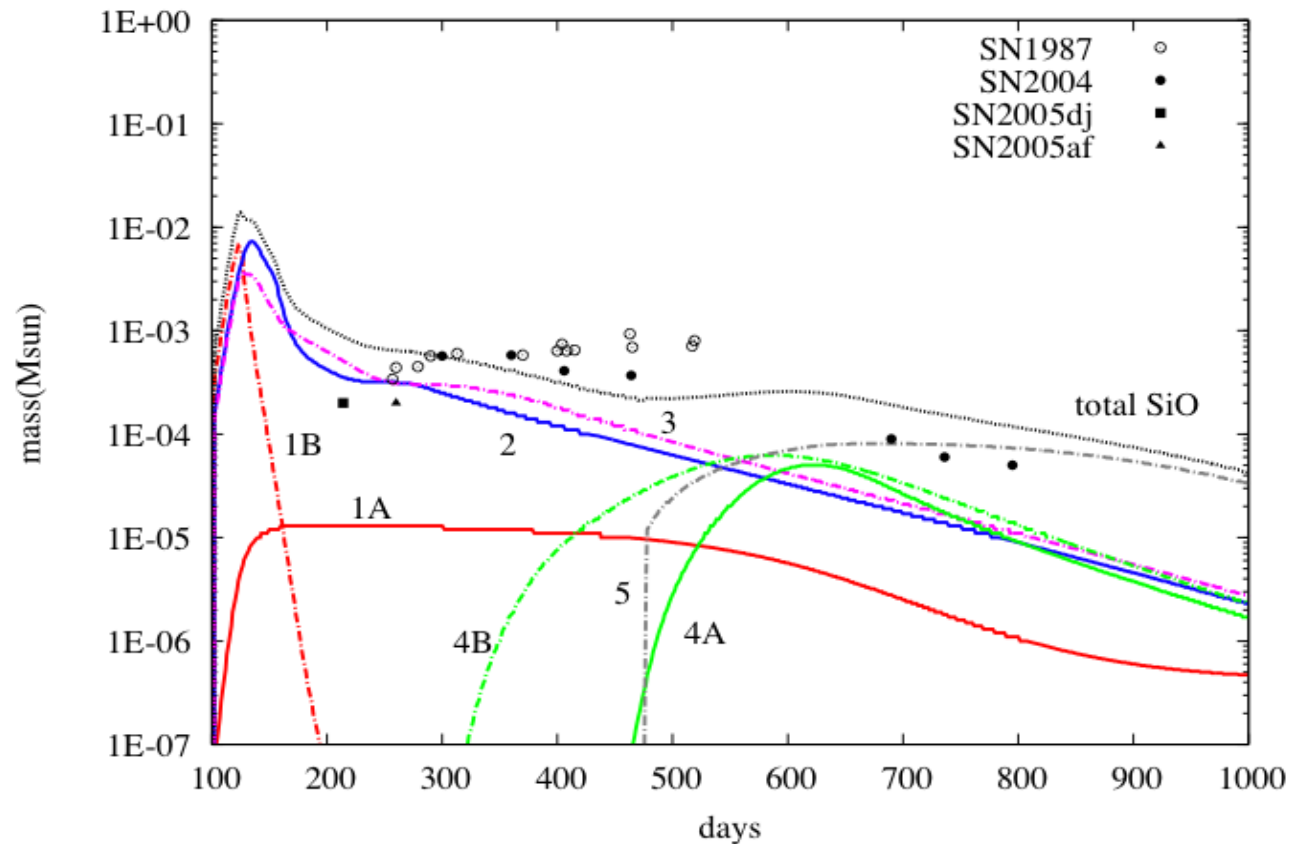
## Pure magnesium



Molecules considered:  
 CO, SiO, SiS, CS, S<sub>2</sub>, SO, O<sub>2</sub>, CO<sub>2</sub>, NO  
 Small clusters and  
 carbon chains/rings

# Results: molecules as tracers of dust synthesis?

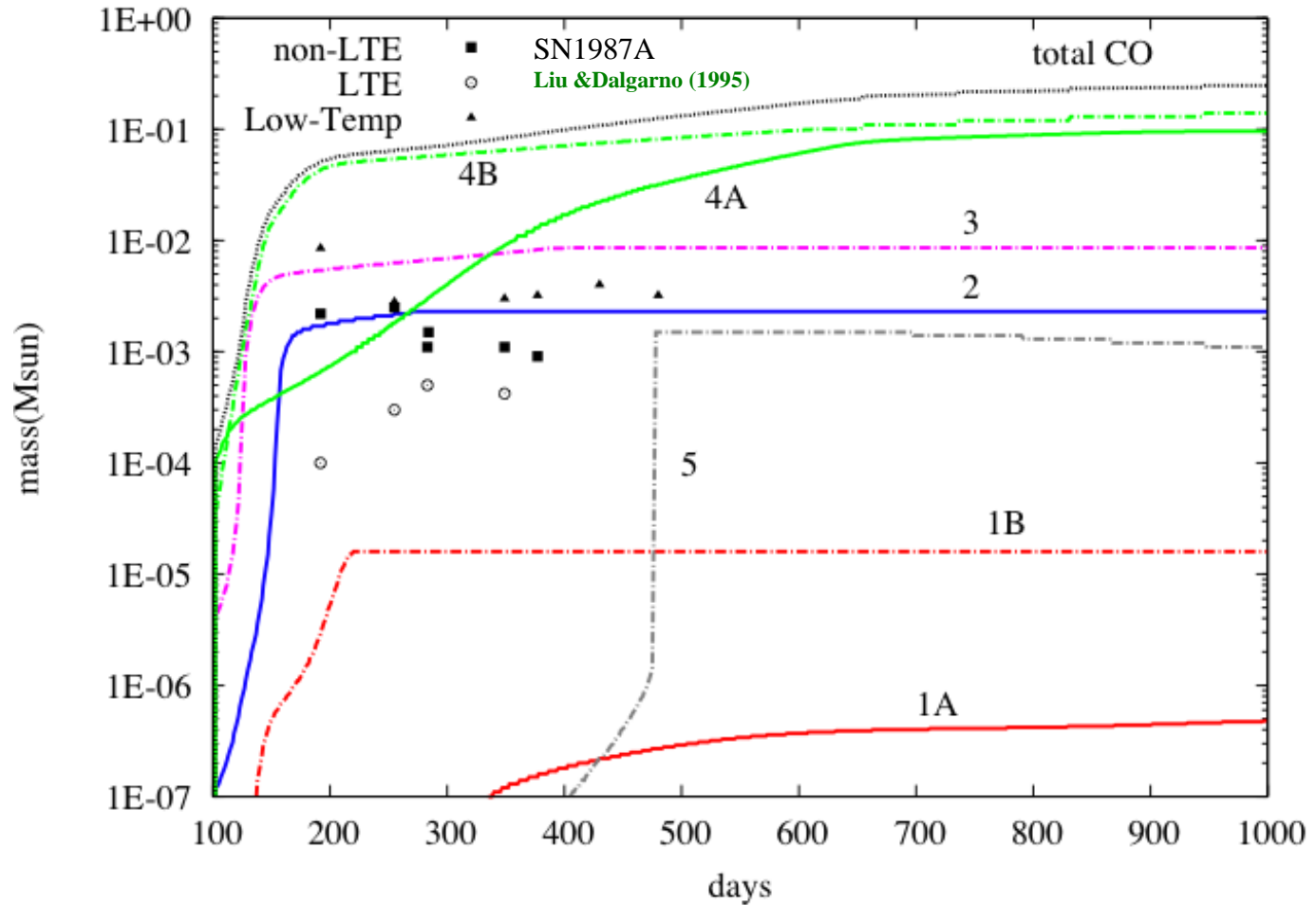
## SiO



- Formation by neutral-neutral & radiative association reactions
- Destruction by thermal fragmentation, Compton  $e^-$ , and cluster formation
- SiO masses are in **good agreement** with observations  $\longrightarrow$  **rapid formation of silica clusters** in innermost mass zones – **SiO tracer!**

# Results: molecules as tracers of dust synthesis?

CO

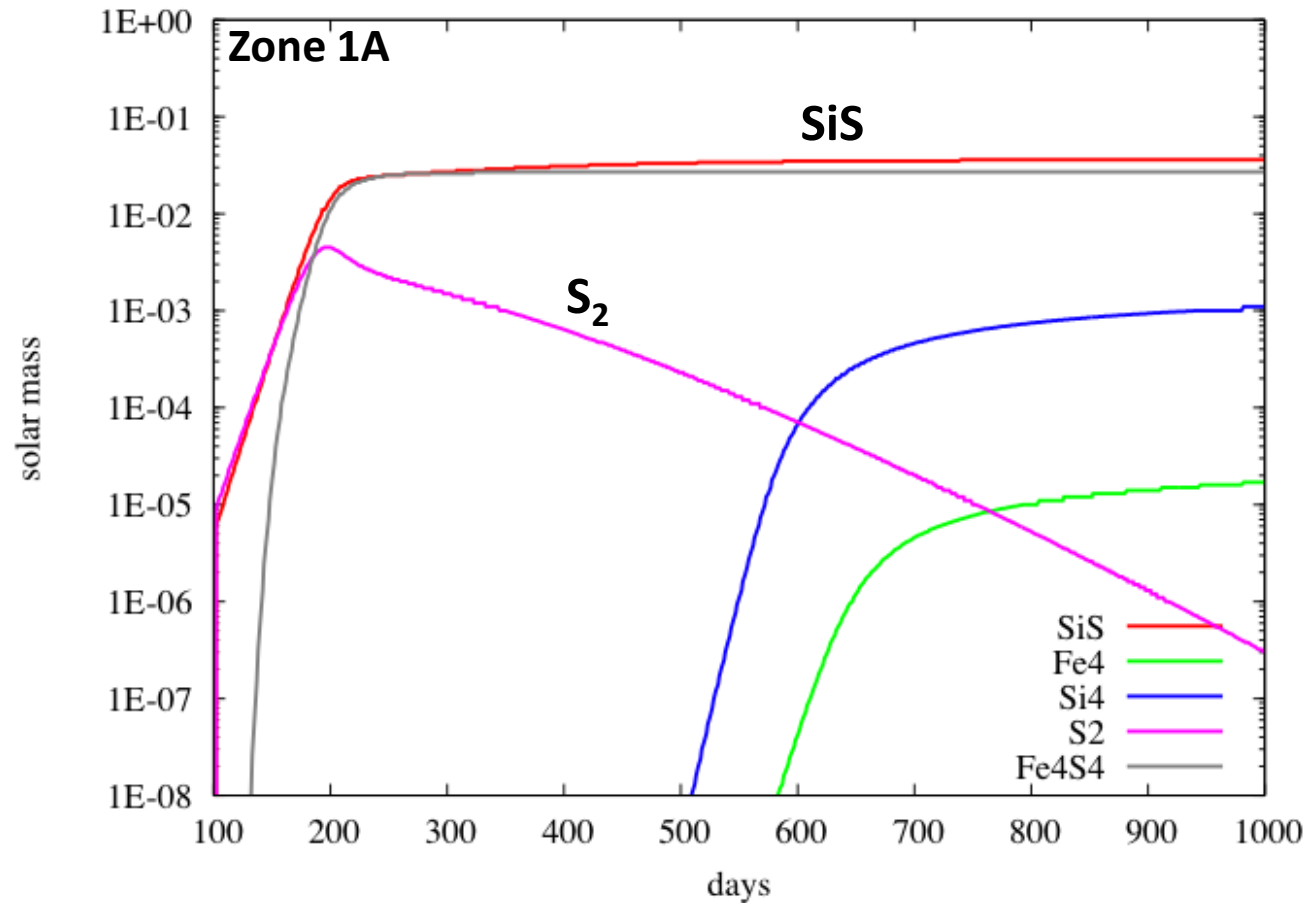


- Formation by neutral-neutral ( $O + C_2 \rightarrow CO + C$ ) and R.A. reactions
- Destruction by  $He^+$  and neutral-neutral reactions
- CO formation as **efficient** as that of SiO but in **different zones** (4A/B)
- **No direct tracer** of dust formation

# Results: molecules as tracers of dust synthesis?

## Other molecules:

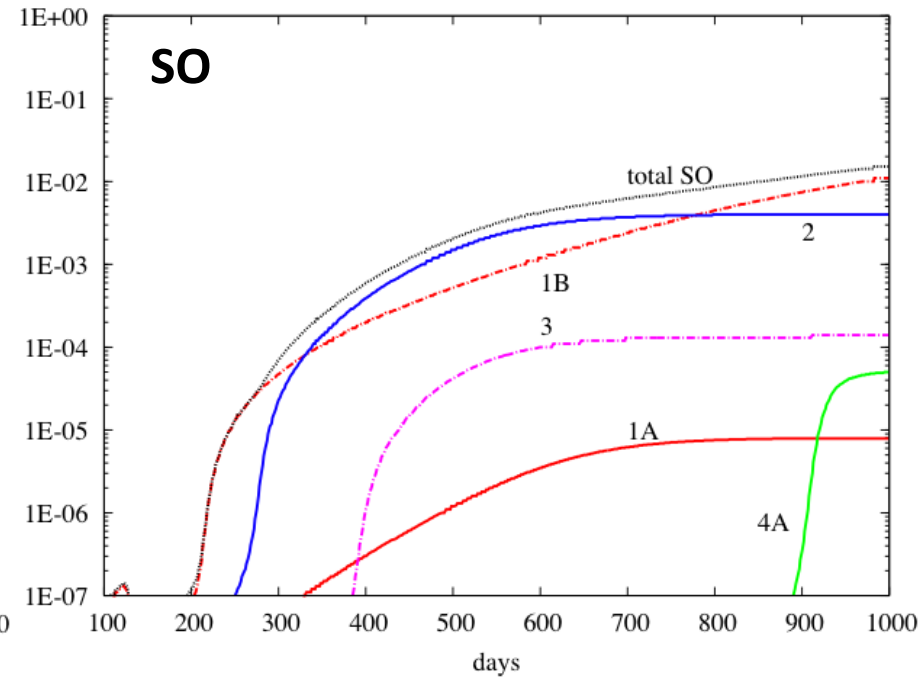
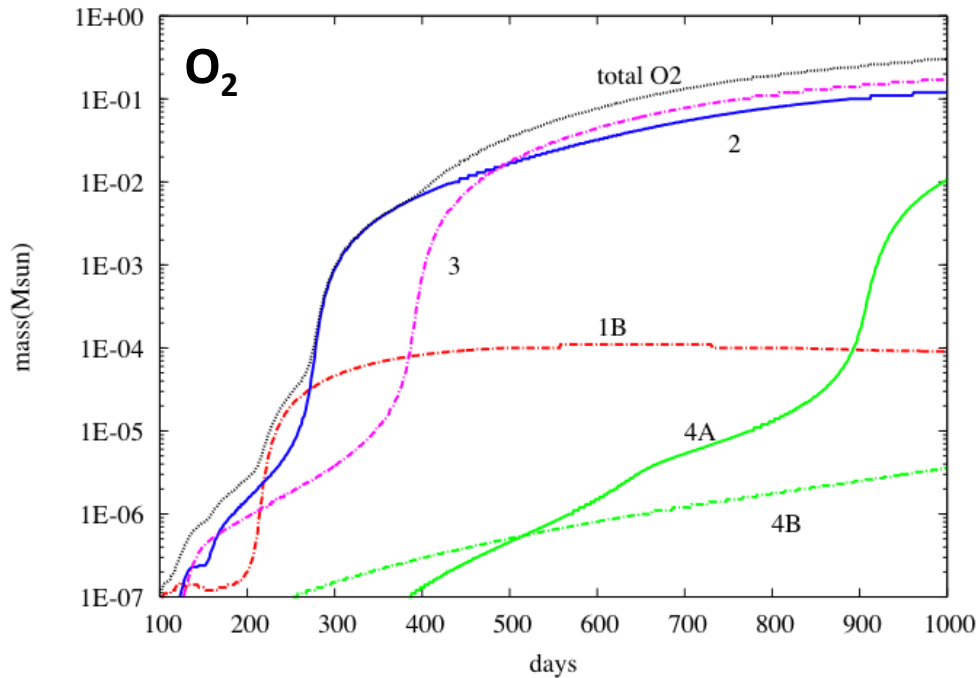
### SiS



- Formation by neutral-neutral and R.A. reactions
- However, **very few rates** – rely on estimated values
- SiS is very efficiently formed and **should be observable** in the IR or in the submm in very young supernova remnants

# Results: molecules as tracers of dust synthesis?

## Other molecules: O<sub>2</sub> and SO



- Formation by neutral-neutral processes – SO related to O<sub>2</sub> via  $S + O_2 \rightarrow SO + O$  in zone 2 (oxygen zone)

# Modelling supernova ejecta: chemistry & mixing

## Summary of molecular budget

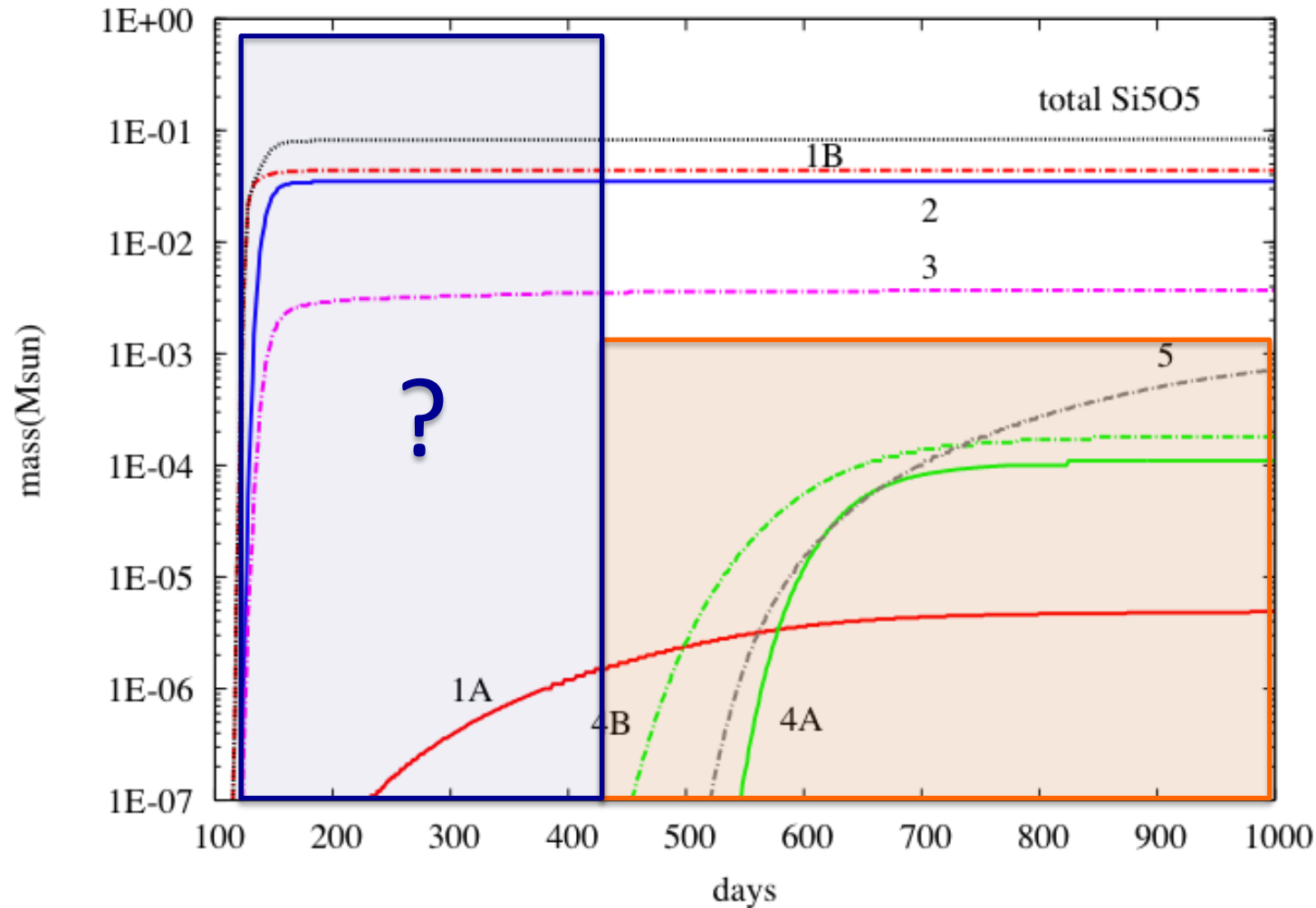
SiO							
CO							
SIS							
O <sub>2</sub>							
SO							
(SiO) <sub>5</sub>							
C <sub>10</sub>							
$m(M_{\text{sun}})$	1.78 - 1.9	1.9 - 1.98	1.98 - 2.3	2.3 - 2.6	2.6 - 2.8	2.8 - 3	3 - 3.8
$M_{\text{zone}}$	0.1	0.095	0.29	0.35	0.19	0.23	0.75
Zone	1A	1B	2	3	4A	4B	5

Molecules are chemical signatures of the various zones in the supernova ejecta

Ejecta molecular phase ~ 30% of ejected mass

# Results: molecules as tracers of dust synthesis?

## SiO clusters

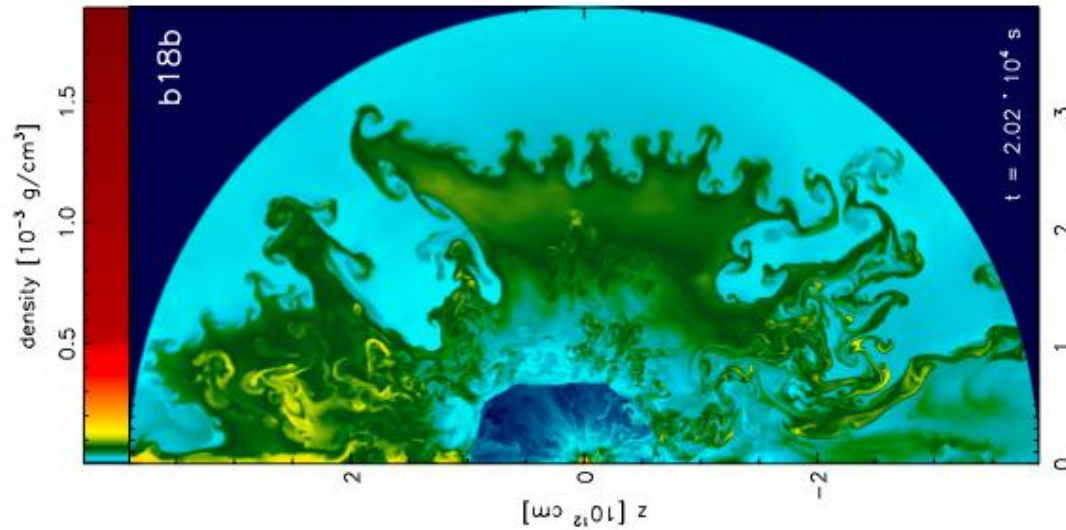


In the infrared, **small dust masses** (silicates + AC) **detected**:  
 $10^{-5} - 10^{-2} M_{\text{sun}}$

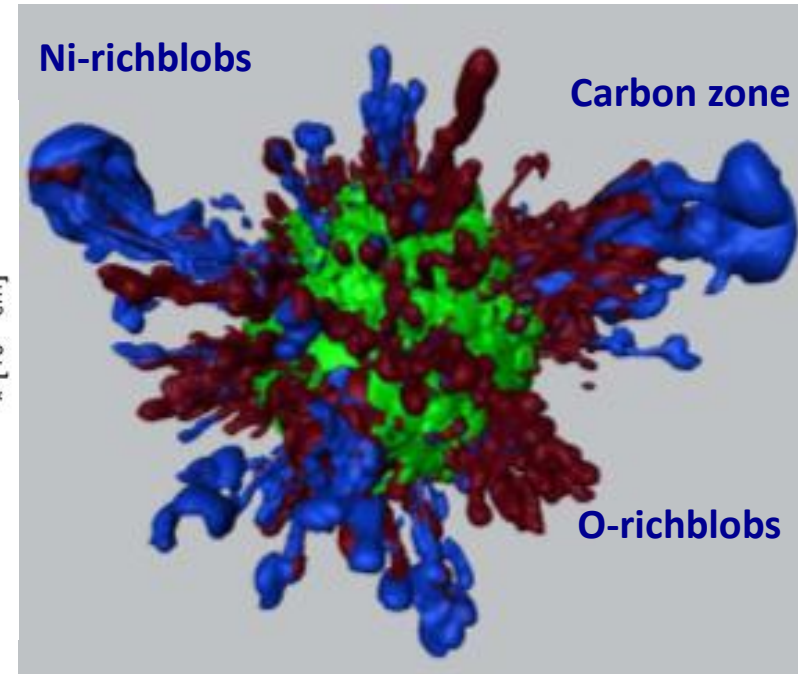


# Results: molecules as tracers of dust synthesis?

## Mixing due to Rayleigh-Taylor instabilities



Kifonidis et al. (2006)



Hammeret al. (2010)

- Early fragmentation of the ejecta— fragments have various velocities
- Homogeneities (blobs, filaments) may have **very different density & temperature histories** than homogeneous flows

**Next step:** follow the chemistry in 3D blobs + condensation of clusters

# Conclusions

- **Efficient formation of molecules** in supernova ejecta
- Prevalent molecules: **O<sub>2</sub>, CO, SO&SiS** - ~ 30% of ejecta
- Agreement of predicted **SiO** masses with observations  
→ implies SiO depletion in ~ 0.1 M<sub>sun</sub> of silica precursors – SiO is a good **dust formation tracer**
- Carbon rings (C<sub>10</sub>) form when no He<sup>+</sup>
- Need for high T chemical rates of key reactions
- Need to model **the chemistry of 3D ejecta fragments** to reconcile predicted dust masses with IR observations

**Implication for the dust and molecular budget of the early universe!**