The molecular chemistry of supernovae

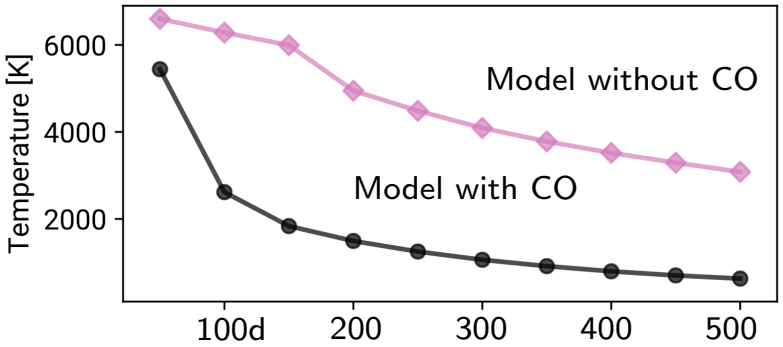
Anders Jerkstrand & Sofie Liljegren

Department of Astronomy, Stockholm University

Why are molecules important?

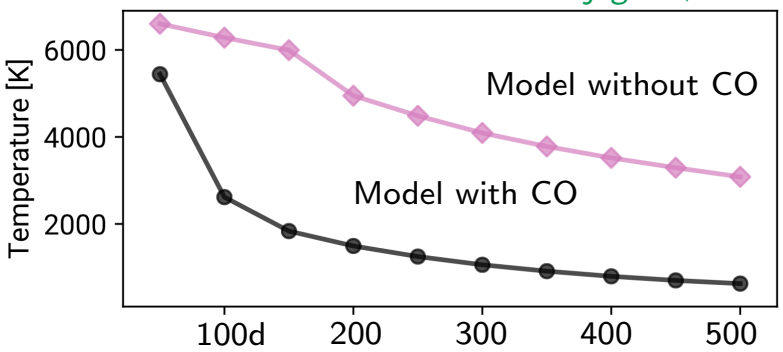
- More efficient coolants than atoms
- $\rightarrow$ can change temperature drastically.

Liljegren+2020



Why are molecules important?

Liljegren+2020

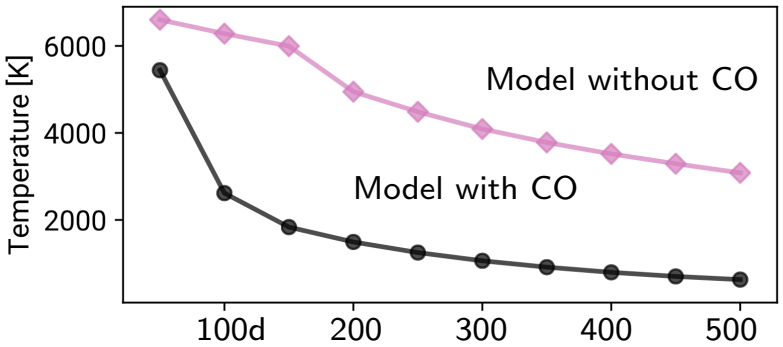


- More efficient coolants than atoms
- $\rightarrow$ can change temperature drastically.

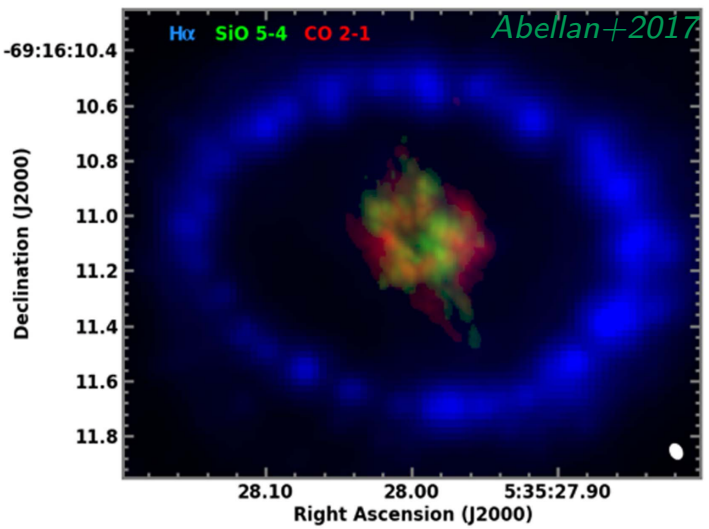
- Governs when and how dust forms by
  - Locking up dust ingredients.
  - Determining when the temperature falls below the dust formation threshold (1000 – 2000 K).

Why are molecules important?

Liljegren+2020

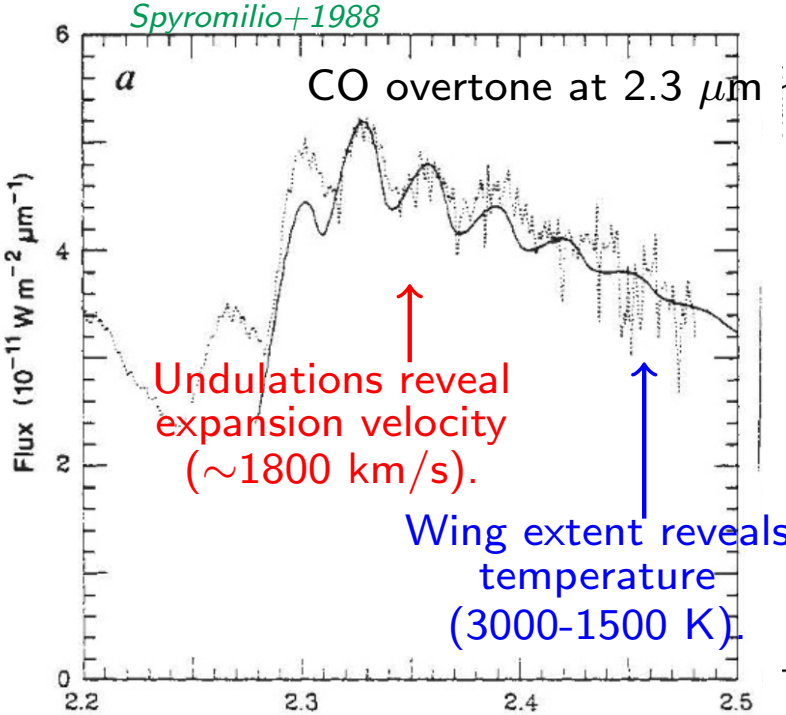


- More efficient coolants than atoms → can change temperature drastically.
- Governs when and how dust forms by
  - Locking up dust ingredients.
  - Determining when the temperature falls below the dust formation threshold (1000 – 2000 K).
- Their molecular IR and radio emission (ALMA, JWST) may be used to probe mixing and morphology.



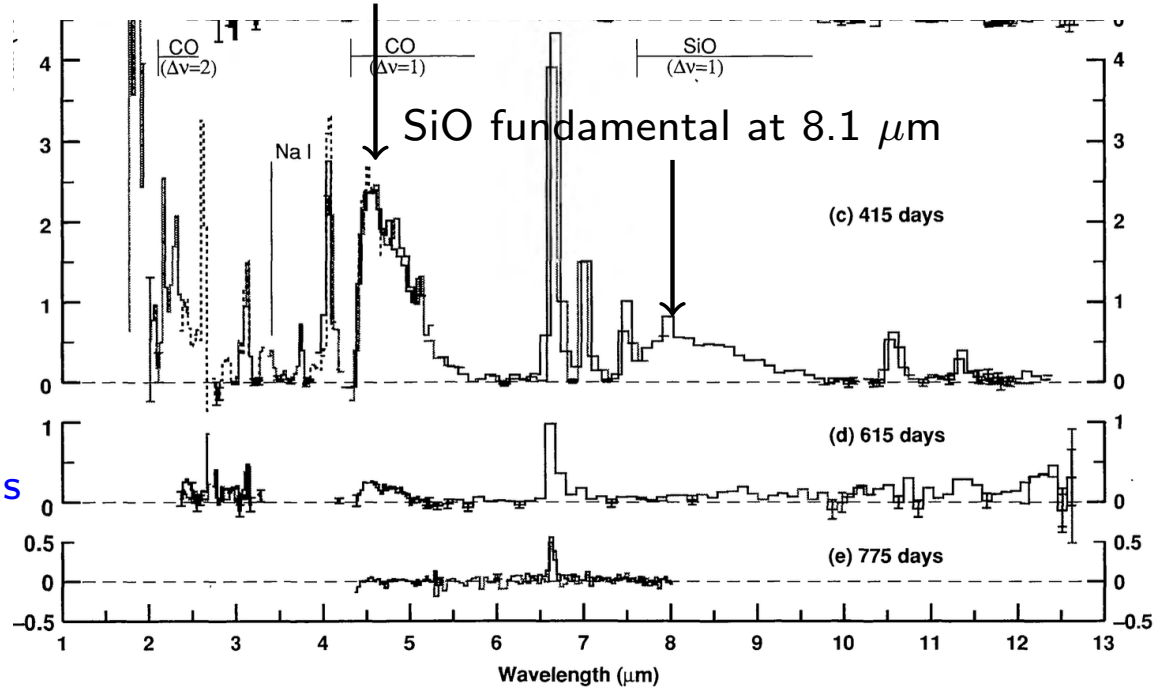
SN 1987A : First detection of molecules in SNe

Spyromilio+1988

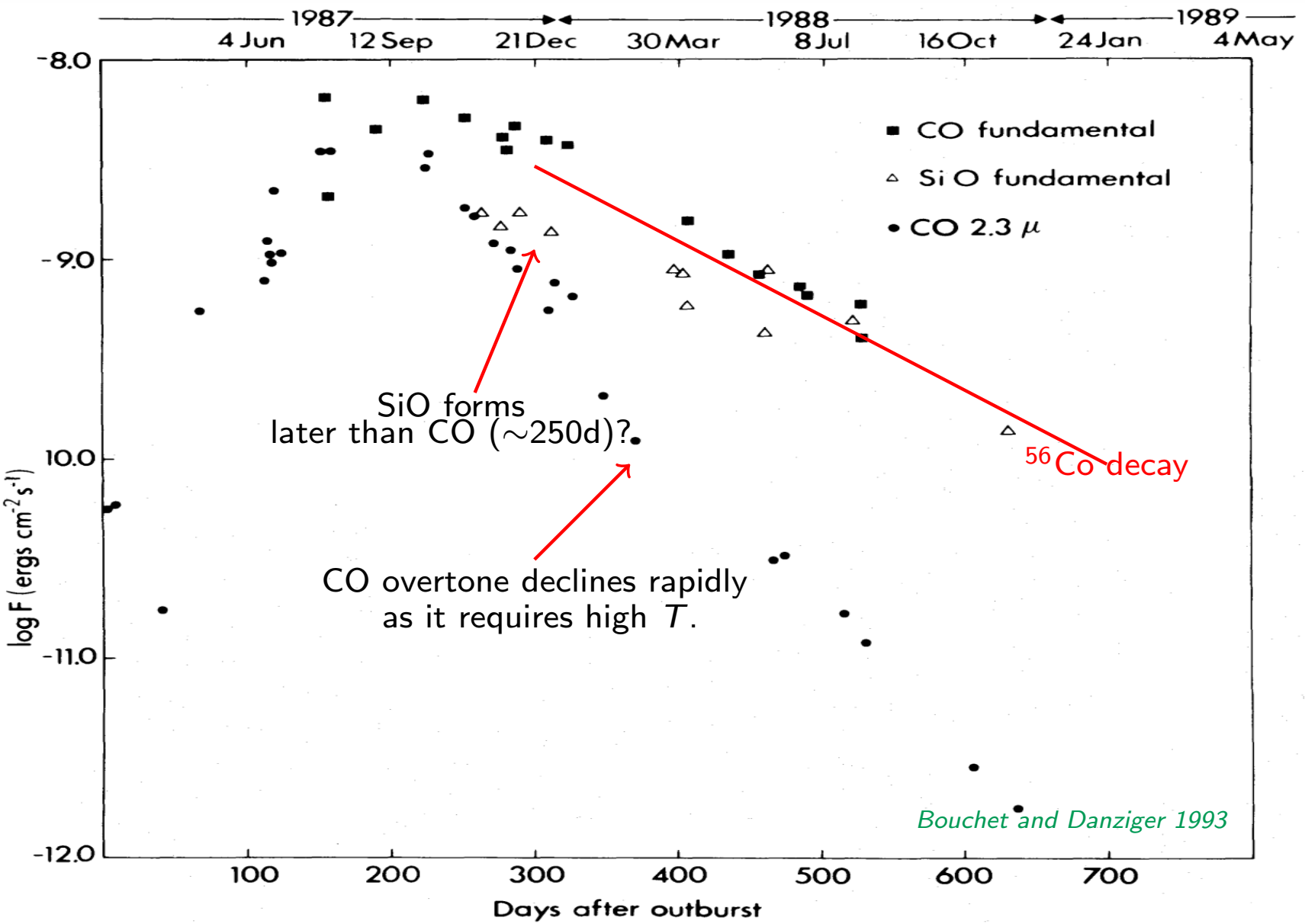


CO fundamental at 4.6 μm

Wooden+1993



SN 1987A : First detection of molecules in SNe



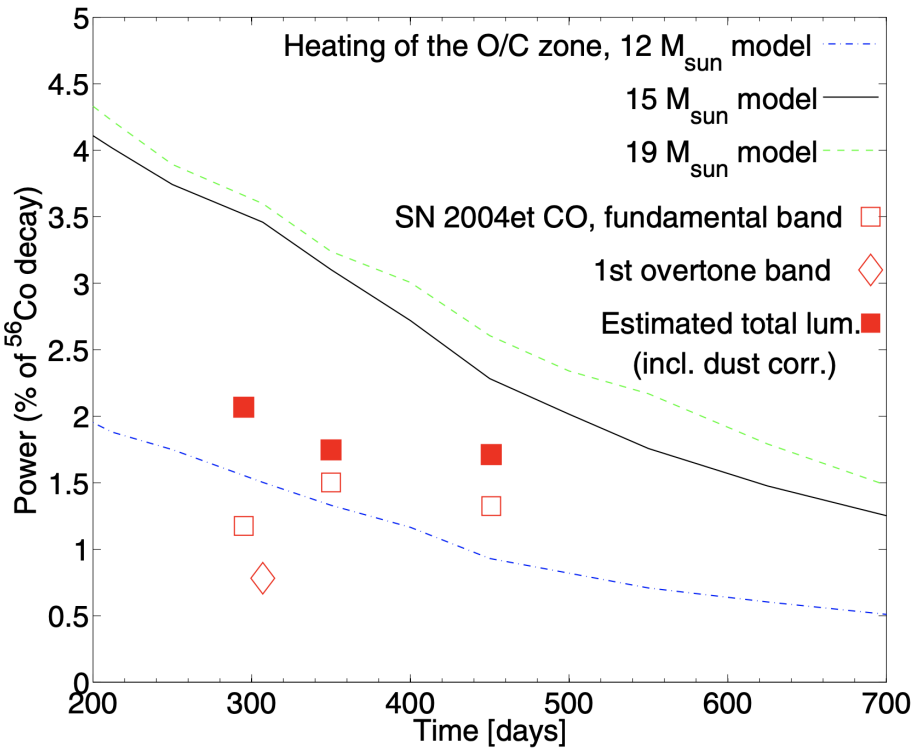
Observations of molecules in other SNe

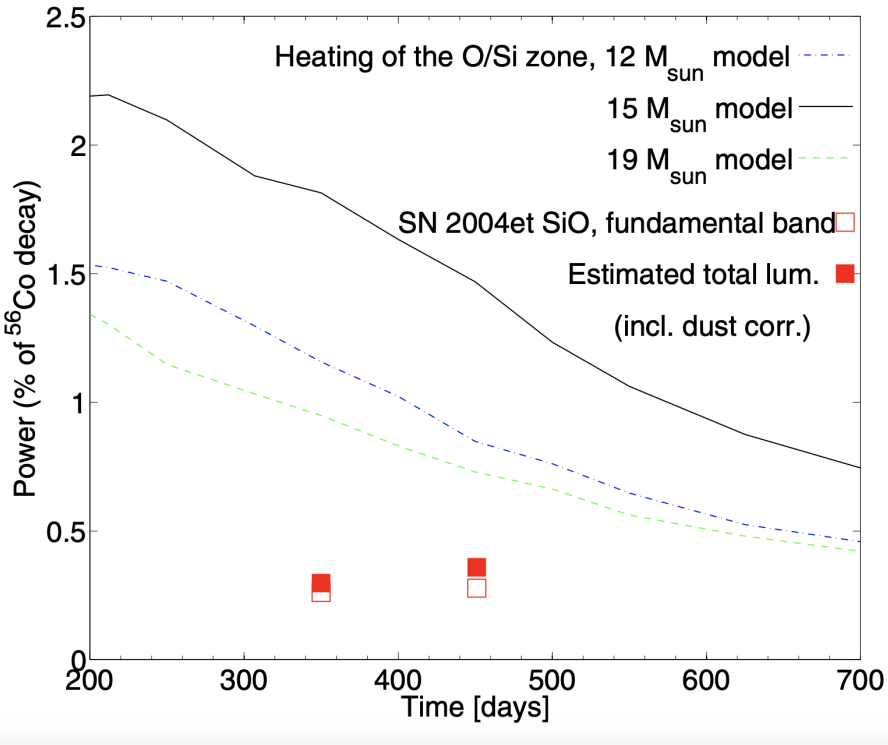
SN	CO 2.3μm	CO 4.6μm	SiO 8.1μm	Reference
Type IIP/pec:				
SN 1987A	x	x	x	Spyromilio+1988, many others
SN 1995ad	x			Spyromilio & Leibundgut 1996
SN 1998dl	x			Spyromilio 2001
SN 1999em	x			Spyromilio 2001
SN 2002hh	x			Pozzo+2006
SN 2004dj	x	x*		Kotak+2005, Szalai+2011
SN 2004et	x	x*	x	Kotak+2009
SN 2005af		x*	x	Kotak+2006
SN 2017eaw	x			Rho+2018
Type IIn:				
SN 1998S	x			Gerardy+2000, Fassia+2001
Type Ib/Ic/IIb:				
SN 2000ew	x			Gerardy+2002
SN 2007gr	x			Hunter+2007
SN 2011dh	x			Ergon+2015
SN 2013ge	x			Drout+2016
SN 2020oi	x			Rho+2020

*Adapted (and expanded) from Cherchneff & Sarangi 2011. * = right side of band.*

Observations of molecules in other SNe

- **SN 2004et** (Kotak+2009) is the only other SN than 1987A where we have complete information about the molecular cooling. Only reemits a moderate fraction of the powering of the O-rich zones.

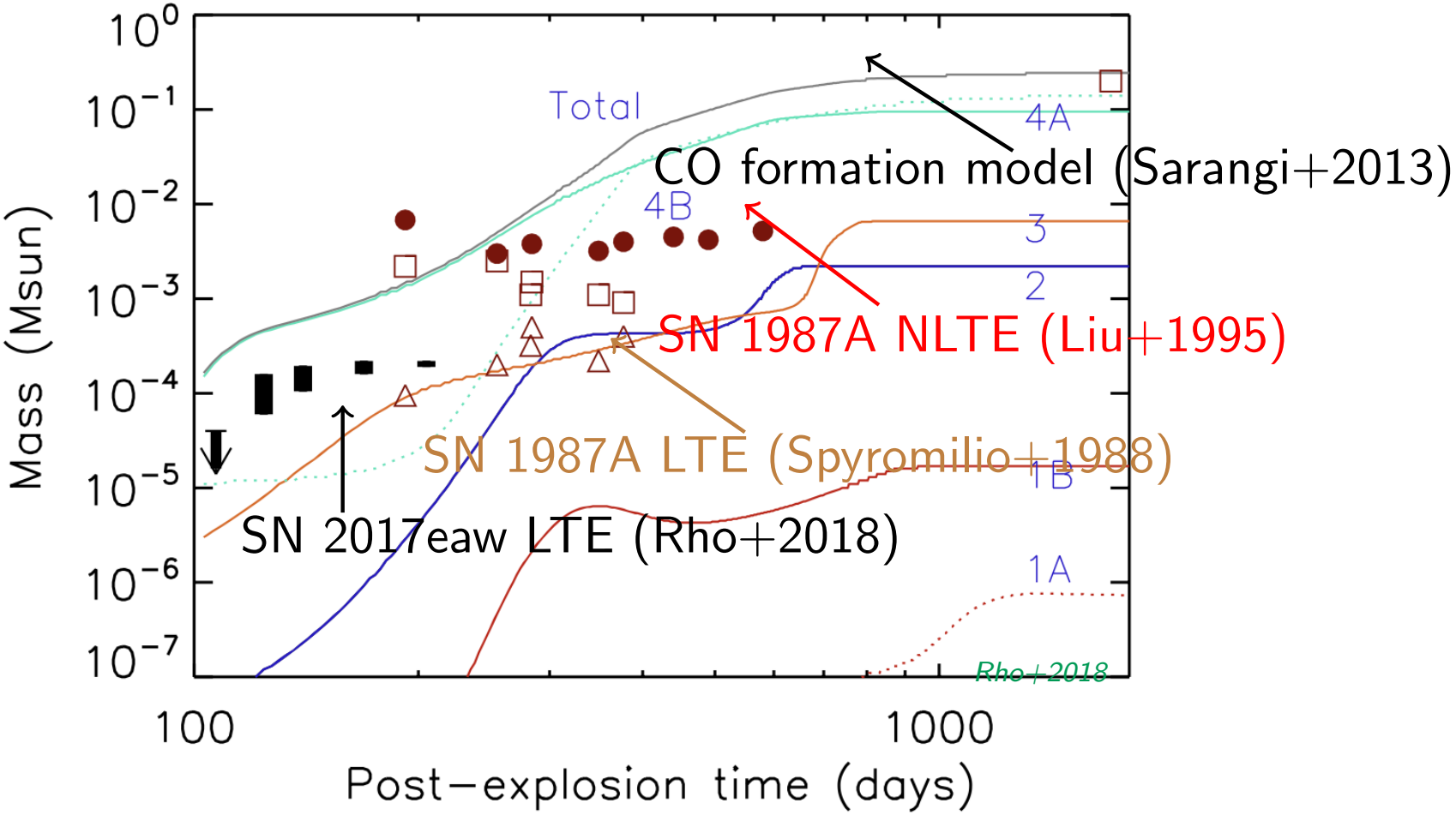




Jerkstrand+2012

Inferred CO masses in SN 1987A and SN 2017eaw

Other SNe have yielded similar estimates.



- There is about 0.1 $M_\odot$ of C available in the O/C zone, 10^{-3} $M_\odot$ in the H-zone..*which zone makes the CO?*

The physics of CO formation, and implementation into the SUMO code *Liljegren+2020,2022*

Currently SUMO has a chemical network of 22 molecules, 115 chemical reactions. Four molecules (CO, SiO, SiS, SO) are part of the time-dependent NLTE machinery.

Reaction	Example	Comment
Formation		
Radiative association	$C + O \rightarrow CO + h\nu$	C mostly ionized in the H, He zone
Formation or destr.		
Neutral-neutral	$C + O_2 \leftrightarrow CO + O$	
Charge exchange	$CO^+ + O \leftrightarrow CO + O^+$	
Destruction		
Compton electrons	$CO + e^-_{fast} \rightarrow C + O, CO^+$	
UV dissociation		To be added.
He^+ attack	$CO + He^+ \rightarrow He + C^+ + O$	Prevents formation in He-zone.

See also Petuchowski 1989, Lepp 1990, Liu 1992,1995,1996, Gearhart 1999, Cherchneff 2008,2009,2010, Sarangi 2013,2015, Höflich (e.g. in Rho 2021,..)

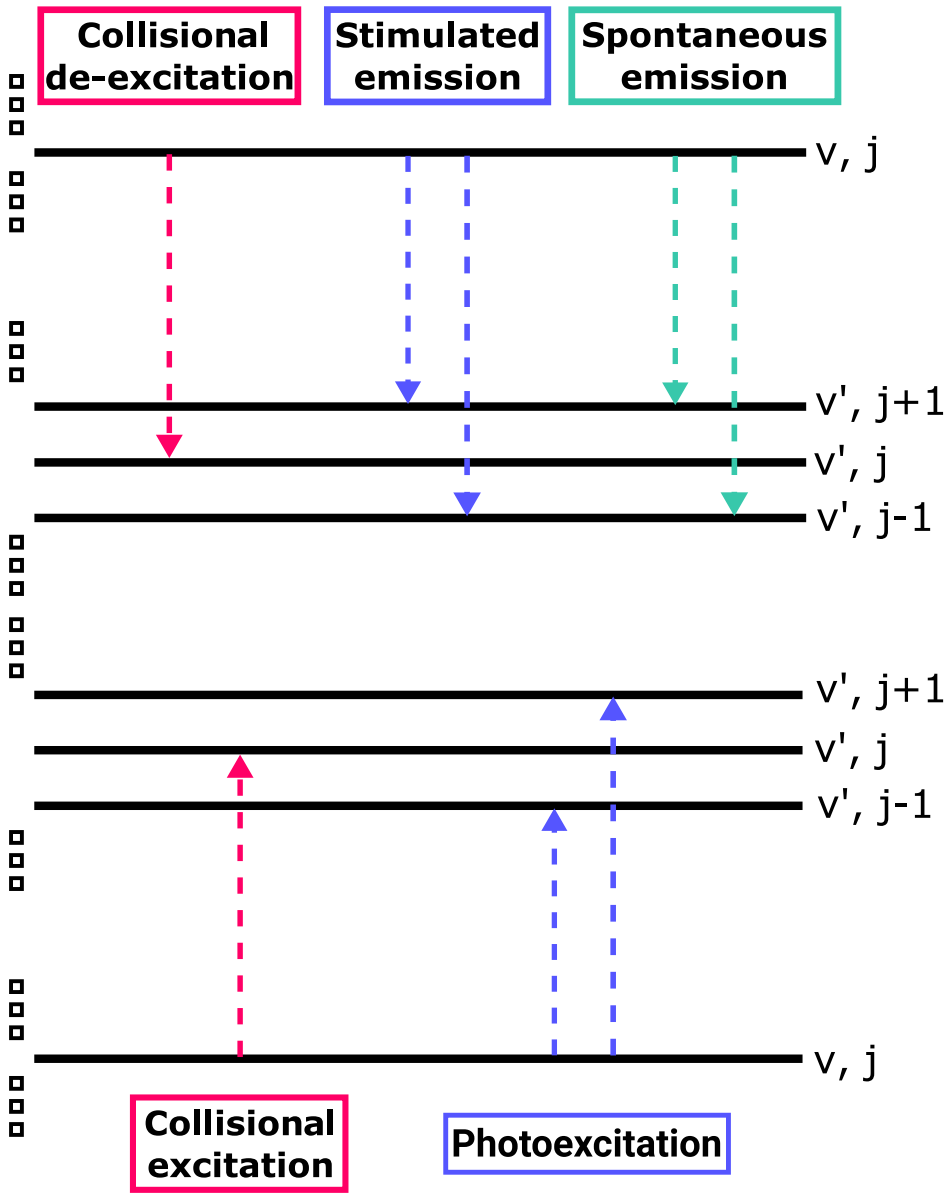
- Conditions favorable in dense, mostly neutral, O/C core region of ejecta.
- Conditions less favorable in H and He-layers, whether in ejecta or CSM.
- *Expected impact of CSI? Not large : radiation cannot reach SN core for decades.*

Molecules in NLTE - cross section issues

- Currently, neither theoretical nor experimental data is available for all the collision rates needed to calculate molecule NLTE statistical ro-vibrational populations in (hot) SNe environments.

Molecules in NLTE - cross section issues

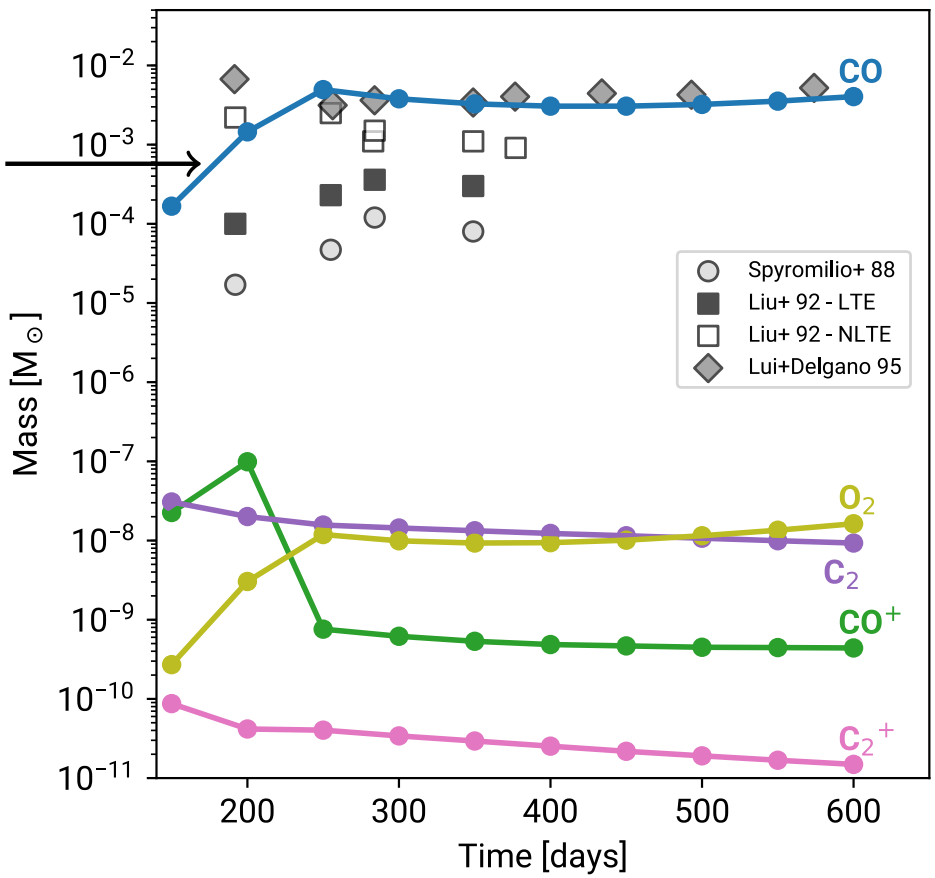
- At least 5 schemes proposed for $\Delta\nu \neq 1$ collision rates. We use Chandra & Sharma 2001.
- To split out the experimental/theory data for vibrational rates to rovibrational, we assume indepedence of j (Laporta 2012). We allocate the rate to $\Delta j = 0$. For now we force rotational LTE so does not really matter.
- For other molecules than CO, no thermal collision data at all available $\rightarrow$ use the CO scheme for all 4 molecules. Data are available for fast electrons.



Carbon monoxide in Type II SN models Liljegren+2020

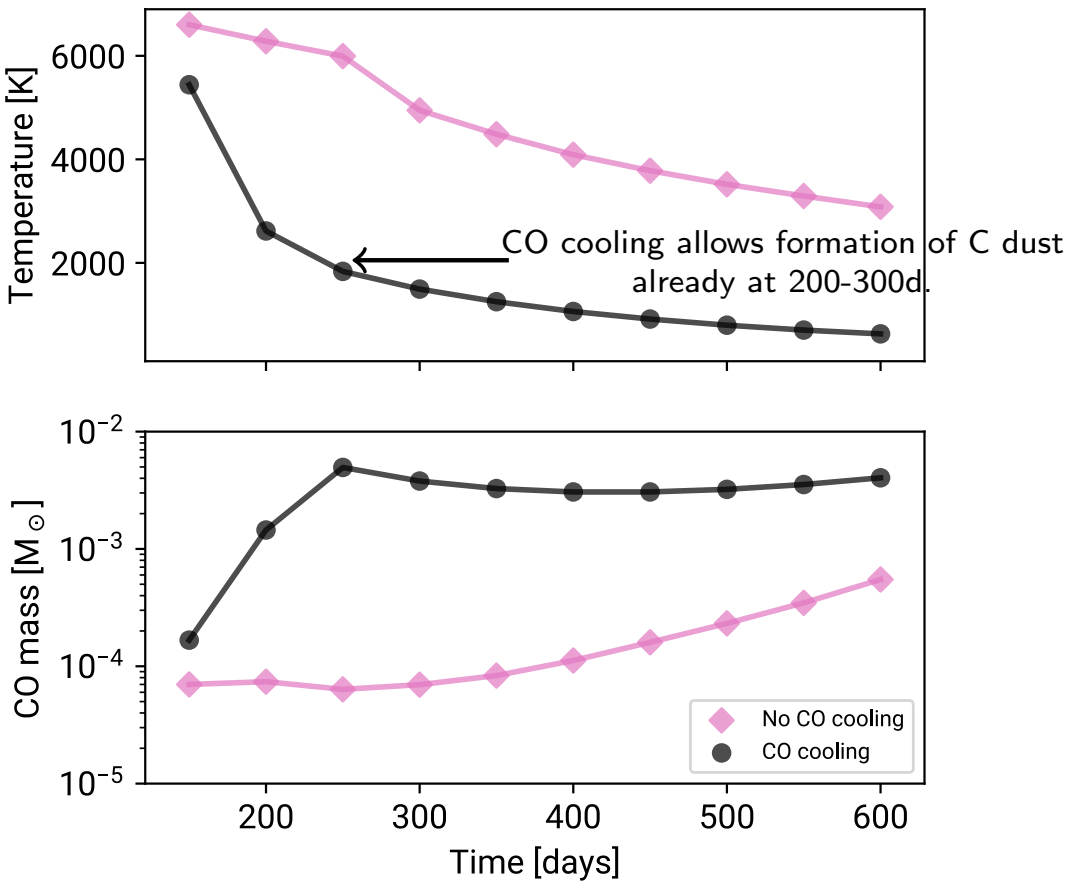
- A 1-zone study with just C and O, but with self-consistent NLTE physics for CO formation and cooling.
- Our standard model forms a few times 10^{-3} $M_\odot$ of CO. The mass grows up to about 250d and is then quite constant in time.

The suppression at early times is mainly due to charge transfer destruction with O^+.



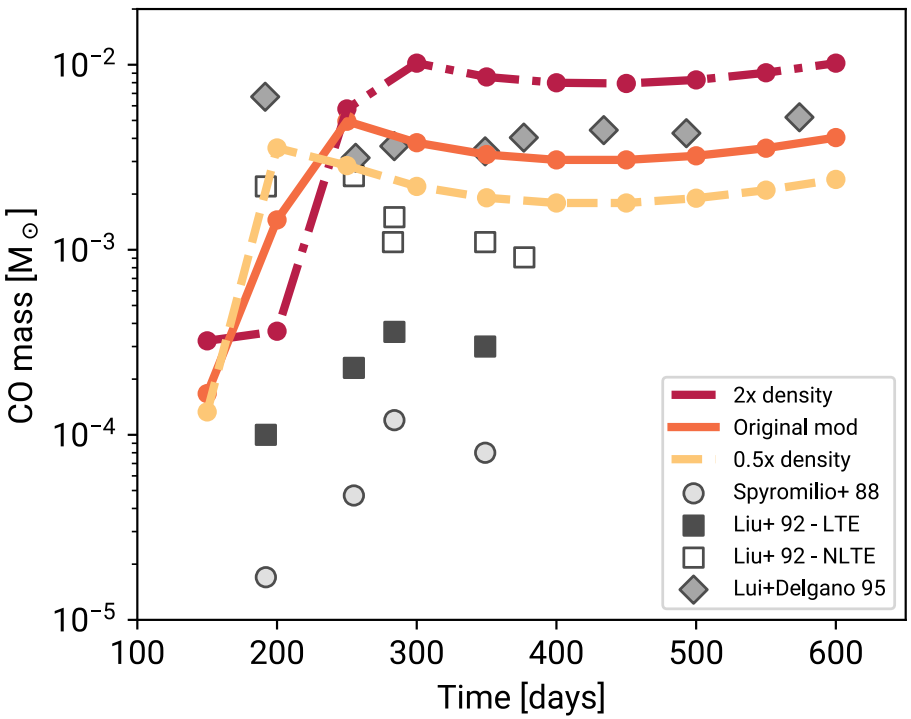
Carbon monoxide in Type II SN models Liljegren+2020

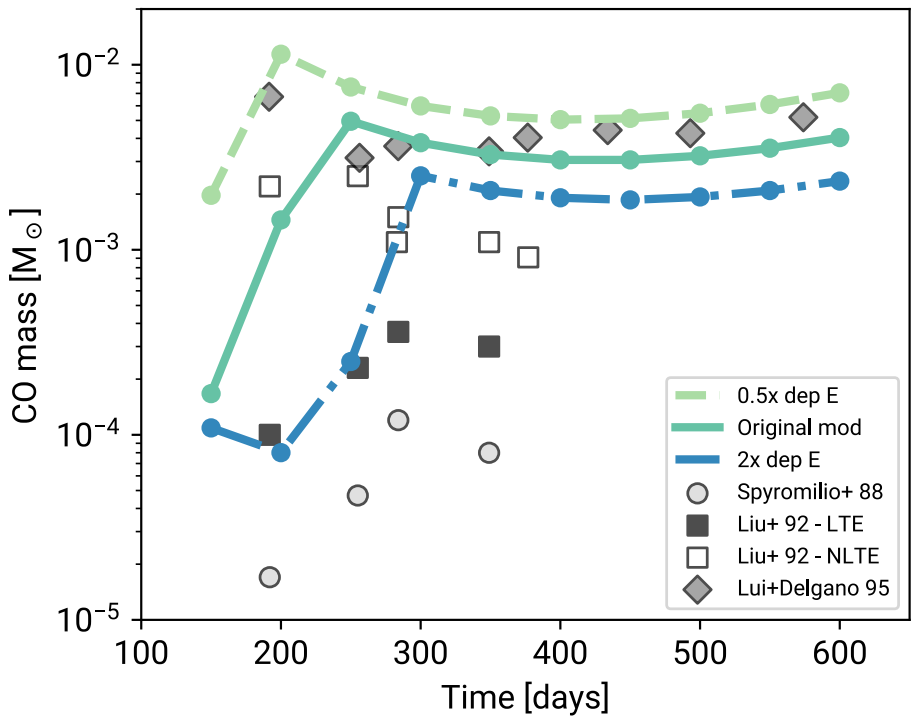
- There is a very strong coupling between molecule **formation** and molecule **cooling** → important to treat both of these self-consistently.



Carbon monoxide in Type II SN models Liljegren+2020

- CO time evolution can probe the **density** and **zone powering**.





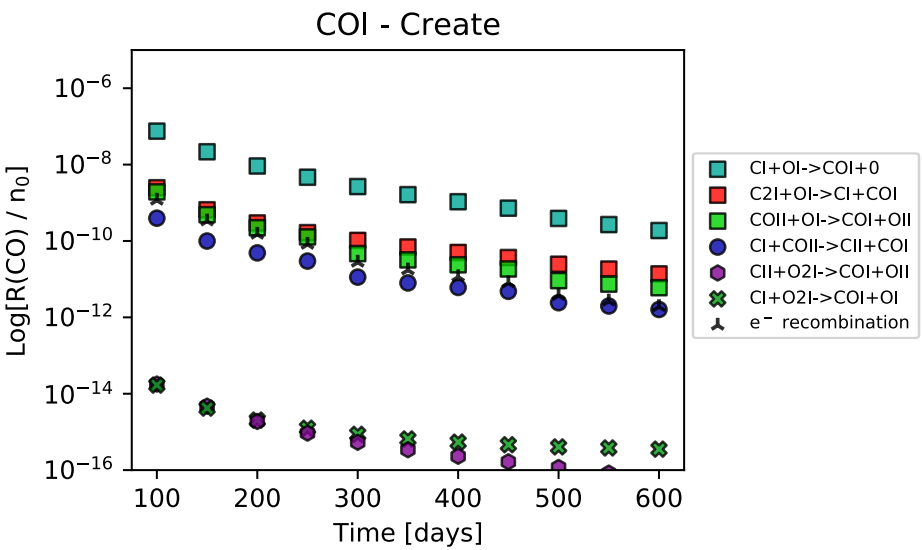
Liljegren & AJ 2022 - molecular chemistry of Type Ibc SNe

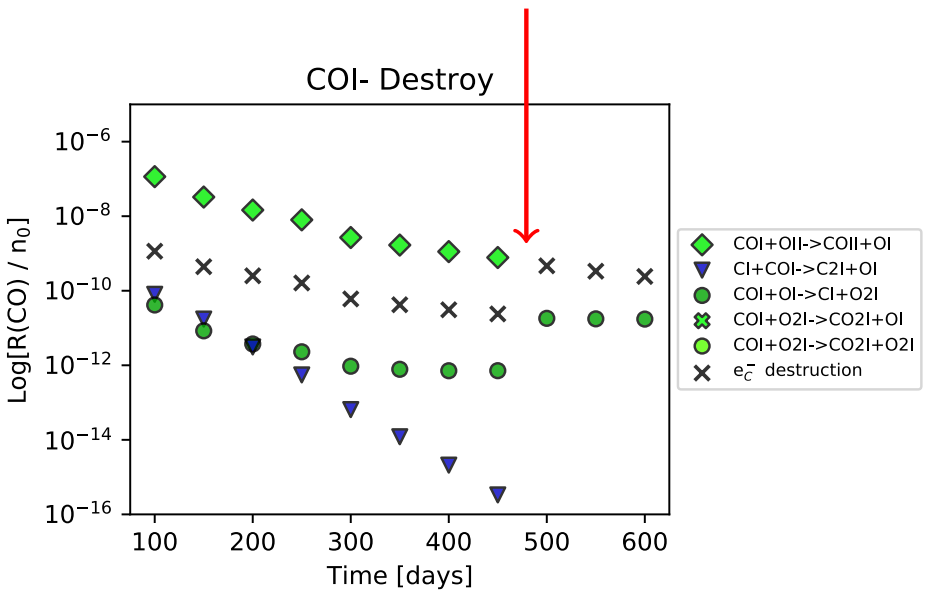
- Improvements
  - Network extended, updates of reaction rates/cross sections. Issue: SN environment is hot $\rightarrow$ molecules excited. Most other applications gas is quite cold $\rightarrow$ molecular data efforts geared toward low temperatures.
  - High-energy cross sections implemented for CO, SiO, SiS, SO.
  - Measured CO thermal collision strengths incorporated.
  - Self-consistent Compton destruction, with high-energy cross sections implemented for CO, SiO, SiS, and SO.
  - Full composition (KEPLER models).
  - Multi-zone modelling (1-zone in L20).
- Upcoming
  - Photoionization/dissociation.

CO formation and destruction in Type Ibc SNe

- **Formation** dominated by radiative association C + O → CO. Latest rate : Gustafsson 2015.
- **Destruction** first by O^+ charge transfer, (Petuchowski 1989) then Compton electrons. (Itikawa 2015.)

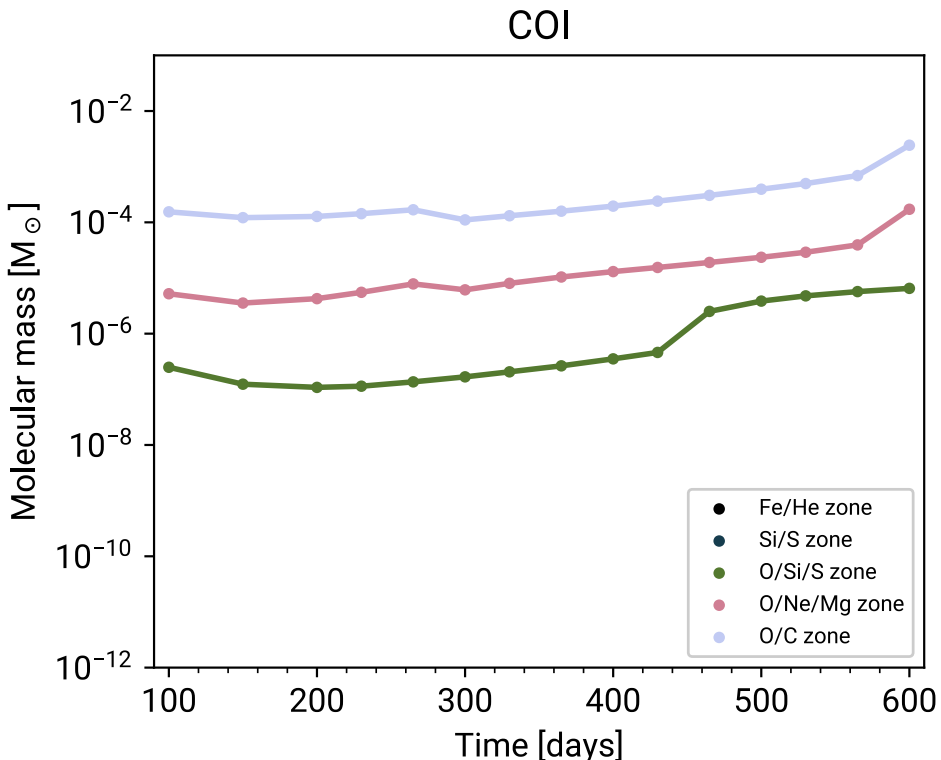
CO growth when O^+ reaction switches off.





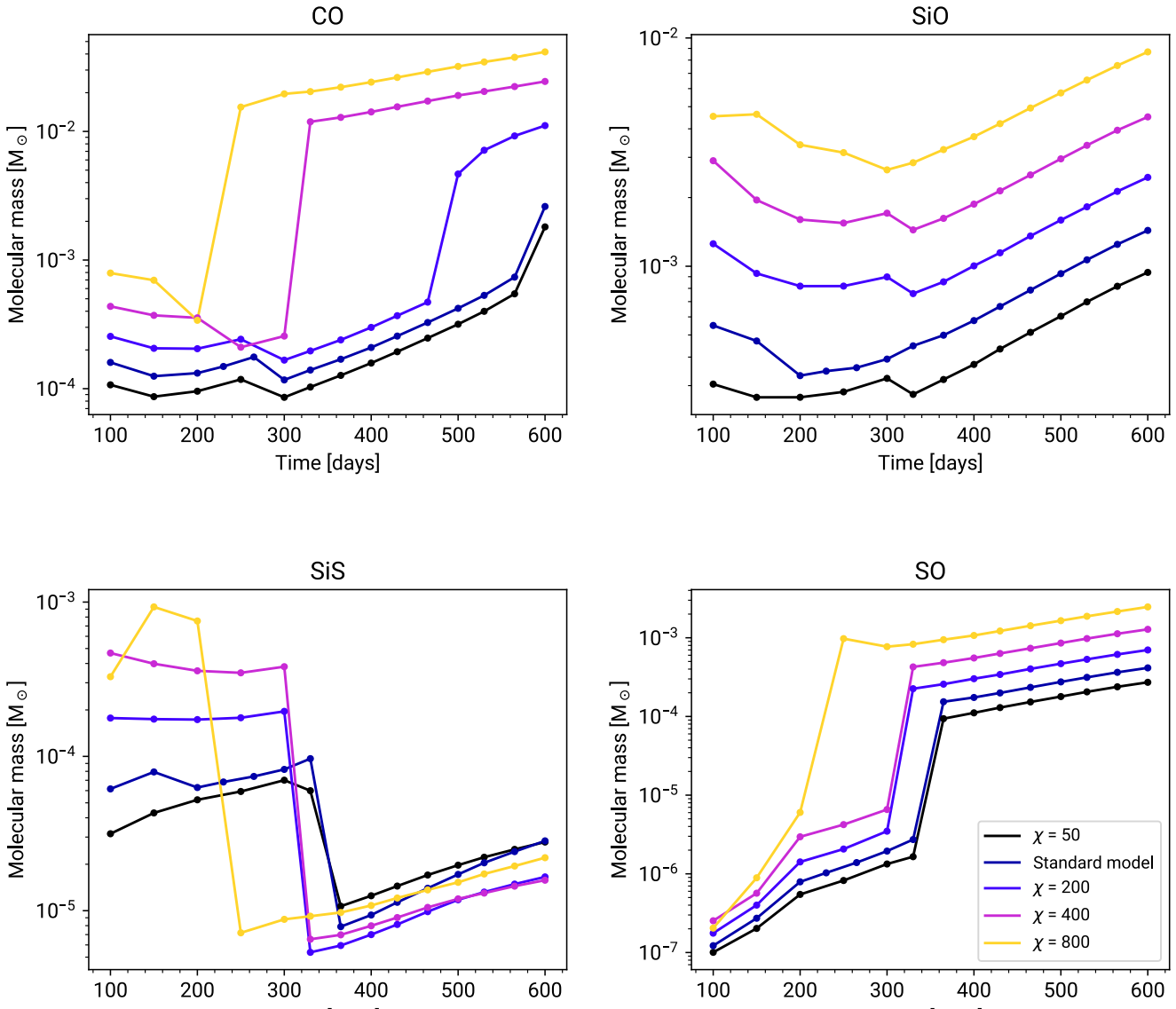
Carbon monoxide in Type Ibc SNe

- CO formation is **significant only in the O/C zone**.
- As in the Type II model, CO mass is quite constant in time. Here a **factor ∼10 lower than in Type II model** due to the lower density, at a few times 10^{-4} $M_\odot$.
- Growth begins at 500-600d as O^+ charge transfer switches off. Chemistry now out of steady state so change is slow.

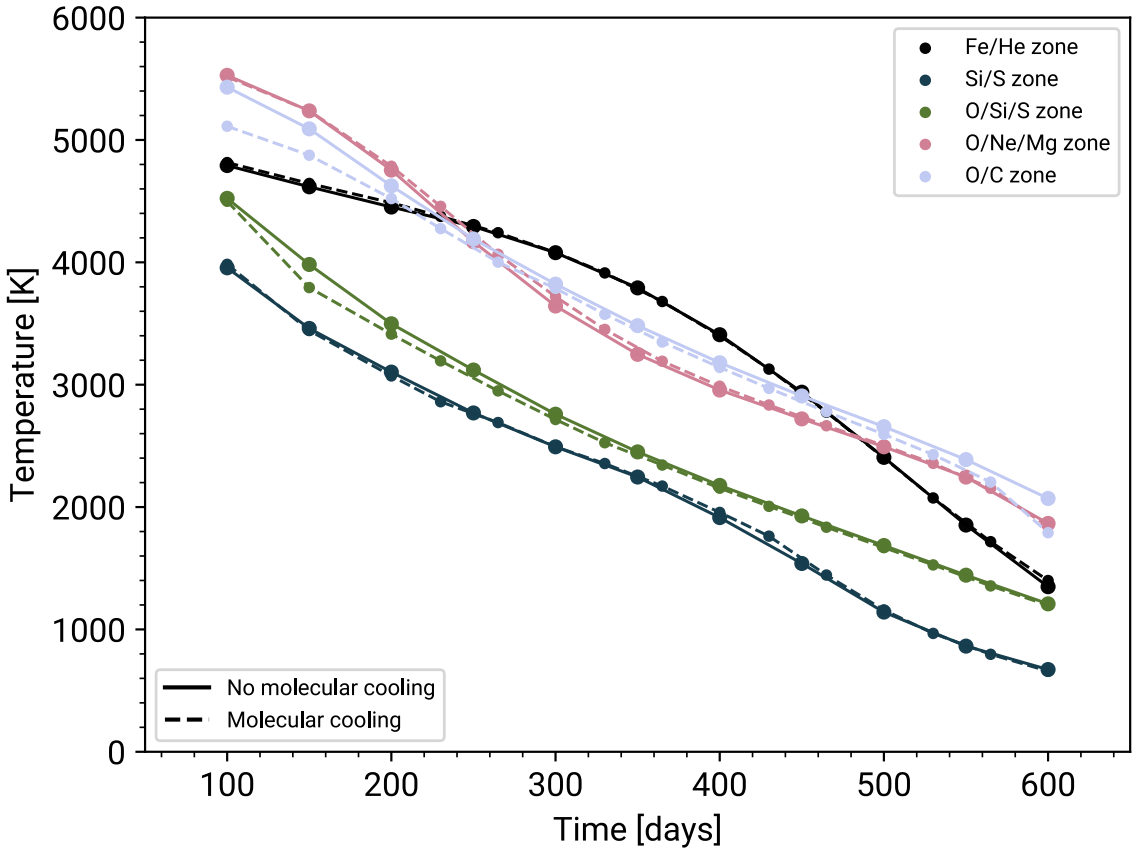


Carbon monoxide in Type Ibc SNe

- But, again, strong density sensitivity.



Impact on temperatures in Ibc SNe : small in standard model.

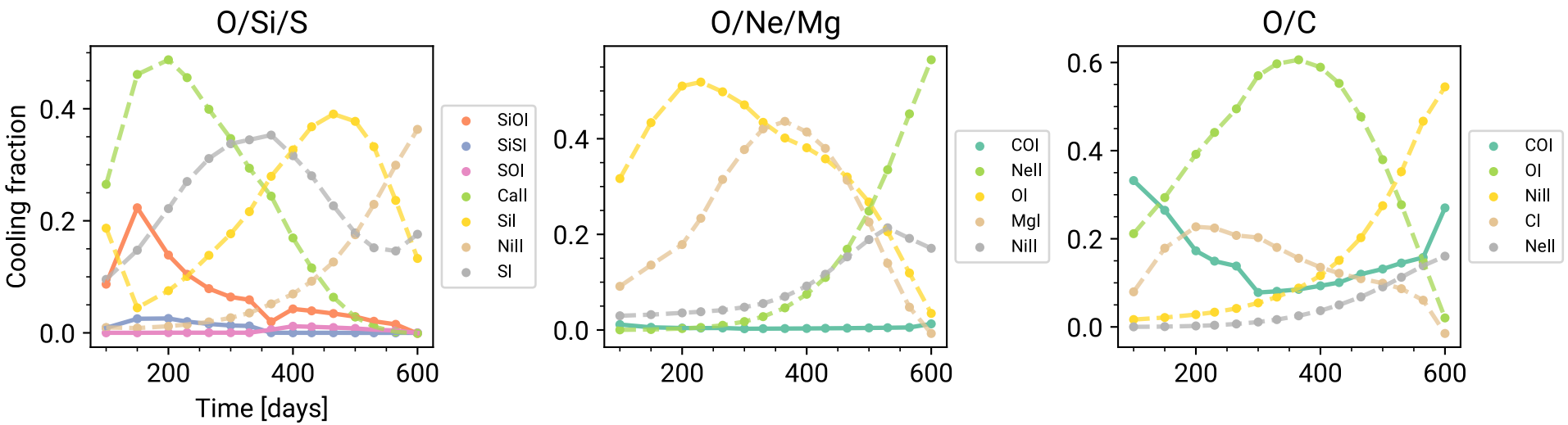


Two contributions:

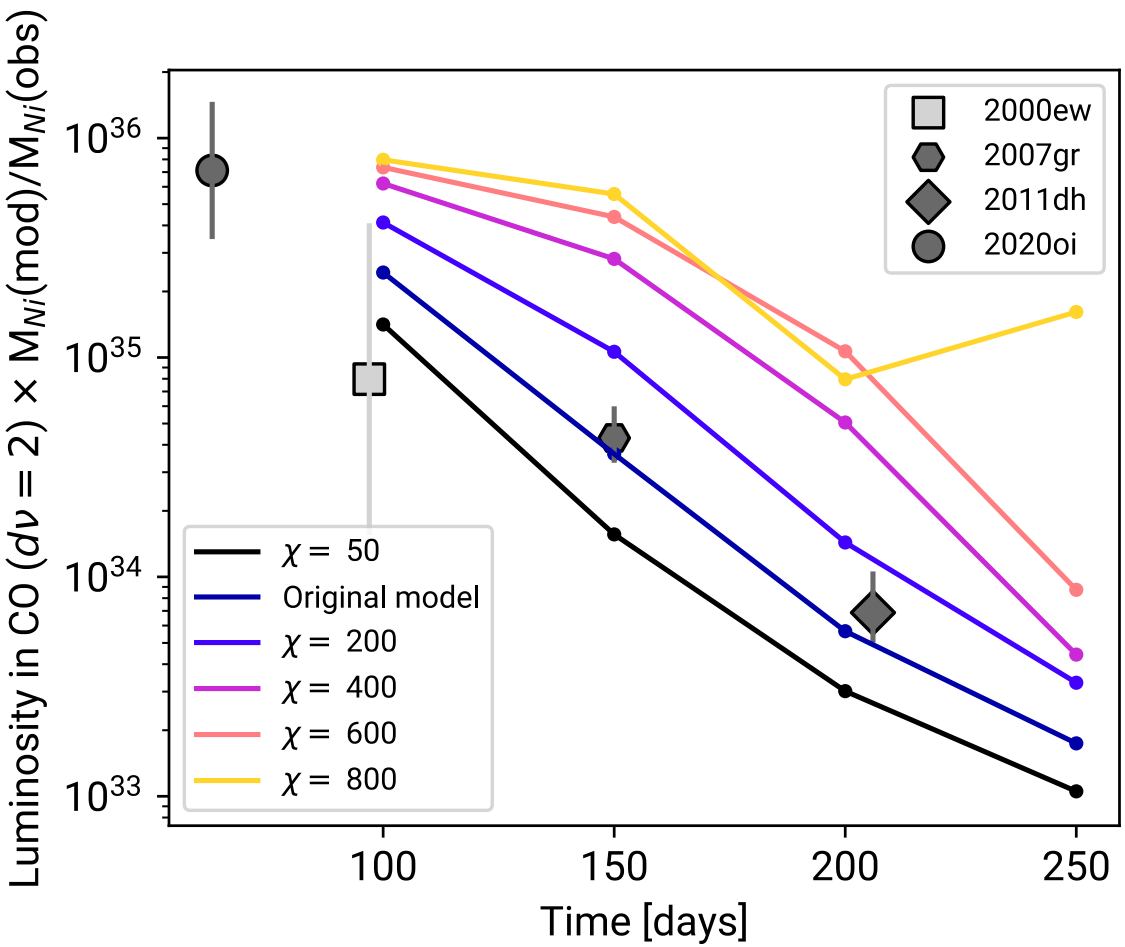
- Lower CO mass formed due to lower density.
- Collisional excitation less efficient with cross section data implemented.

Carbon monoxide in Type Ibc SNe

- CO does not affect emission from the important O/Ne/Mg zone (or the O/Si/S zone). This is important because it suggests low metal masses inferred from nebular atomic lines (e.g. AJ+2015) is robust.
- It does significant, but still only partial, cooling of the O/C zone : 10-40%.

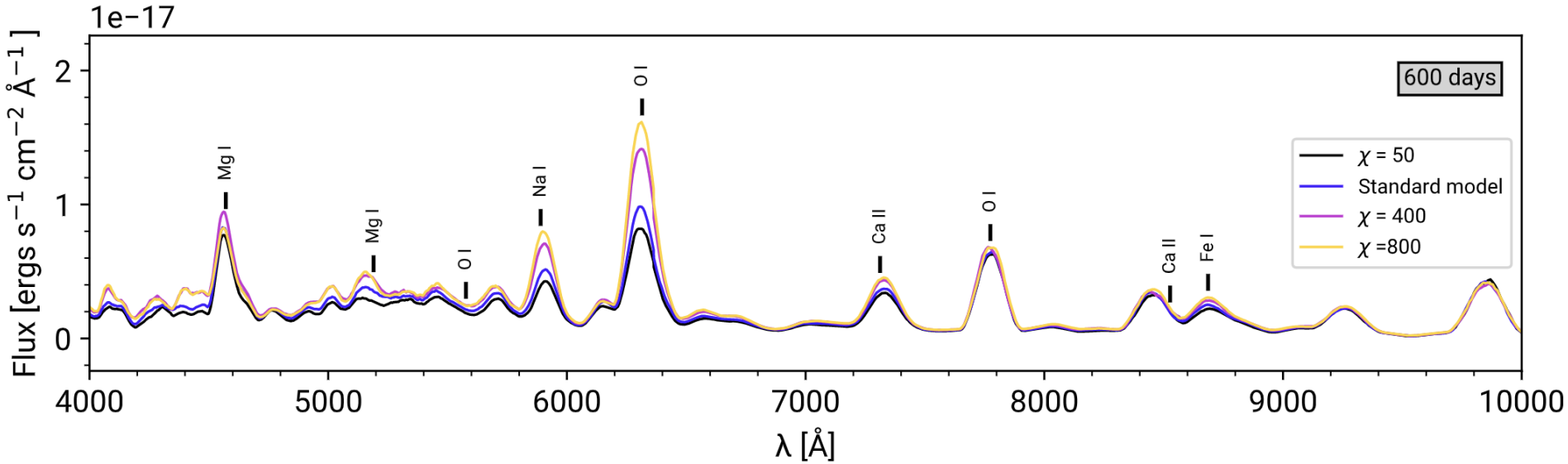


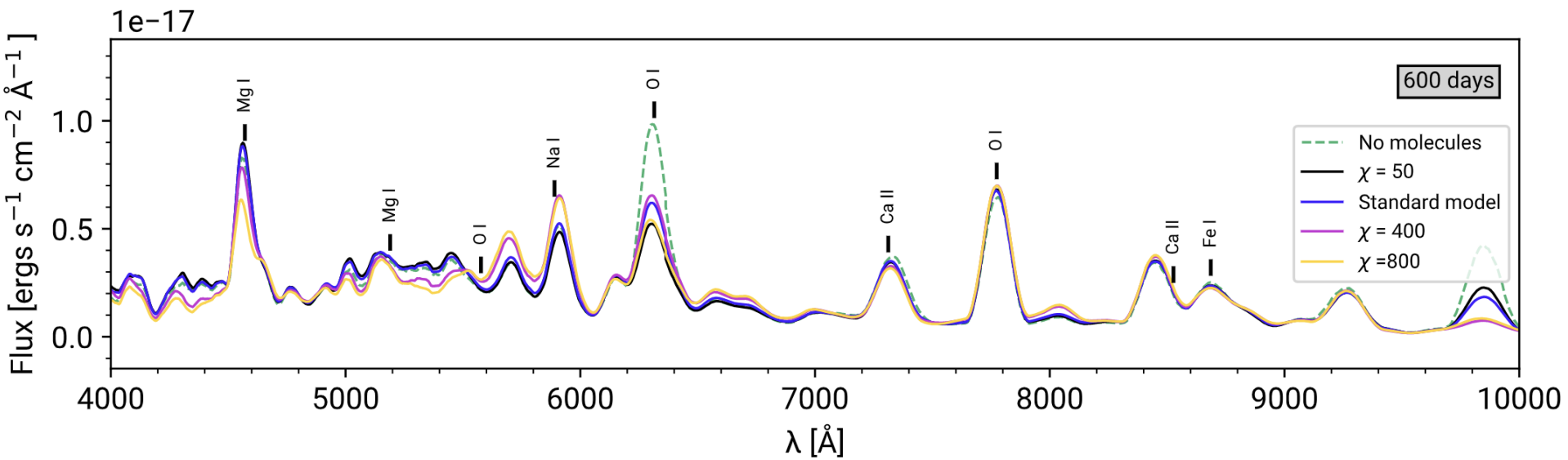
Comparison to CO overtone observations in Ibc SNe



- Too little data to draw any particular conclusions : hopefully JWST will improve situation.

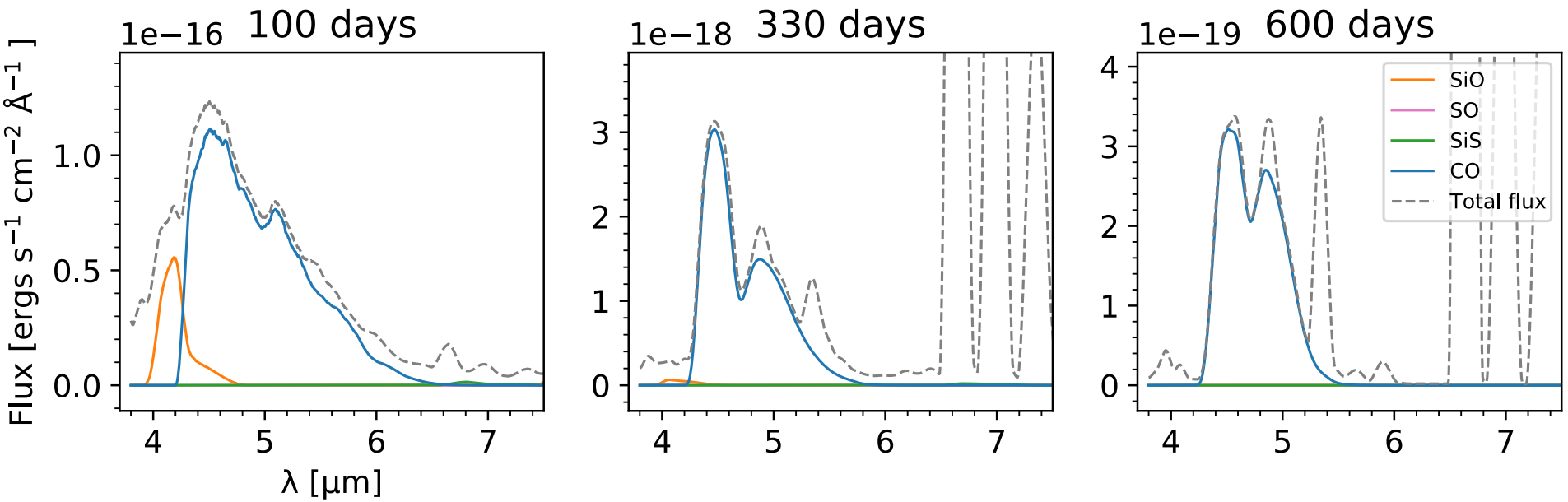
Impact on optical spectra





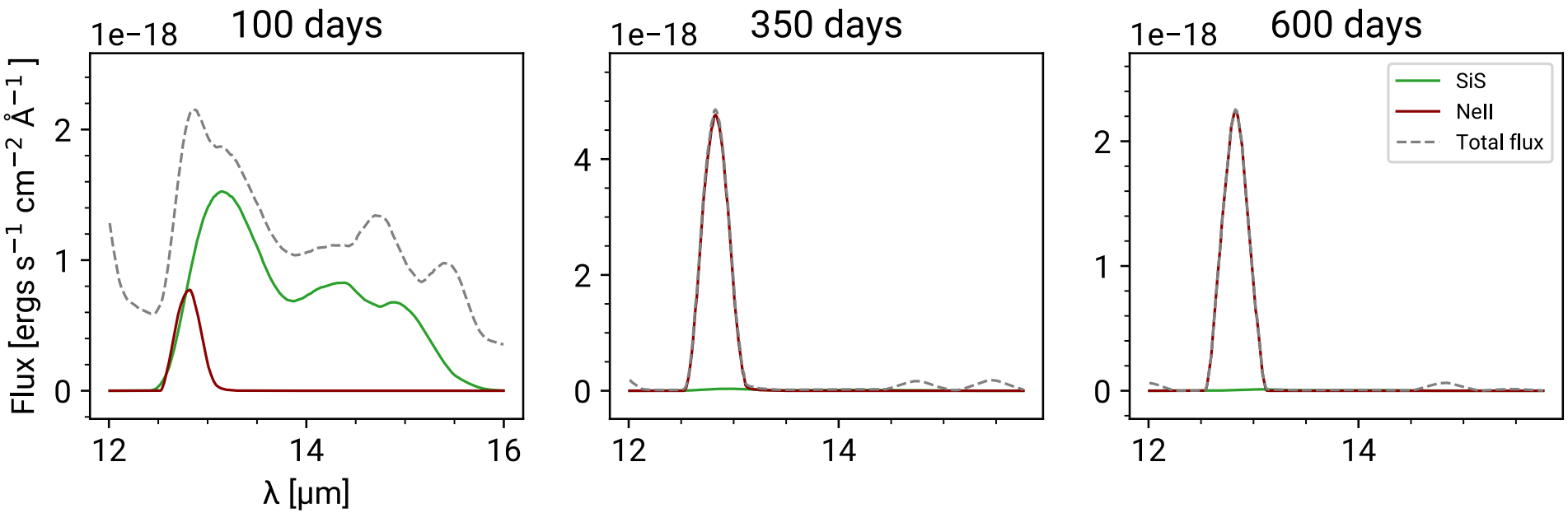
MIR predictions relevant for JWST

- CO fundamental band ; with SiO overtone at early times.

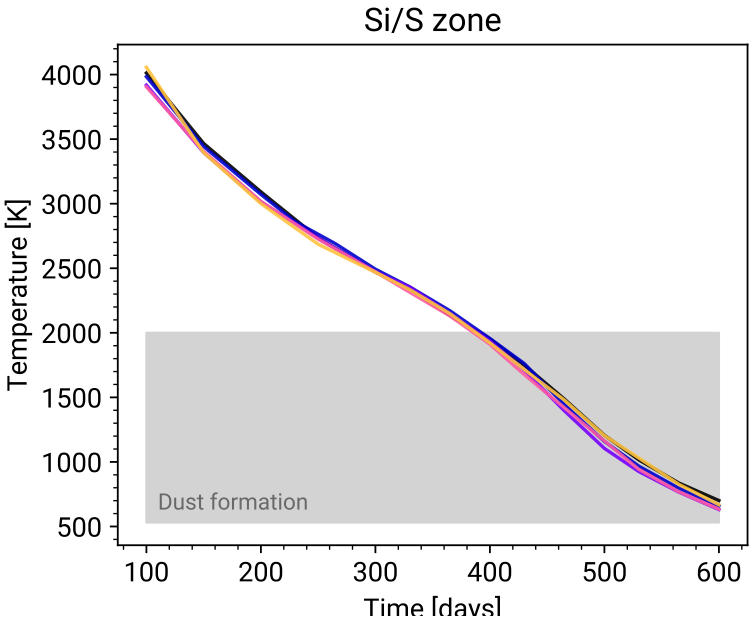


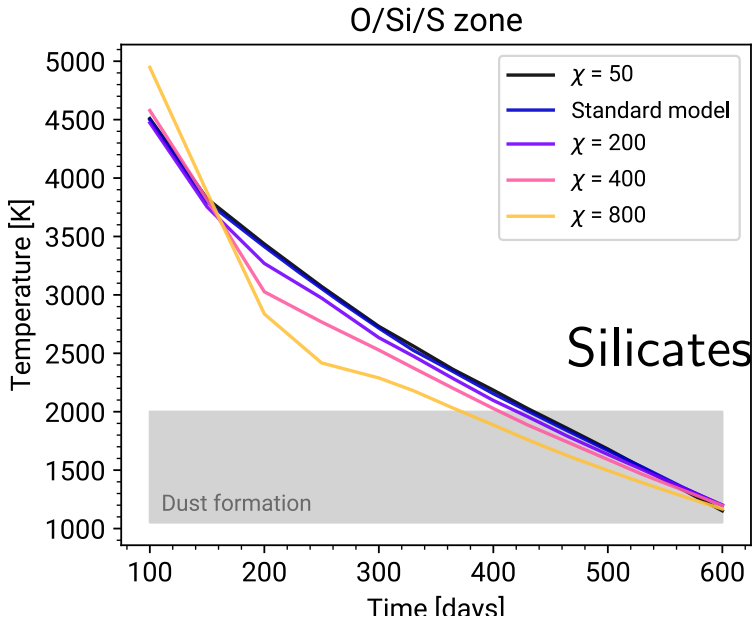
MIR predictions relevant for JWST

- SiS fundamental band : detectable early on, swamped by [Ne II] later.

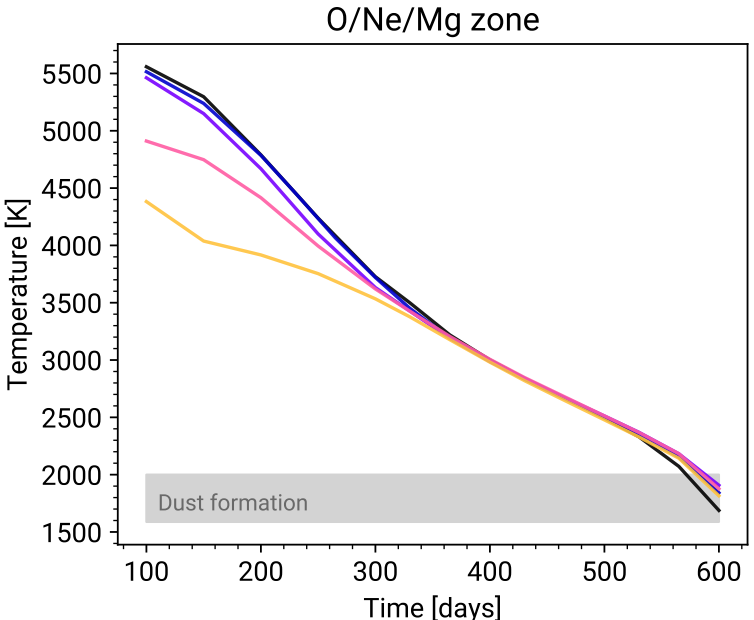


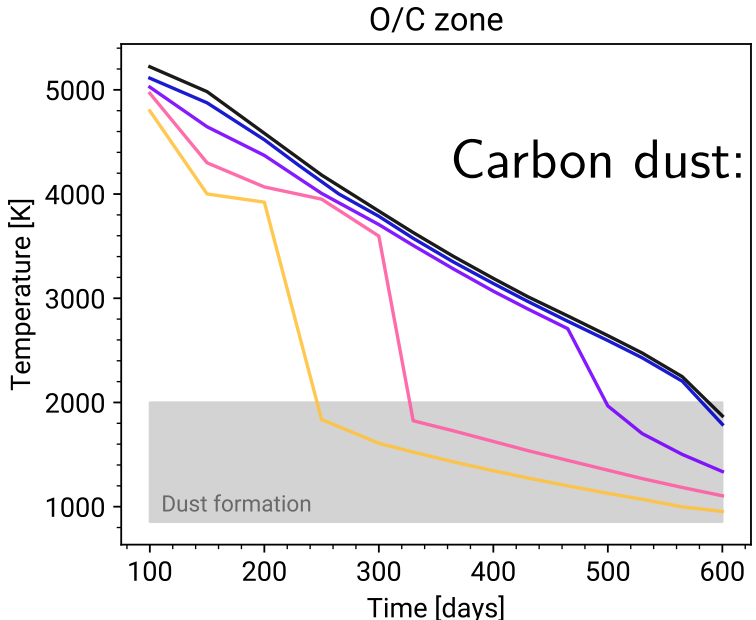
Predicted dust formation epochs





Silicates: ∼400d.





Carbon dust: ∼300 - 600d.

Summary

- Observations show that molecules, in particular SiO and CO, appear to form in all types of SN ejecta. Their large cooling abilities means they can dramatically change the temperature evolution of the layers where they form.
- This in turn means they governs when dust formation can begin ($T \lesssim 2000$ K).
- A molecular chemical network, and NLTE cooling of CO, SiO, SiS and SO, have been implemented into the SUMO spectral synthesis code.
- A first 1-zone carbon-oxygen study tailered to Type II SNe shows formation of $\sim 10^{-3}\ M_{\odot}$ of CO, but strong variations with assumed density (clumping).
- A full ejecta model for a Type Ibc SN has also been investigated. The lower densities in Ibc ejecta leads to less efficient molecular cooling - the standard model shows only small changes to temperature evolutions. However, the higher clumping models show larger effects.
- The models give predictions for MIR emission and guidance for what JWST data may tell us.