

On the roles of molecules for dust formation

Takaya Nozawa

(National Astronomical Observatory of Japan)

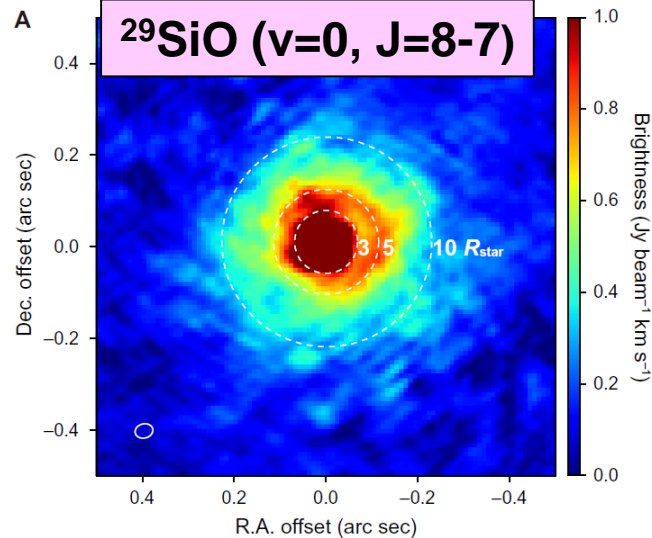
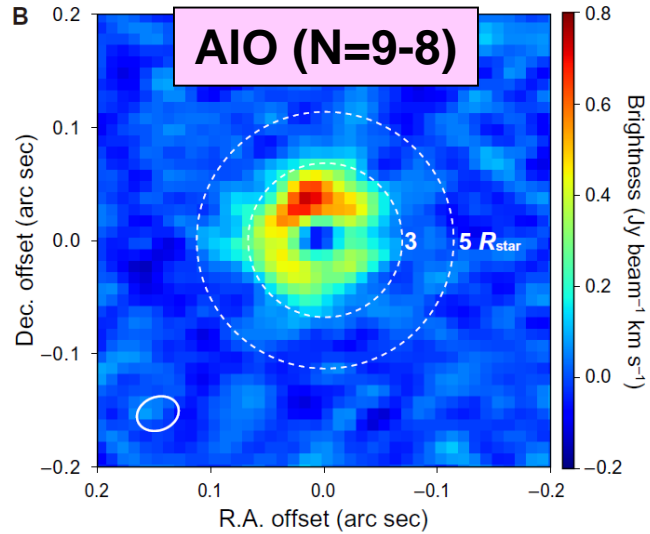
Topics of this talk

(1) Molecules as precursors of dust grains

(2) Molecules as efficient coolants of warm gas

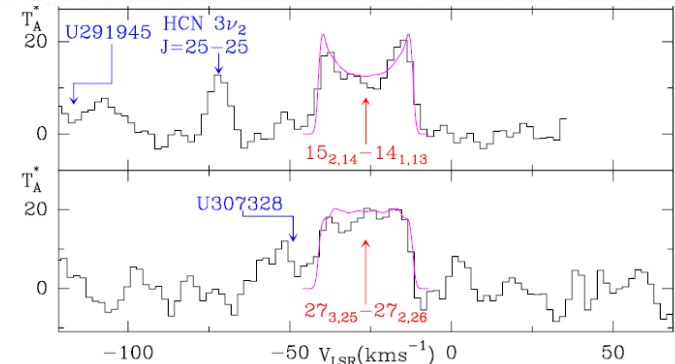
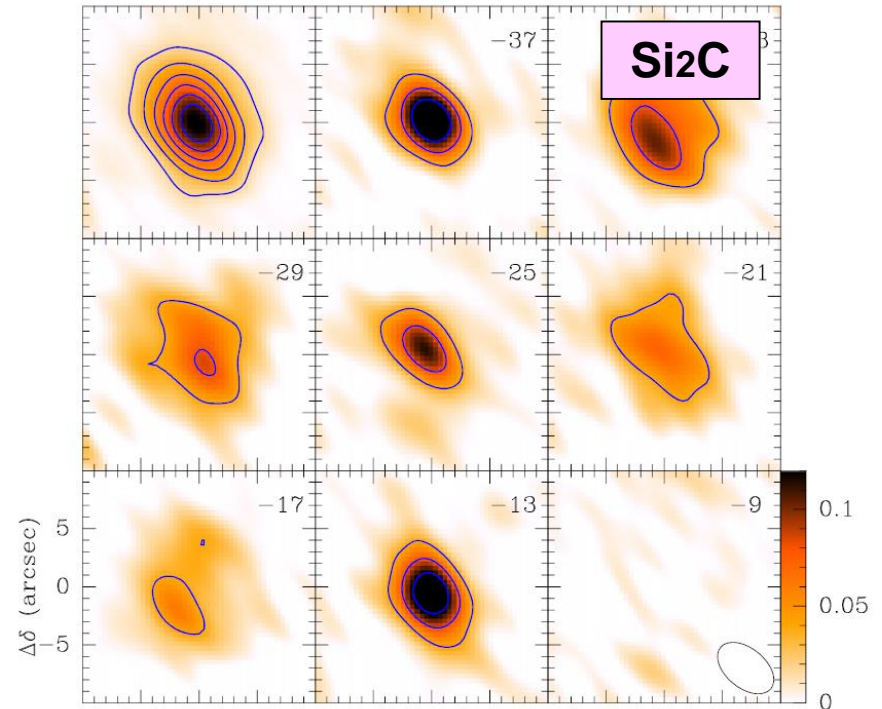
1-1. Molecules in AGB stars

O-rich star (W Hya)



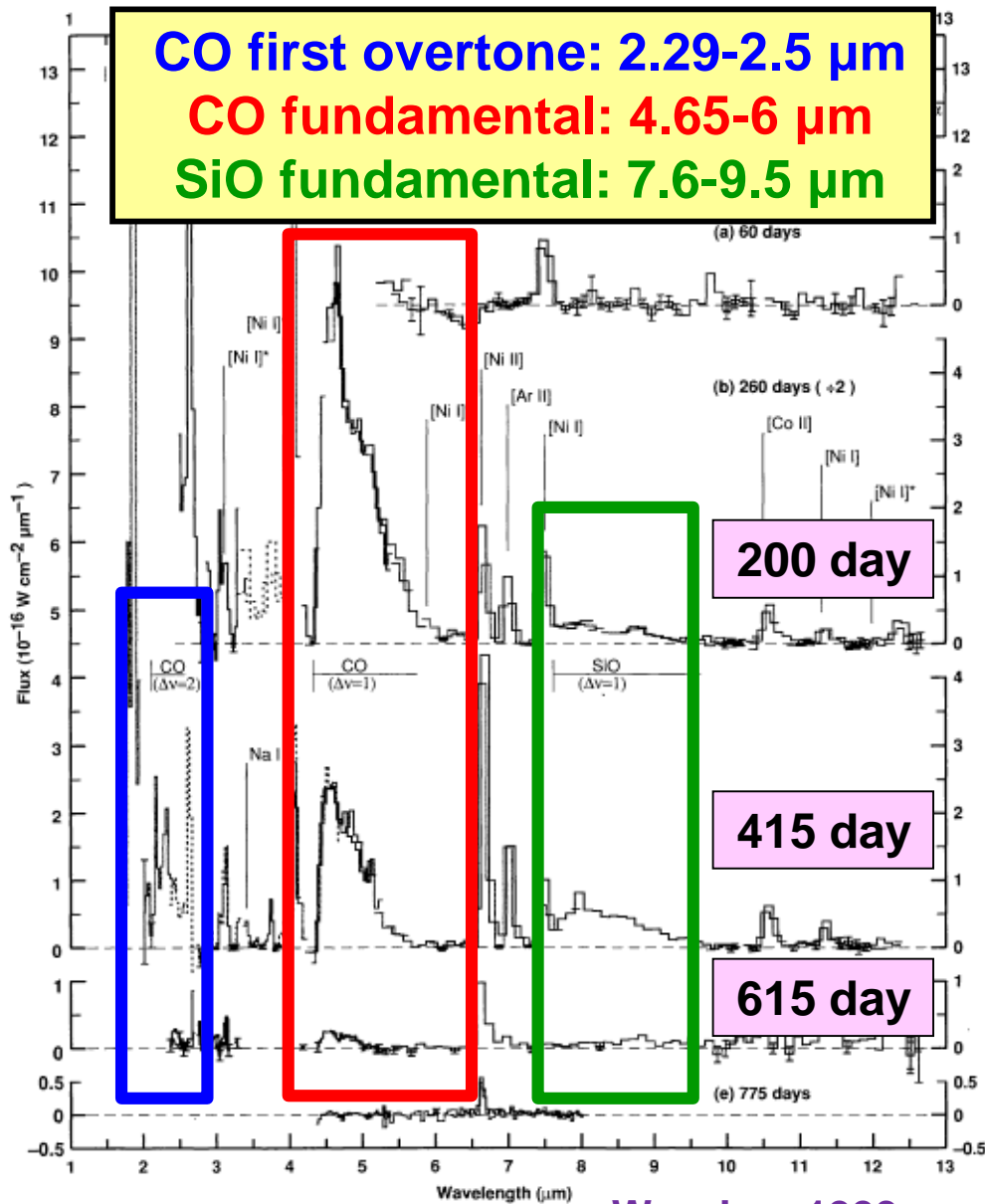
Takigawa+2016

C-rich star (IRC+10216)

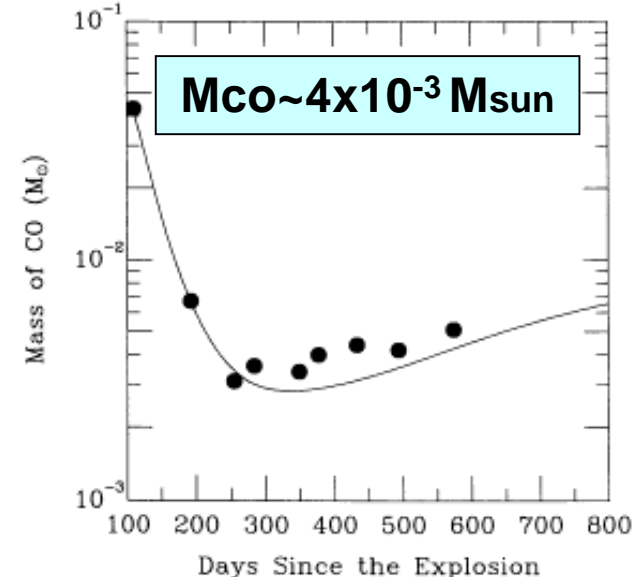


Cernicharo+2015

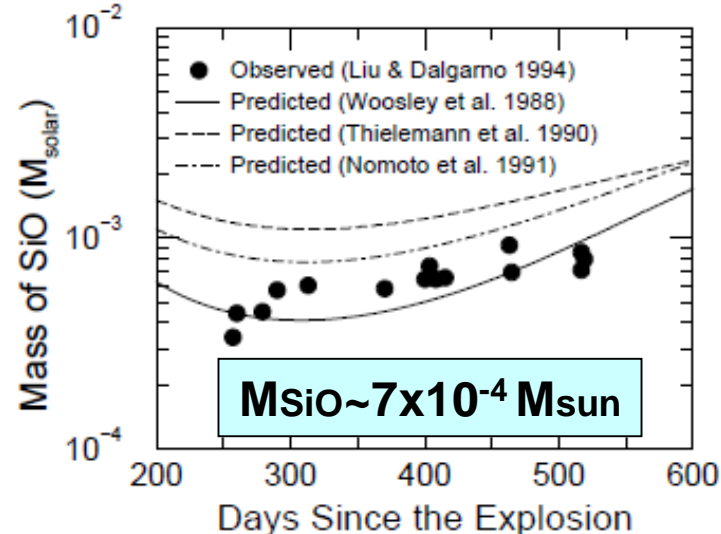
1-2. CO and SiO molecules in SN 1987A



Wooden+1993

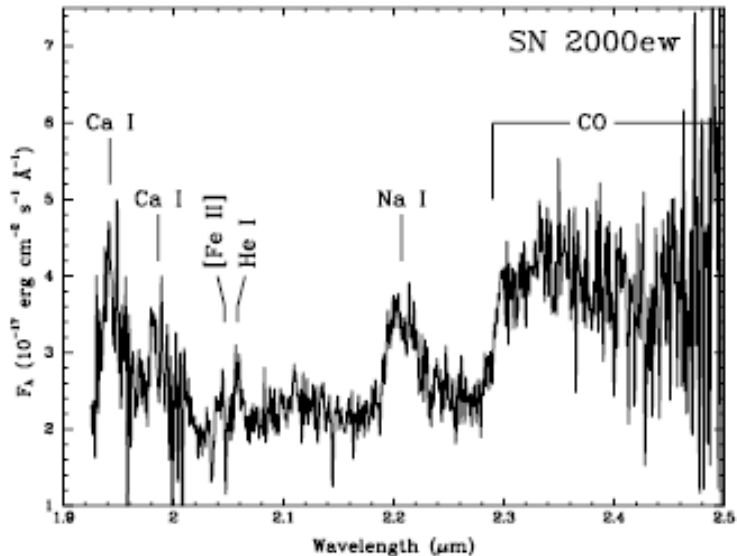


Liu+1995

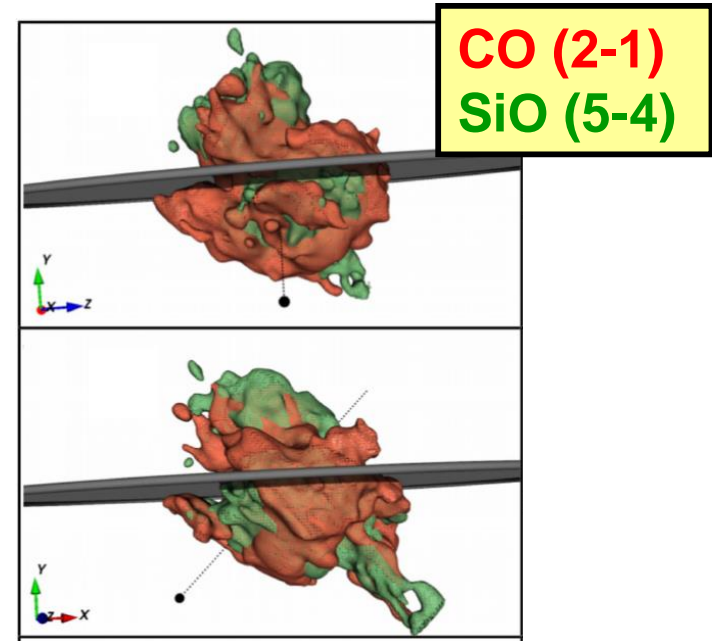
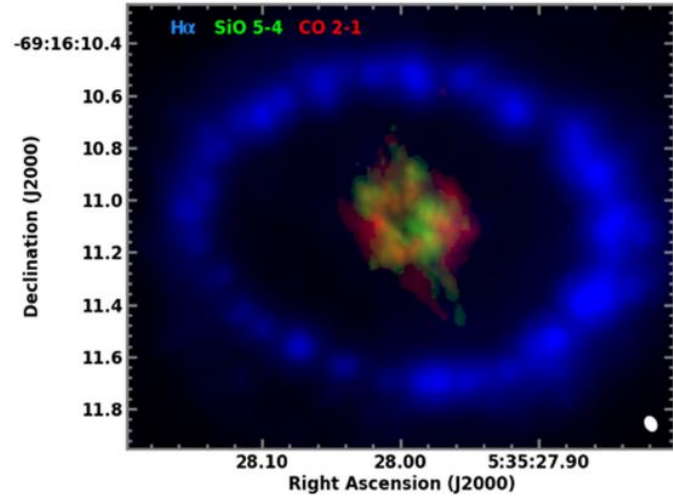


Liu & Dalgarno 1996

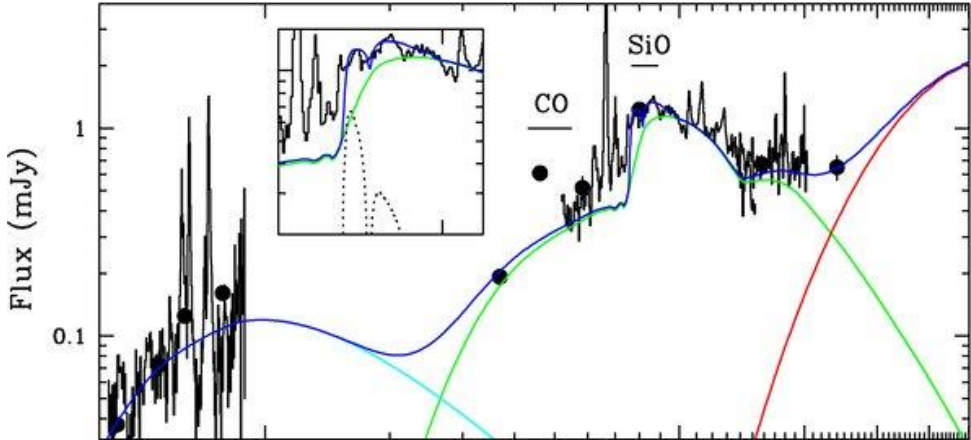
1-3. CO and SiO detection in other SNe



Gerardy+2002, SN2000ew at ~100 day



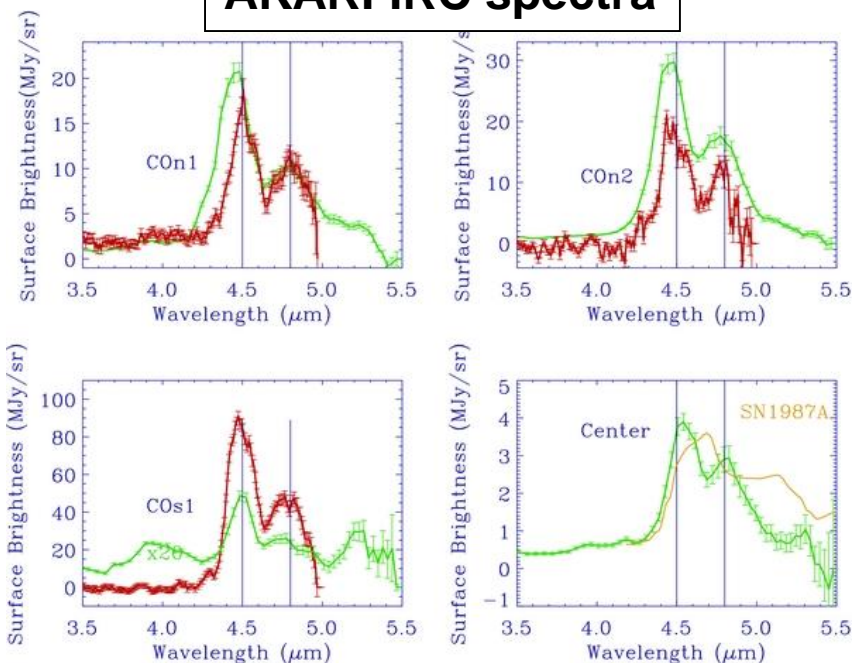
Abellan+2017, SN 1987A at ~28 yr



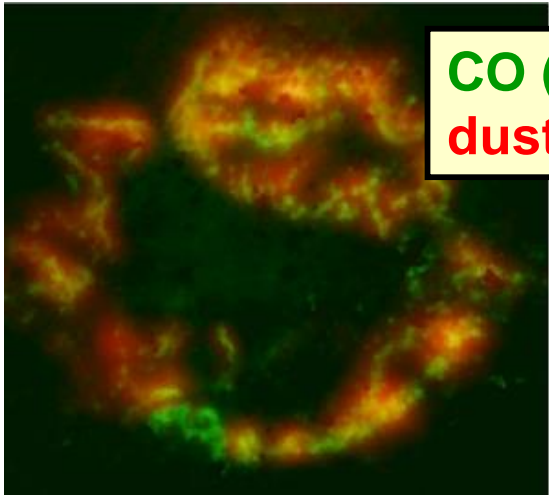
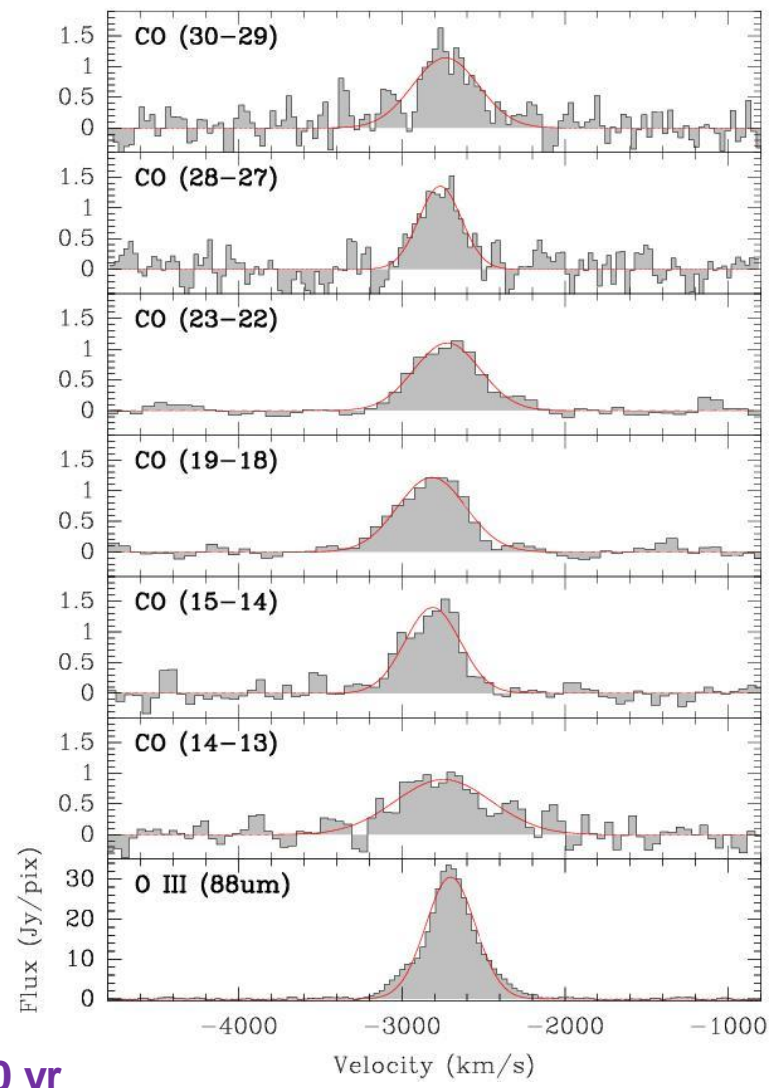
Kotak+2009, SN 2004et at ~400 day

1-4. CO detection in Cassiopeia A SNR

AKARI IRC spectra



Herschel PACS



**CO (4.5 μm)
dust (21 μm)**

Rho+2012
Cas A at ~ 330 yr

Wallstrom+2013

1-5. Observations of molecules in AGB/SNe

- (1) O-rich ($C/O < 1$) star : **CO**, **SiO**, **AlO**, **MgO**, ...
C-rich ($C/O > 1$) star : **CO**, **CS**, **HCN**, **Si₂C**, **SiC₂**, ...
- (2) N-MIR emissions by **CO** and **SiO** ro-vibration
100-600 days in several SNe
- (3) FIR-submm emission by **CO** and **SiO** rotation
28 yr in SN 1987A
- (4) **CO** in Cas A (330 yr) → survive? or re-formation?

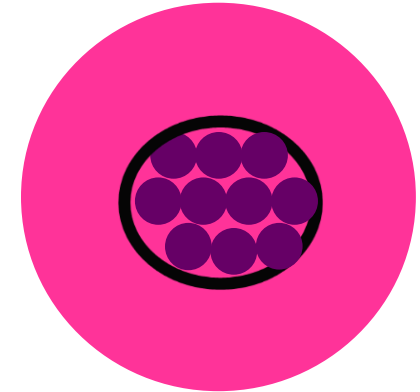
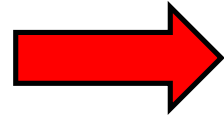
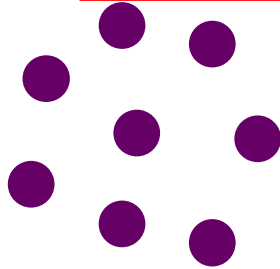
○ CO : inhibiting dust formation

**○ SiO, AlO, MgO, Si₂C, SiC₂:
precursor molecules for dust formation**

2-1. Theory of nucleation and grain growth

1. Nucleation

(formation of stable clusters)



Steady-state nucleation rate

$$J_s(t) = \alpha_s \Omega \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} \Pi c_1^2(t) \exp \left[-\frac{4}{27} \frac{\mu^3}{(\ln S)^2} \right]$$

Growth rate of dust grains

$$\frac{da}{dt} = s \Omega_0 \left(\frac{kT}{2\pi m_1} \right)^{\frac{1}{2}} c_1 \left(1 - \frac{1}{S} \right)$$

number of stable clusters formed per volume per sec

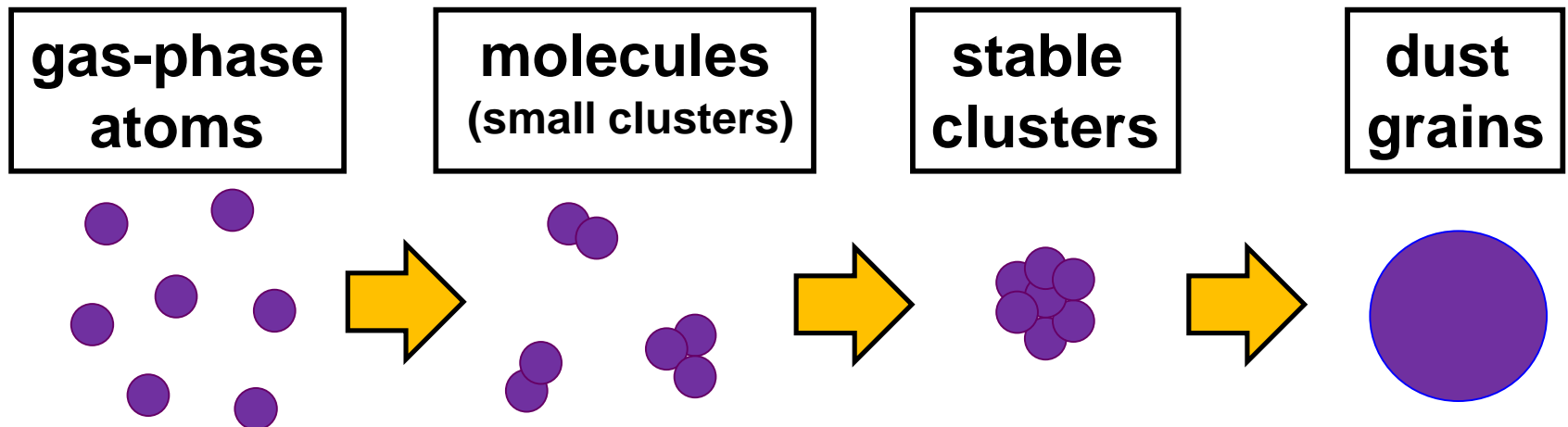
2-2. Base of nucleation theory

○ Nucleation : the first-order phase transition (condensation from gas-phase to solid-phase)

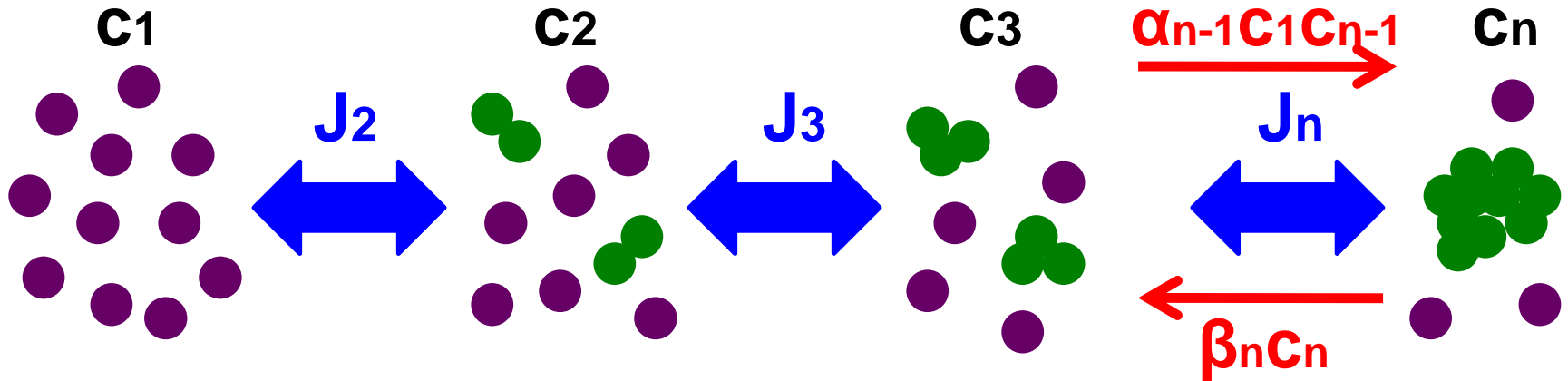
- described by the change of Gibbs free energy

- **Need to specify the chemical reaction**

ex. silicate : $\text{Mg(g)} + \text{SiO(g)} + 2\text{O(g)} \implies \text{MgSiO}_3\text{(s)}$



2-3. Non-steady-state (kinetic) nucleation



Master equations

$$\frac{dc_n}{dt} = J_n(t) - J_{n+1}(t) \quad \text{for } 2 \leq n \leq n_*,$$

$$J_n(t) = \alpha_{n-1}c_1 [c_{n-1} - c_n \exp(\gamma_n)]$$

$$\alpha_n = \eta_s 4\pi a_0^2 n^{\frac{3}{2}} \left(\frac{kT}{2\pi m_n} \right)^{\frac{1}{2}}$$

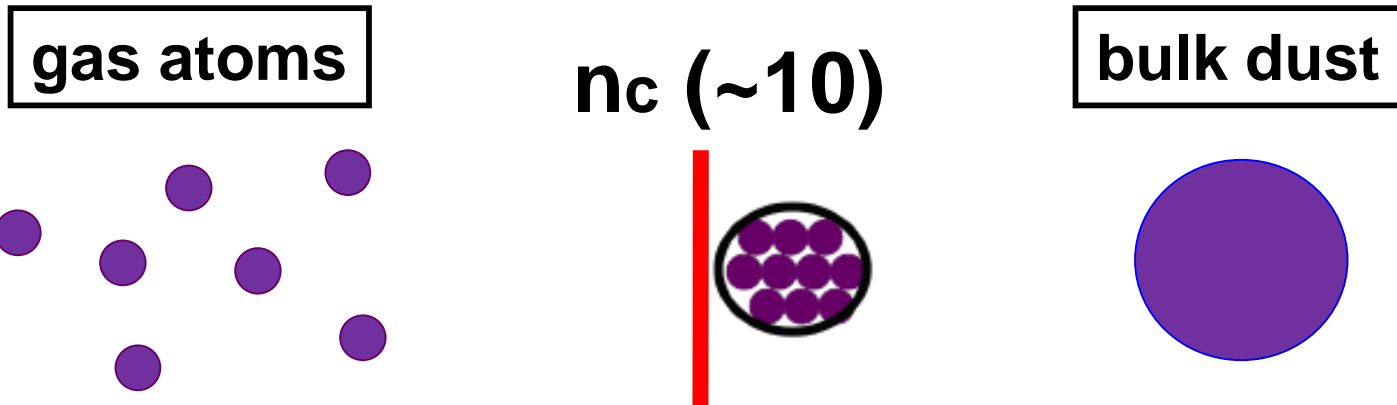
sticking coefficient, $\eta_s = 1$

$$\gamma_n = \frac{1}{kT} (E_{\text{surf},n} - E_{\text{surf},n-1}) - \ln S$$

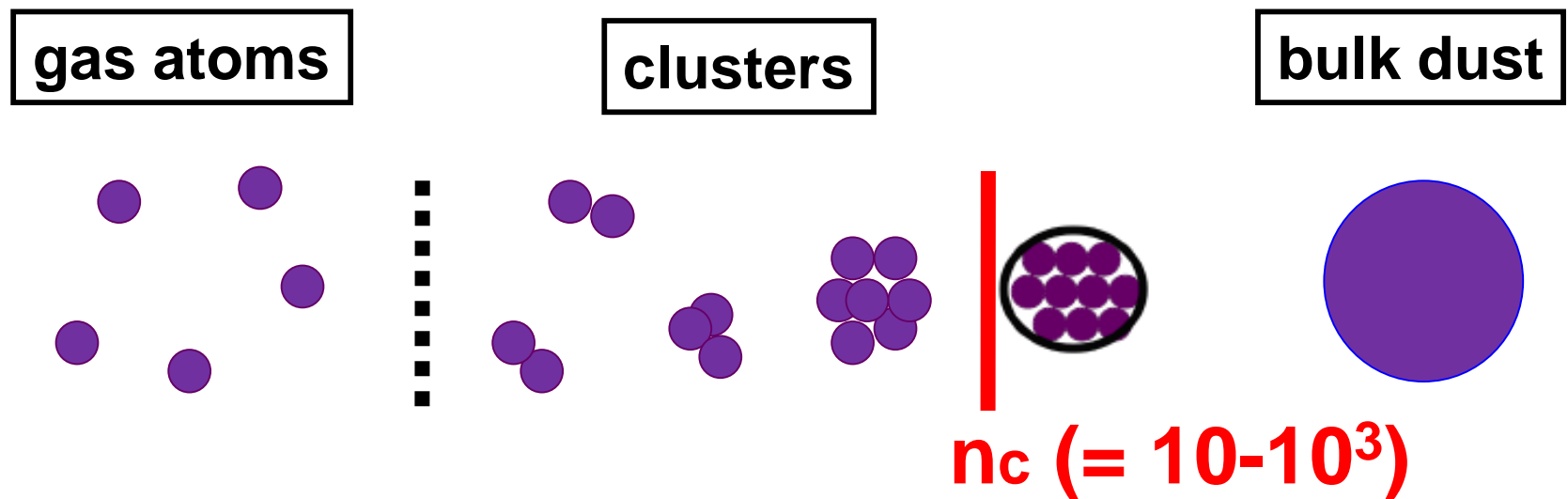
energy barrier : ~ 10

2-3-1. Concept of non-steady-state nucleation

○ steady-state nucleation rate: J_s



○ non-steady-state nucleation rate: J^*



2-4. Reaction coefficients of carbon clusters

Arrhenius form

$$\frac{dc_k^{\text{mol}}}{dt} = k_{ij}(T)c_i c_j$$

$$k_{i,j} = A_{i,j} \left(\frac{T}{300 \text{ K}} \right)^\nu \exp \left(-\frac{E_{\text{act}}}{kT} \right)$$

Carbon - C

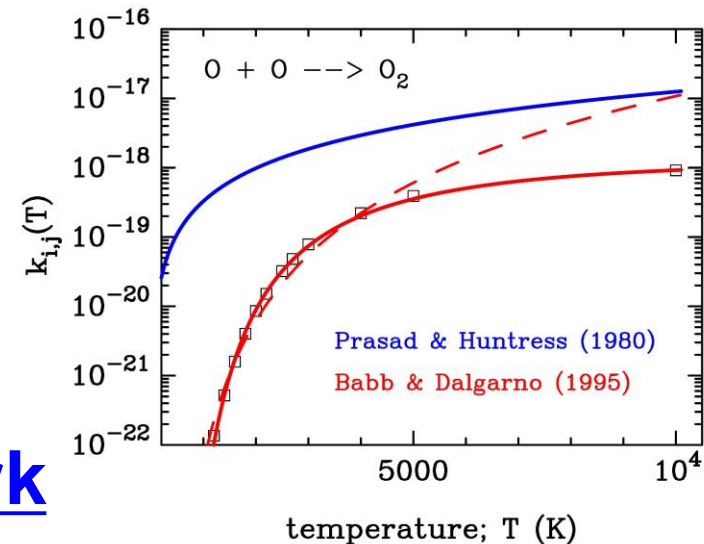
C1	C + C	→	C ₂ + hν	4.36 × 10 ⁻¹⁸	0.35	161.3	Andreazza & Singh 1997
C2	C + C ₂	→	C ₃ + hν	1.00 × 10 ⁻¹⁷	0	0	Clayton et al. 1999
C3	C + C ₃	→	C ₄ + hν	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C4	C + C ₄	→	C ₅ + hν	1.00 × 10 ⁻¹³	0	0	Clayton et al. 1999
C5	C + C ₄	→	C ₂ + C ₃	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C6	C + C ₅	→	C ₆ + hν	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C7	C + C ₆	→	C ₇ + hν	1.00 × 10 ⁻¹³	0	0	Clayton et al. 1999
C8	C + C ₆	→	C ₂ + C ₅	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C9	C + C ₆	→	C ₃ + C ₄	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C10	C + C ₇	→	C ₈ + hν	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C11	C + C ₈	→	C ₉ + hν	1.00 × 10 ⁻¹³	0	0	Clayton et al. 1999
C12	C + C ₈	→	C ₂ + C ₇	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C13	C + C ₈	→	C ₃ + C ₆	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C14	C + C ₈	→	C ₄ + C ₅	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999
C15	C + C ₉	→	C ₁₀ + hν	1.00 × 10 ⁻¹⁰	0	0	Clayton et al. 1999

Cherchneff & Dwek (2010)

2-5. Drawbacks of chemical nucleation

○ Unknown reaction coefficients

- no data for gas species and clusters of interest
→ **most of reaction coefficients assumed**
- experimental data mainly < 300 K
→ **Extrapolation to high-T may involve large uncertainties**



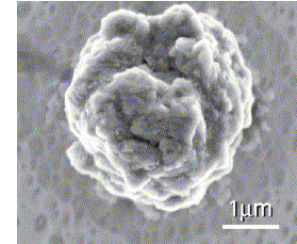
○ Incomplete chemical network

- **need to treat the destruction processes**
- if important (bottleneck) reactions are missed, the results may change dramatically

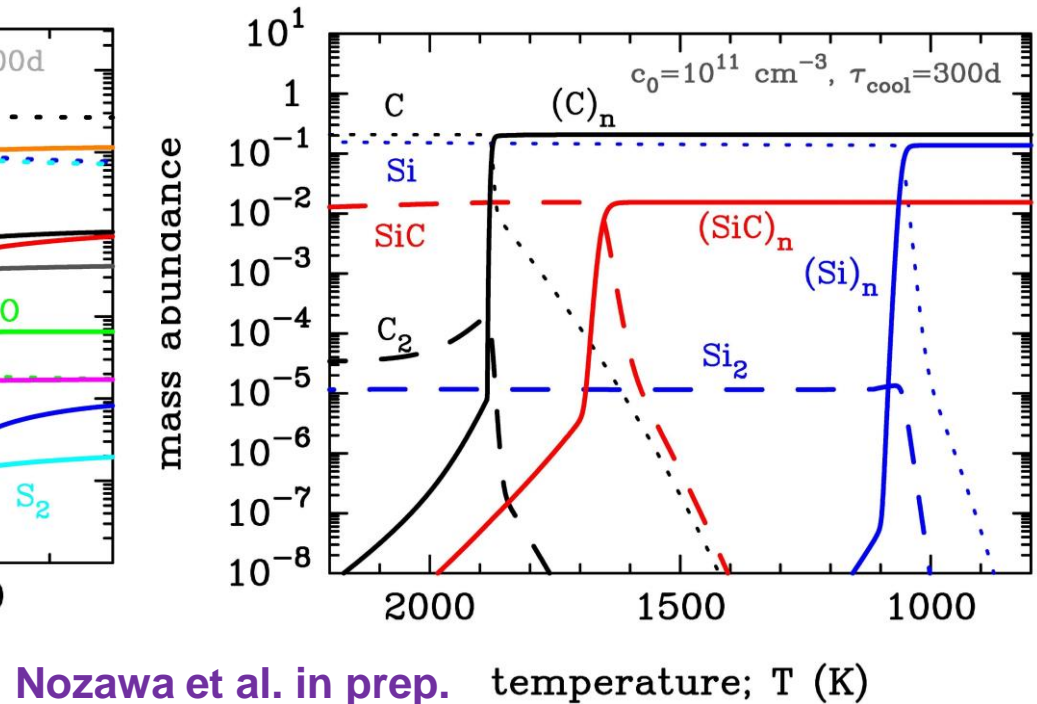
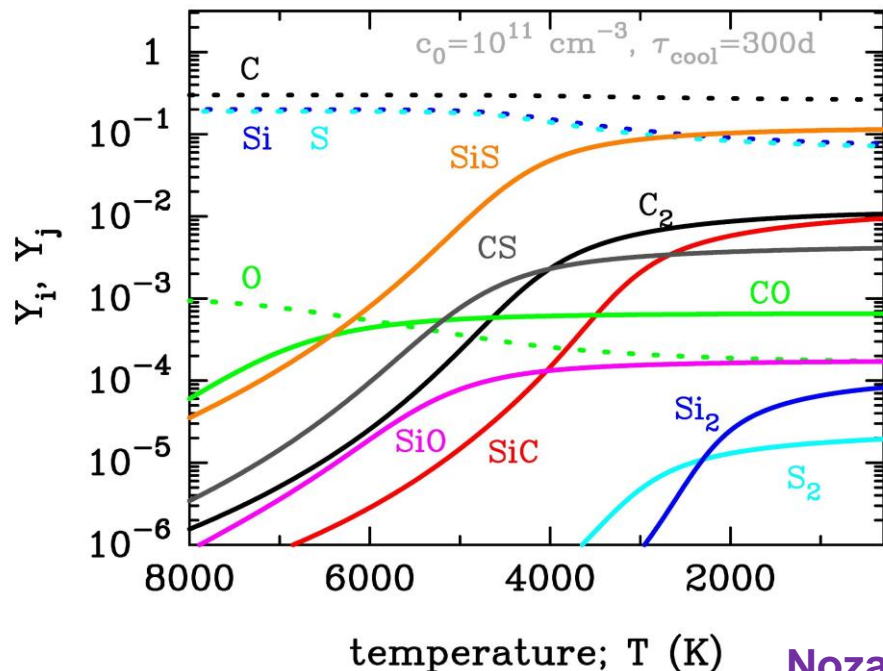
2-6. Hybrid nucleation model

○ Hybrid nucleation model

- formation of diatomic molecules
 - simple chemistry
- nucleation theory
 - kinetics and thermodynamics

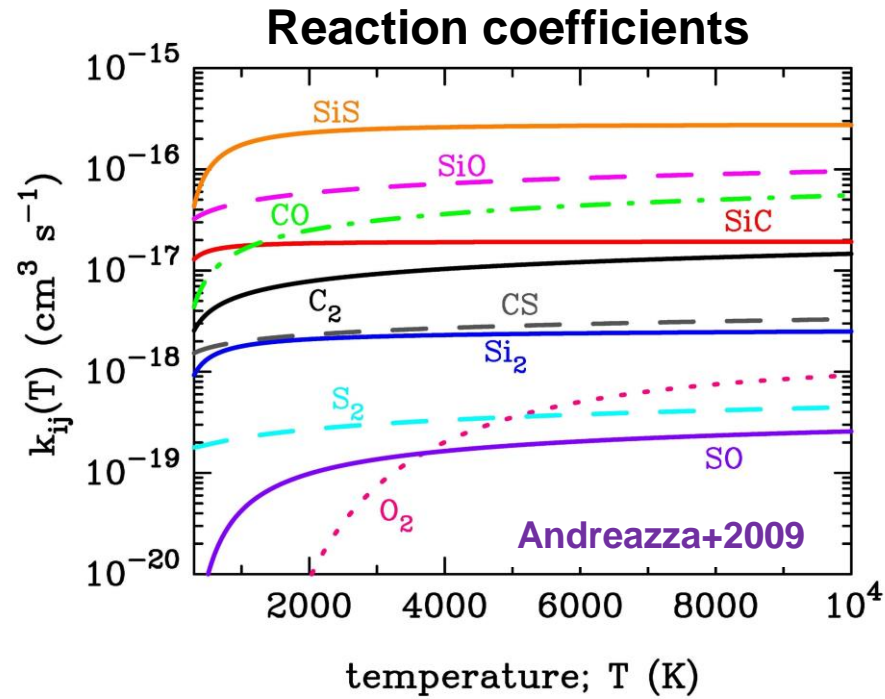


SN-origin presolar SiC Grains (Nittler 2003)



Nozawa et al. in prep. temperature; T (K)

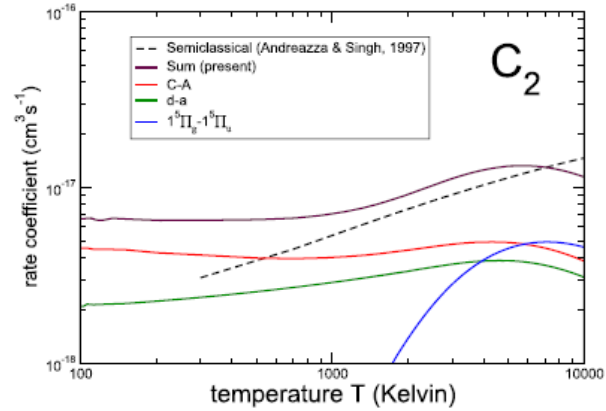
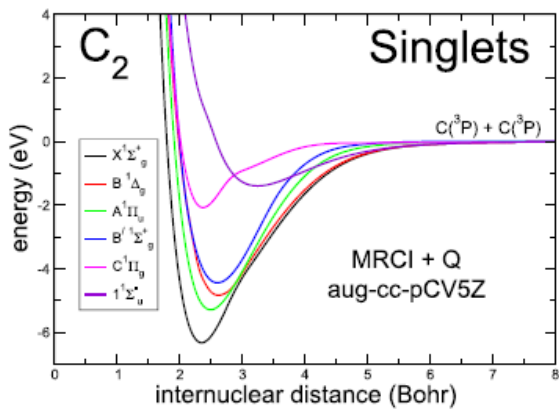
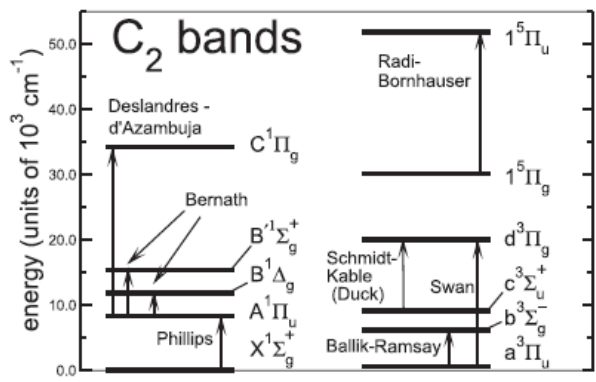
2-7. Insufficient data on reaction coefficients



- Wanted reaction data**
- C-bearing grains
→ C₃, C₄, ... Si₂C, SiC₂
 - silicate/oxide grains
→ MgO, SiO₂, AlO, ...
 - Fe-bearing grains
→ Fe₂, FeO, FeS, ...

○ Quantum chemistry calculation

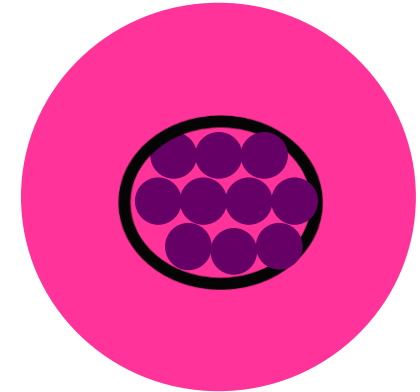
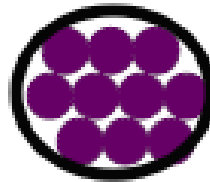
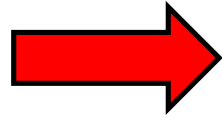
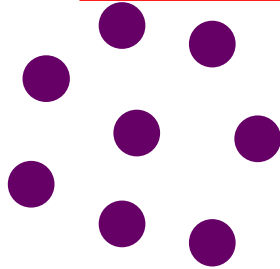
Babb+2019, ApJ, 876, 38



3-1. Theory of nucleation and grain growth

1. Nucleation

(formation of stable clusters)



▪ steady-state nucleation rate

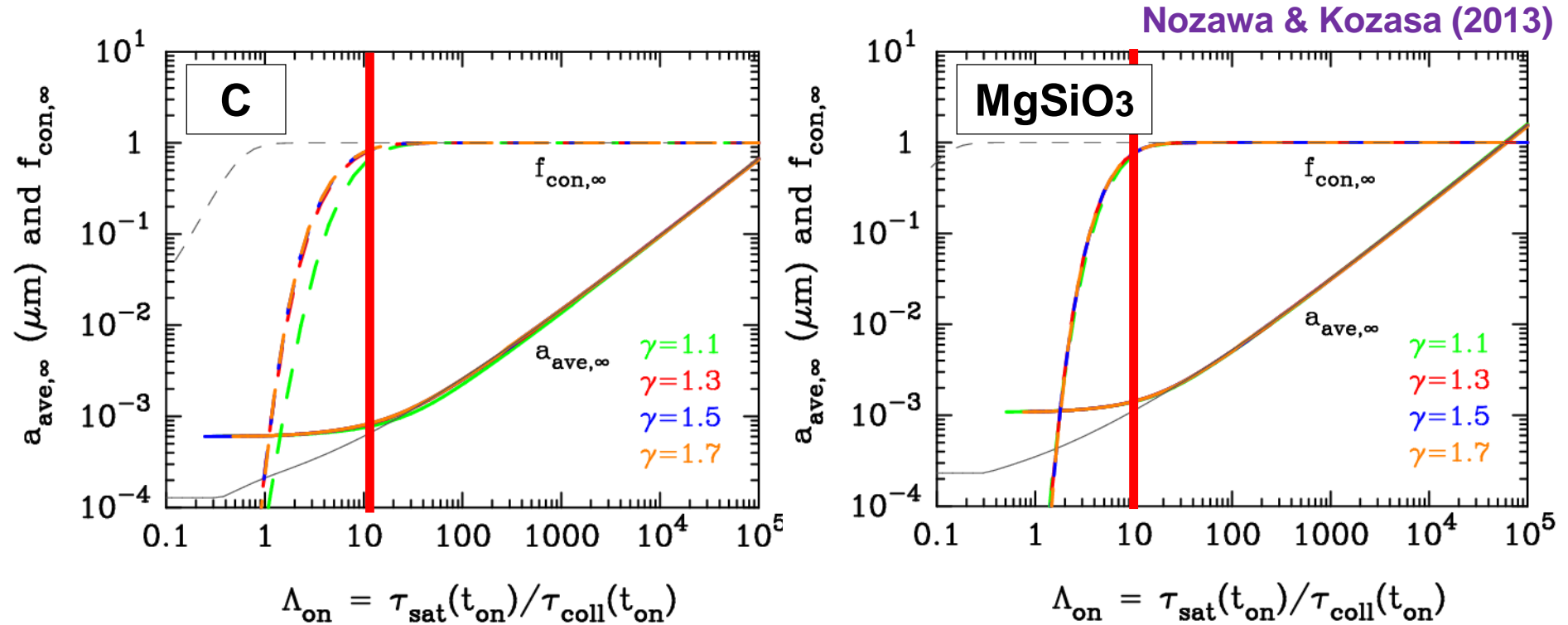
$$J_s(t) = \alpha_s \Omega \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} \Pi c_1^2(t) \exp \left[-\frac{4}{27} \frac{\mu^3}{(\ln S)^2} \right]$$

▪ Growth rate of dust grains

$$\frac{da}{dt} = s \Omega_0 \left(\frac{kT}{2\pi m_1} \right)^{\frac{1}{2}} c_1 \left(1 - \frac{1}{S} \right)$$

number of stable clusters
formed per volume per sec

3-2. Scaling relation of average grain radius



$\Lambda_{\text{on}} = \tau_{\text{sat}}/\tau_{\text{coll}} \propto \tau_{\text{cool}}/\tau_{\text{grow}}$

→ the ratio of supersaturation timescale to gas collision timescale at the onset time (t_{on}) of dust formation

- $\tau_{\text{sat}} \propto \tau_{\text{cool}}$: timescale of nucleation**
- $\tau_{\text{coll}} \propto \tau_{\text{grow}}$: timescale of grain growth**

3-3. Sizes of newly formed grains

(1) larger T_{cool}/T_{grow}

grain growth proceeds much more rapidly than nucleation

→ larger grains



<https://ja.wikipedia.org/wiki/雪だるま>

(2) smaller $T_{cool}/T_{grow} (> 10)$

T_{grow} is moderately shorter than timescale of nucleation

→ smaller grains



<http://asahi-ginza.jugem.jp/?eid=395>

(3) $T_{cool}/T_{grow} < 1$

→ no dust formation



<https://ja.wikipedia.org/wiki/雪>

3-4. Temperature evolution of gas

○ Supernovae

$$T(t) = T_0 \left(\frac{t}{t_0} \right)^{-3(\gamma-1)}$$

○ Stellar winds (AGB stars)

$$T(r) = T_* \left(\frac{r}{R_*} \right)^{-\frac{1}{2}}$$

○ Others

$$T(t) = T_0 \exp \left(-\frac{t - t_0}{\tau_{\text{cool}}} \right)$$

3-5. Cooling rates around 1000 K

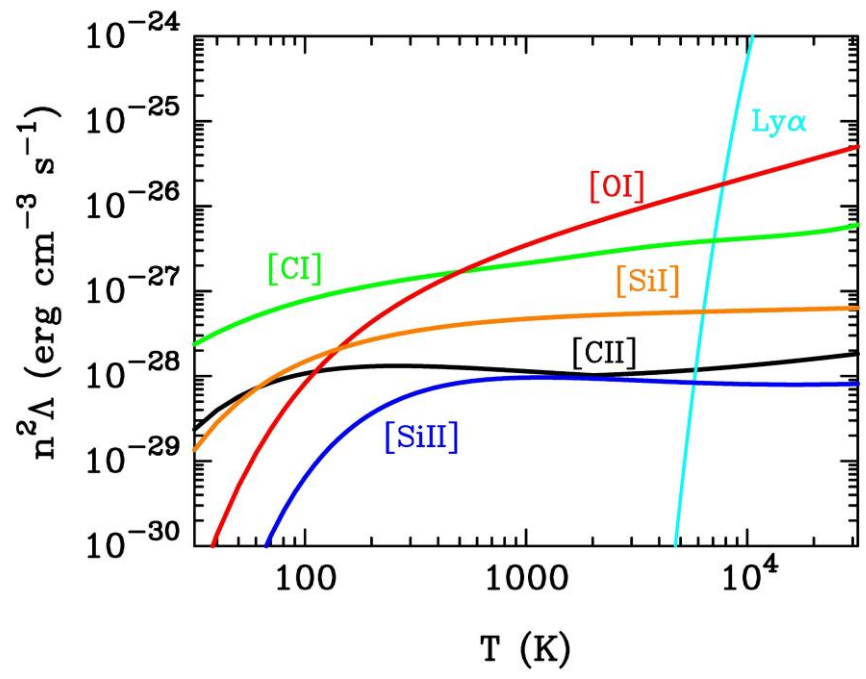
Cooling rate by emission lines

$$\Lambda_i = n_u A_{ul} E_{ul} \beta(\tau_{ul}),$$

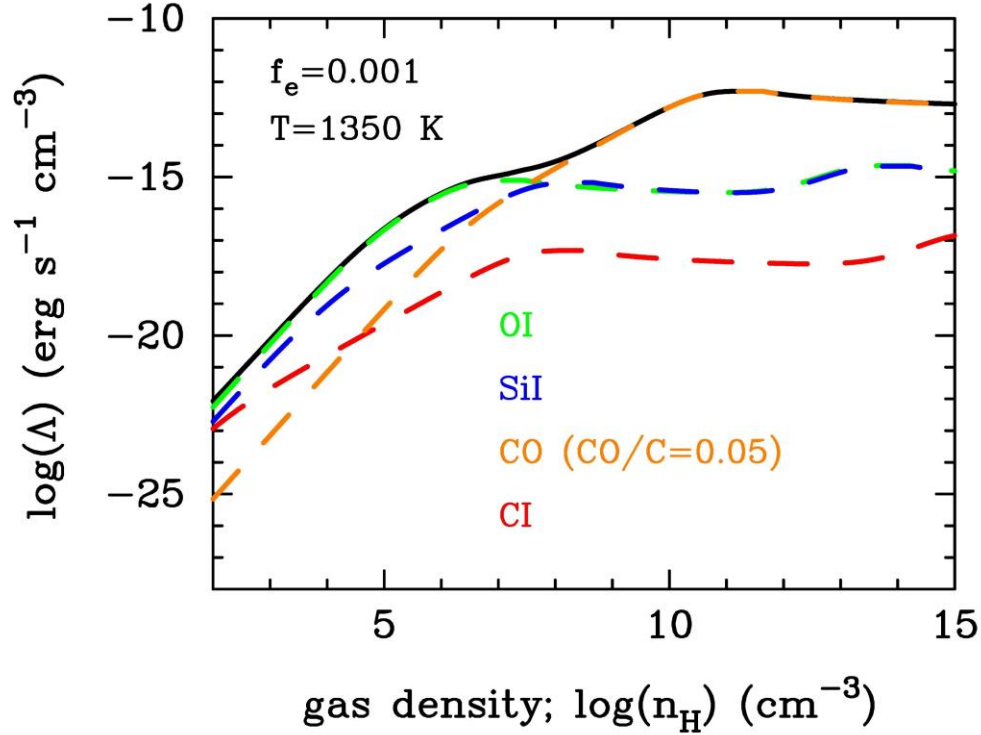
Gas cooling by CO vibration would be great in dense gas



Cooling function in diffuse medium



Cooling function in dense medium



4. Conclusions

(1) Molecules as precursors of dust grains

- important for nucleation process of dust grains
- hybrid nucleation model
 - following only formation of diatomic molecules
- wanted data :
 - reaction rate coefficients of AlO, MgO, Fe₂, FeO, ...

(2) Molecules as efficient coolants of warm gas

- accelerate cooling, affecting size of newly formed dust
- wanted data :
 - Einstein coefficients of CO/SiO ro-vibration transition