Molecular layers in the dust formation zone of AGB stars

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Seminar

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Overview

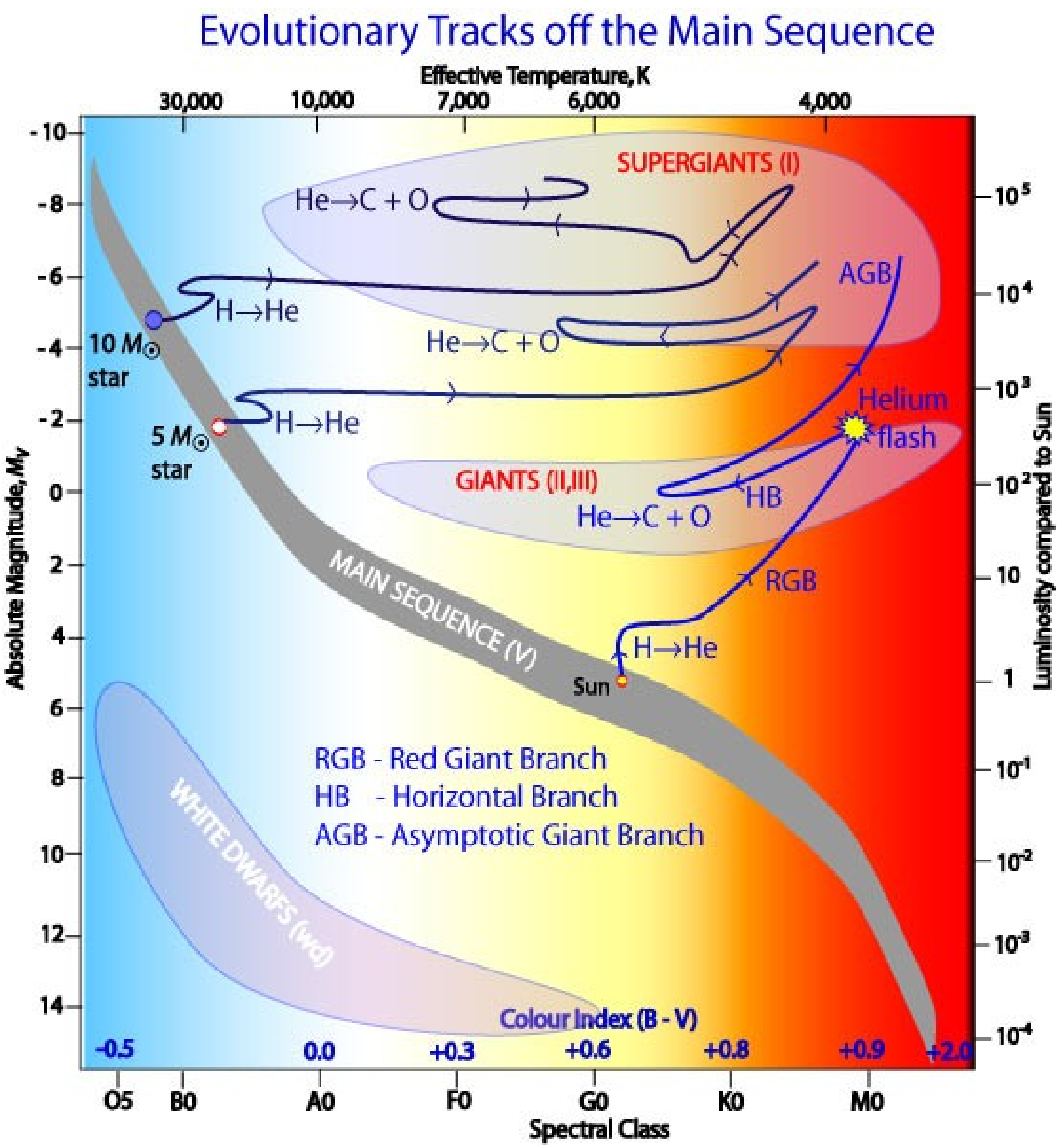
- AGB stars: types & evolution
- The inner wind of AGB stars
- Stationary wind vs. Dynamic pulsations
- Chemical model for the gas phase, cluster formation routes and dust grains
- Results on molecules & dust clusters
- Dust condensation & grain size distributions
- Outlook & Conclusions

AGB stars

Late stage evolution of low- and intermediate stars ($M_*^{ZAMS} < 8\ M_\odot$)

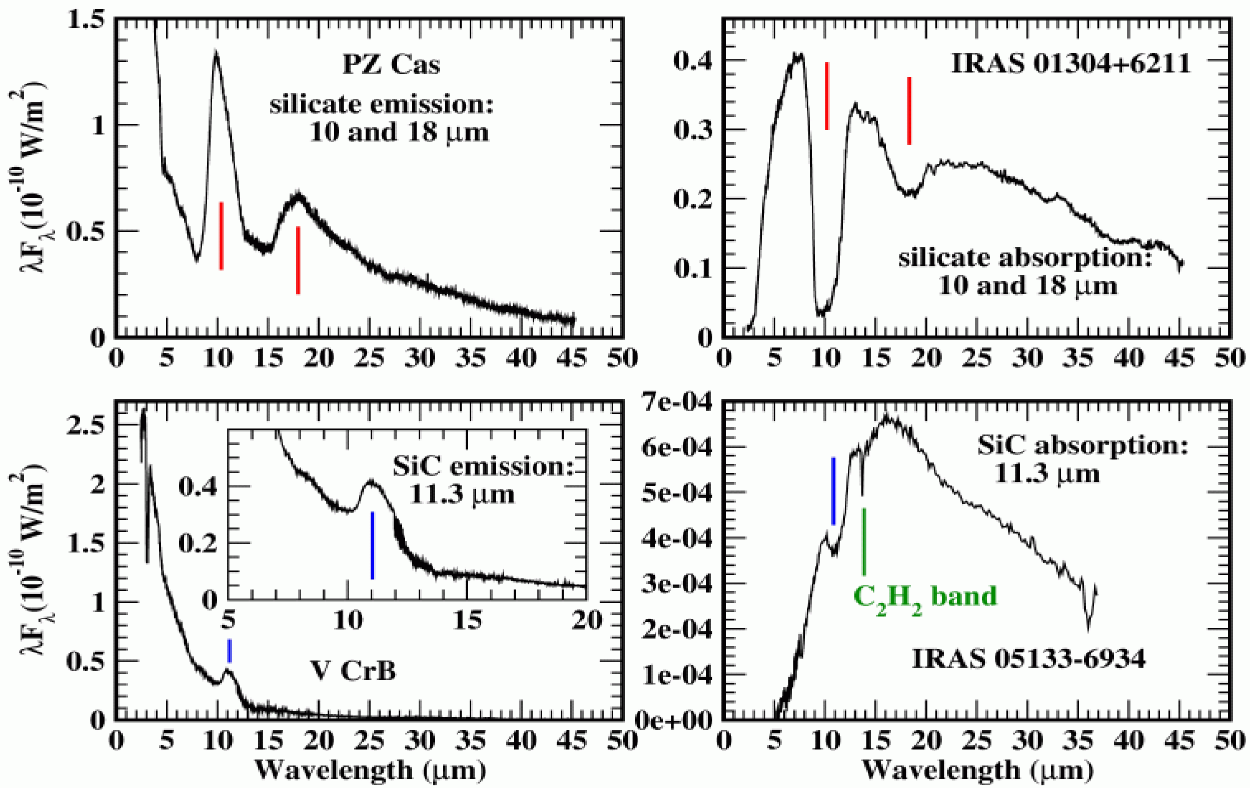
Cool photospheres (T = 2000 - 3000 K) and high luminosities ($L \sim 10^3 - 10^4\ L_\odot$)

High mass loss rates ($10^{-7} - 10^{-4}\ M_\odot/yr$) due to the presence of dust



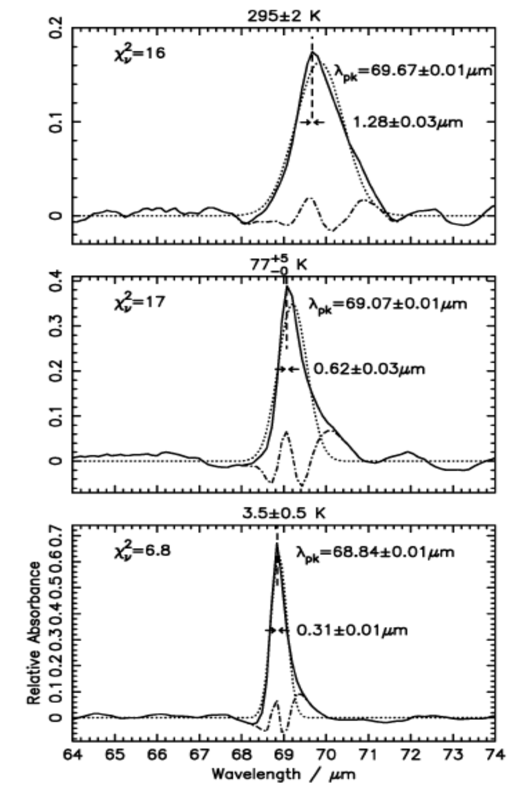
Evidence for dust

Spectral dust features (Silicates & SiC):



Homepage StSci, K. Volk

Forsterite (Mg_2SiO_4) in the lab (69 μm):



Bowey 2013

In addition: MgS at 30 μm
PolyAromatic Hydrocarbons (PAHs) at 3.3,6.2,7.7,8.8,12.7 and 16.4 μm → (hydrogenated) amorphous carbon

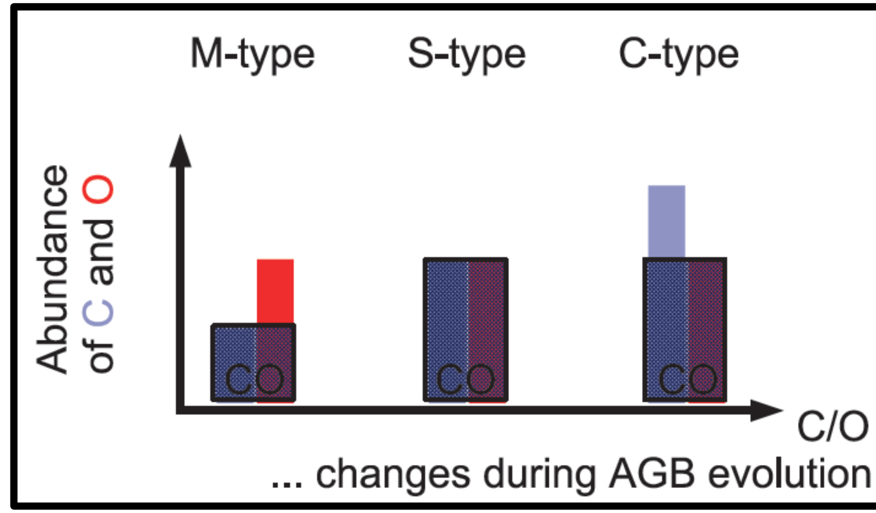
Chemical types of AGB stars

M-type: oxygen-rich, C/O < 1

S-type: C/O ~ 1

C-type: carbon-rich, C/O > 1

... at the photosphere



Hoefner 2009

Low mass: 3rd dredge up mixes carbon to the photosphere → C/O increases

Intermediate mass: Hot bottom burning converts C in N and other CNO products

→ C/O decreases

C/O ratio: molecules

Thermodynamic equilibrium (TE) predicts the presence of:

CO, C, HCN, CS, C_2H_2, CH, CN in the C-rich case

Tsuij 1973

CO, H_2O, SiO, OH, TiO in the O-rich case

→ $E_{bind}(CO) = 11.2$ eV → locks up lesser abundant element

BUT observed are also:

C-bearing molecules in O-rich AGBs:

HCN, CS, OCS, CN, CO_2

Deguchi 1985, Lindqvist 1988, Omont 1993, Bujarrabal 1993, Justtanont 1998, Decin 2010

O-bearing species in carbon stars:

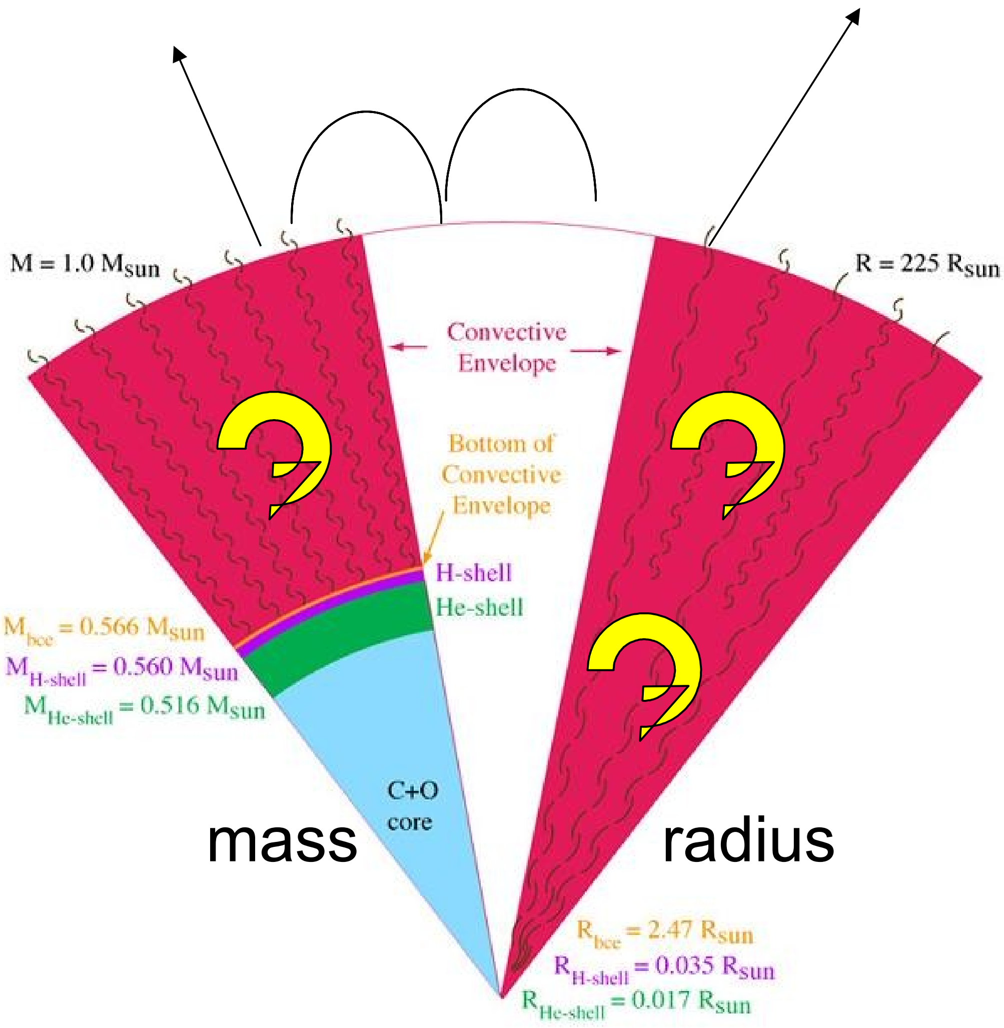
H_2O, OH, SiO

Melnick 2011, Hasegawa 2006, Ford 2004, Schoeier 2006

TE cannot account for these observed molecules

=> Kinetic description is necessary for the chemistry

AGB star structure



Lattanzio 2004

Stellar wind driven by pulsations and dust grains

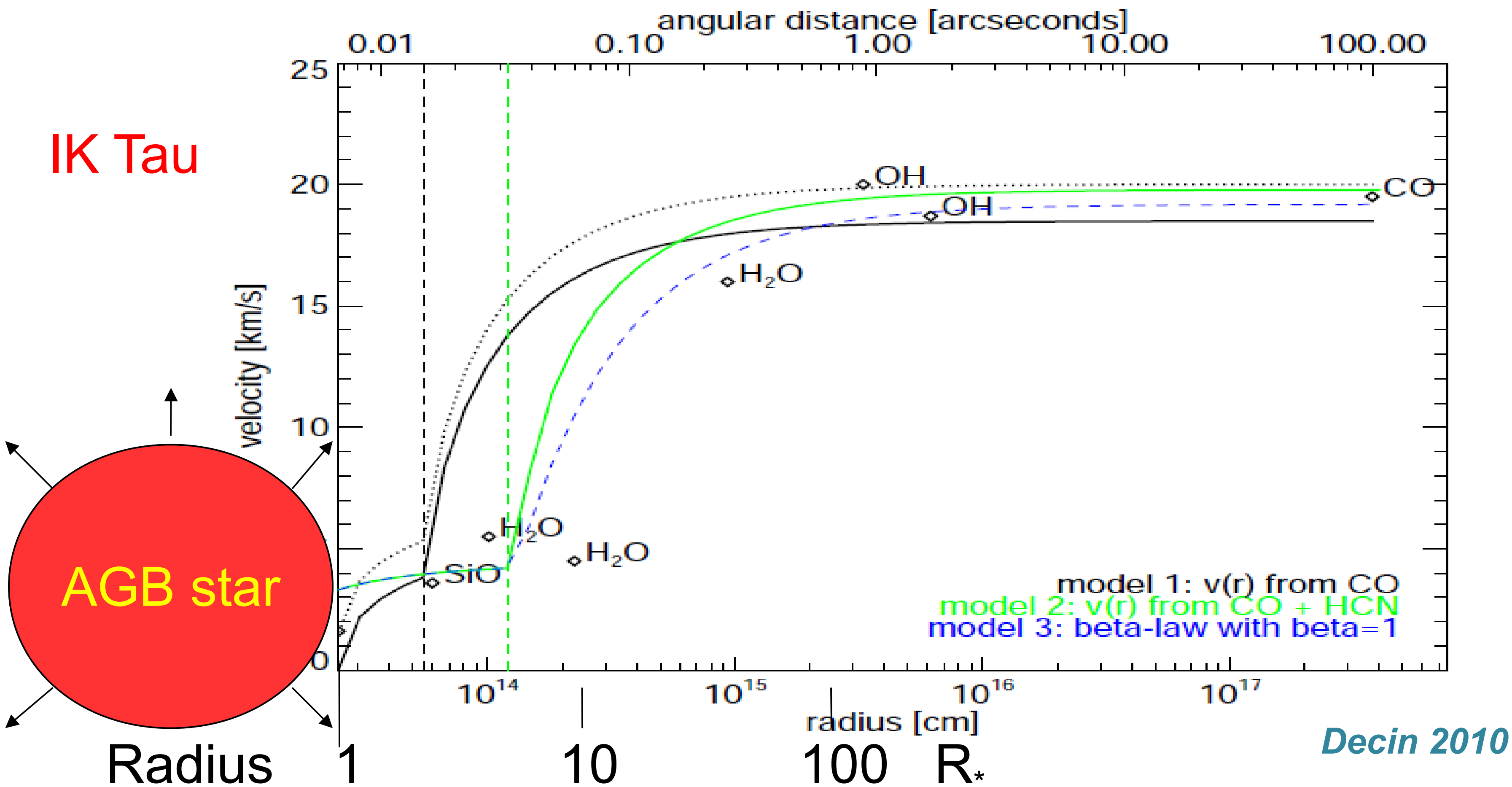
Large convective envelope

Energy generation proceeds in thin burning shells

Degenerate (non-burning) core consisting of carbon and oxygen

The inner wind of AGBs

IK Tau



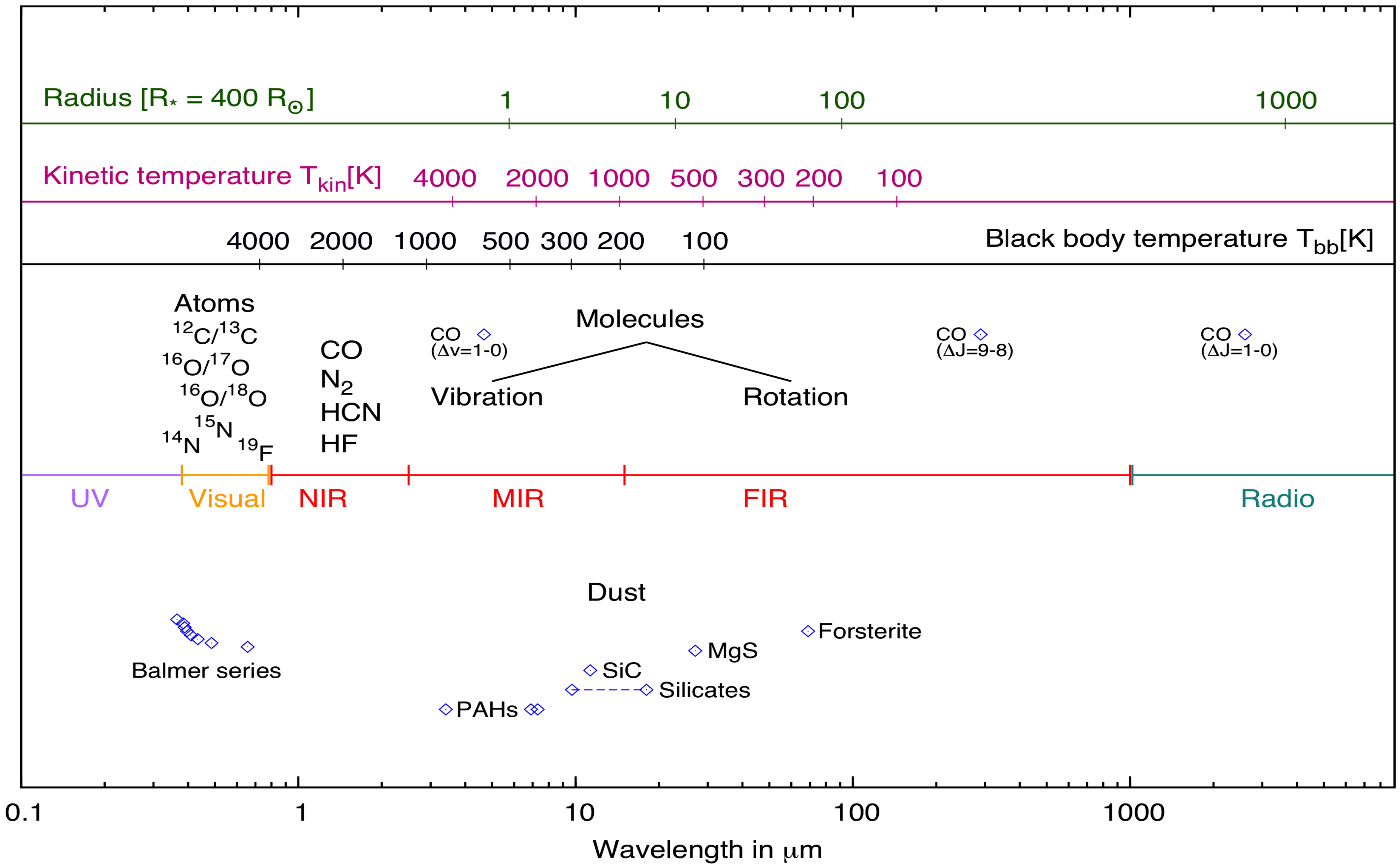
Decin 2010

Pulsating Photosphere	Inner envelope Dust formation	Fully accelerated wind
T = 2200 K	**500-42'000 K**	**100 K**
N = 10^{14} cm^{-3}	**10^6 – 10^{16} cm^{-3}**	**10^6 cm^{-3}**
CO, H_2O, SiO	HCN, CS, CO_2, SiS, PN, AlOH	NH_3, SO_2, H_2S

Interstellar UV radiation

daughter species produced by photo reactions of mother species

Energy scale in the wind



Timescales for AGB stars

Main sequence: ~ 10^7 - 10^{10} years

Time on the (TP) AGB: ~ 10^6 years

Time between dredge-up (mixing) episodes:
~ 10^4 years *Maercker 2009*

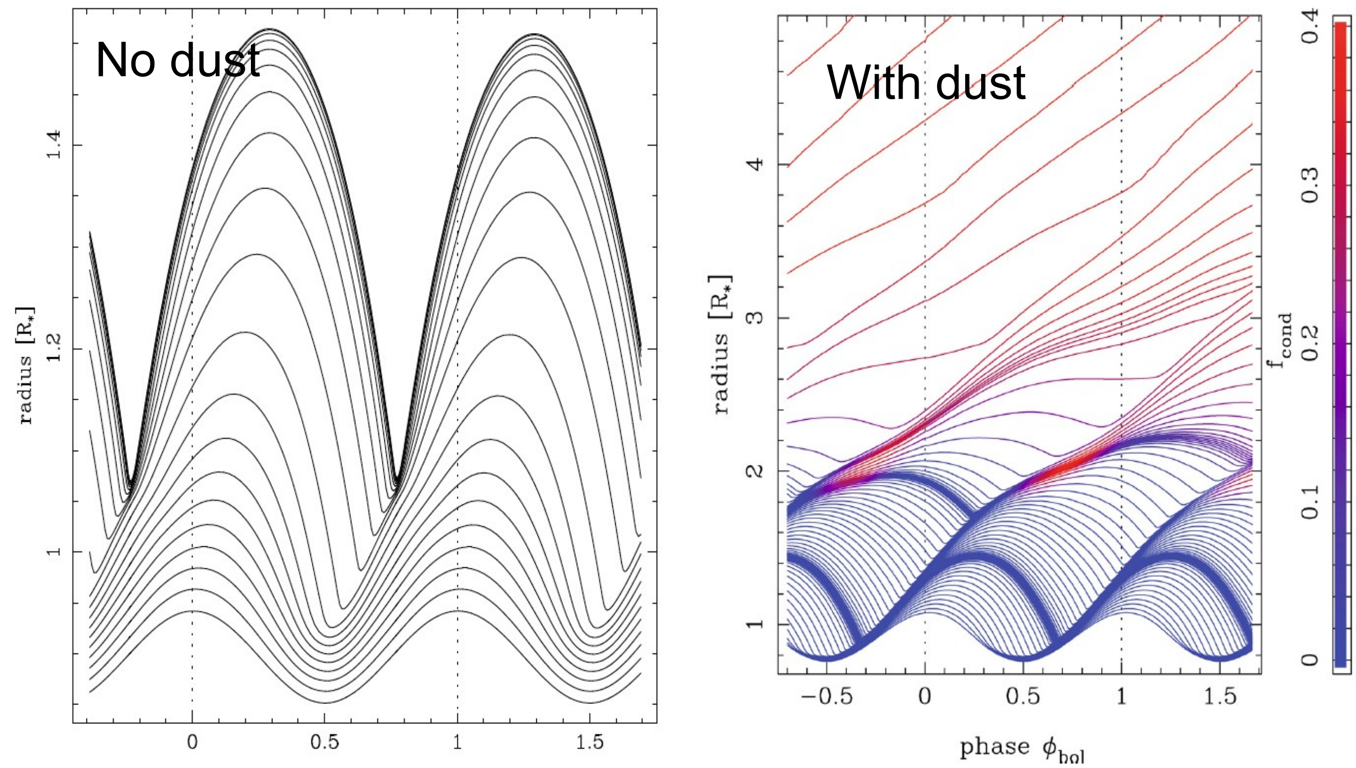
Timescale in the wind:

- Expansion timescale: R_{env} /V_{exp} ~
- Time between pulsations: ~ 1 year
- Chemical reactions: 1/k ~ ms to hours
- Dust growth: coagulation & surface growth

Physics of the inner wind

Periodic shocks cross the stellar atmosphere

→ ambient gas is compressed, heated and accelerated



Nowotny 2010

→ formation of dense and warm gas layers gravitationally bound to the star

→ favourable conditions for molecule, cluster & dust grain formation *Cherchneff 1996/2006/11/12, Willacy & Cherchneff 1998, Duari 1999*

→ ***Pulsations & dust are necessary for mass loss***

Periodic pulsation model for a galactic Mira star: IK Tau

Pre-shock profiles:

Temperature

$$T(r) = T_* \left(\frac{r}{R_*}\right)^{-0.6}$$

number density

$$n(r) \propto n_* \exp\left(\frac{-r}{H}\right)$$

Scale height

$$H = \frac{k_B T}{\mu m_H g} = \frac{k_B T R^2}{\mu m_H G M}$$

Willson&Bowen 1984, Cherchneff 1992

Post-shock profiles:

- Rankine-Hugoniot jump conditions
- Gas excursions on ballistic trajectories

Based on mass, momentum, and energy conservation

$$\frac{d\rho}{dt} \equiv \left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial z}\right)\rho = -\rho(\nabla \cdot \boldsymbol{v}) \, ,$$

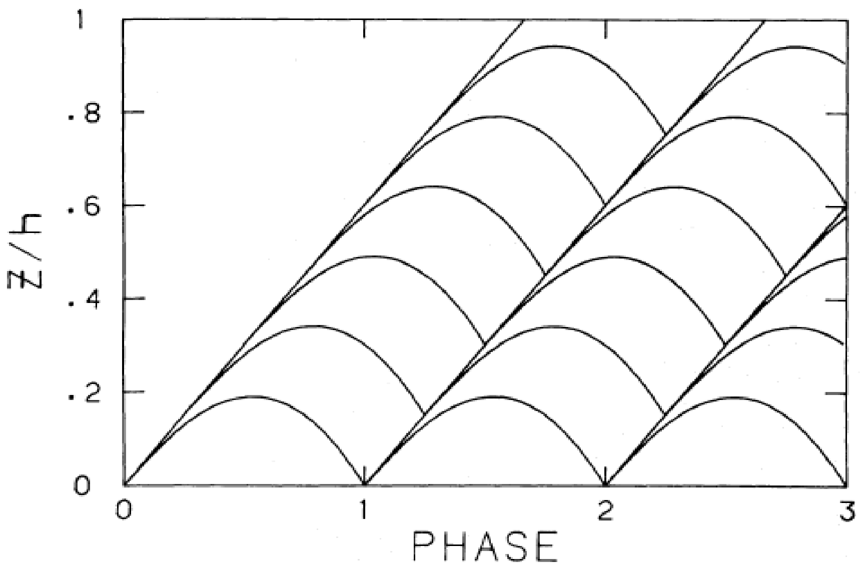
$$\frac{dv}{dt} + \frac{1}{\rho}\frac{\partial p}{\partial z} = -g \, ,$$

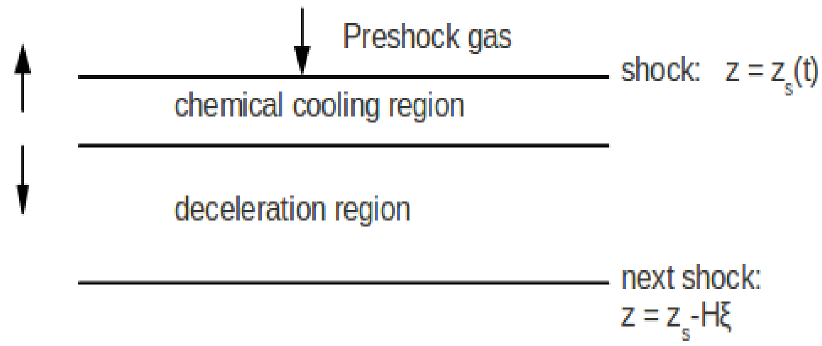
$$\frac{dp}{dt} + \gamma p(\nabla \cdot \boldsymbol{v}) = 0 \, .$$

Parameters for IK Tau

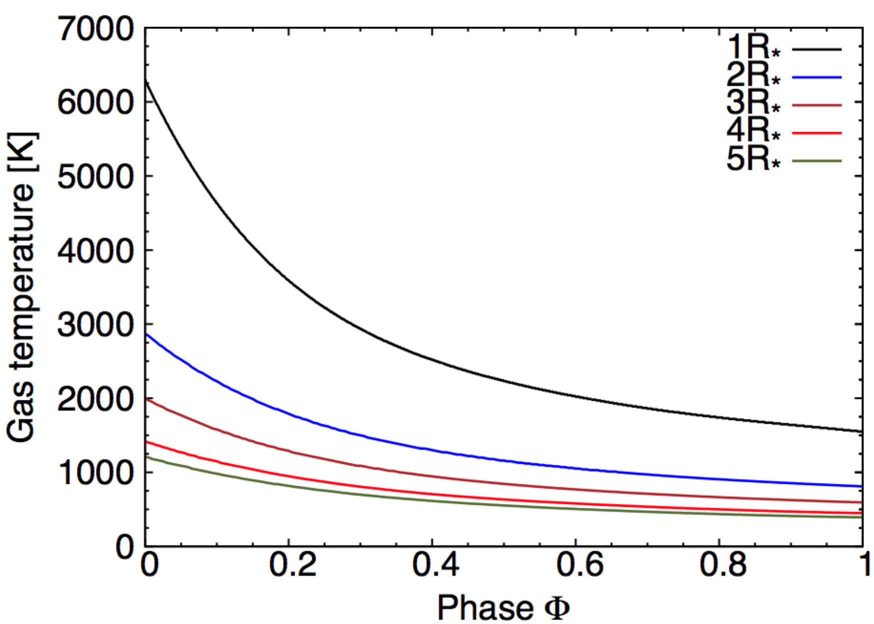
Parameter	Value
T_*	2200 K
M_*	$1 M_\odot$
R_*	2.5×10^{13} cm
v_s	$25 - 32$ kms^{-1}
P	470 days
$n(1R_*)$	3.6×10^{14} cm^{-3}
r_s	1 R_*
C/O	0.75
$\dot{M}$	$(0.4 - 3) \times 10^{-5}$ $M_\odot$/yr
Ψ	1.9×10^{-2}

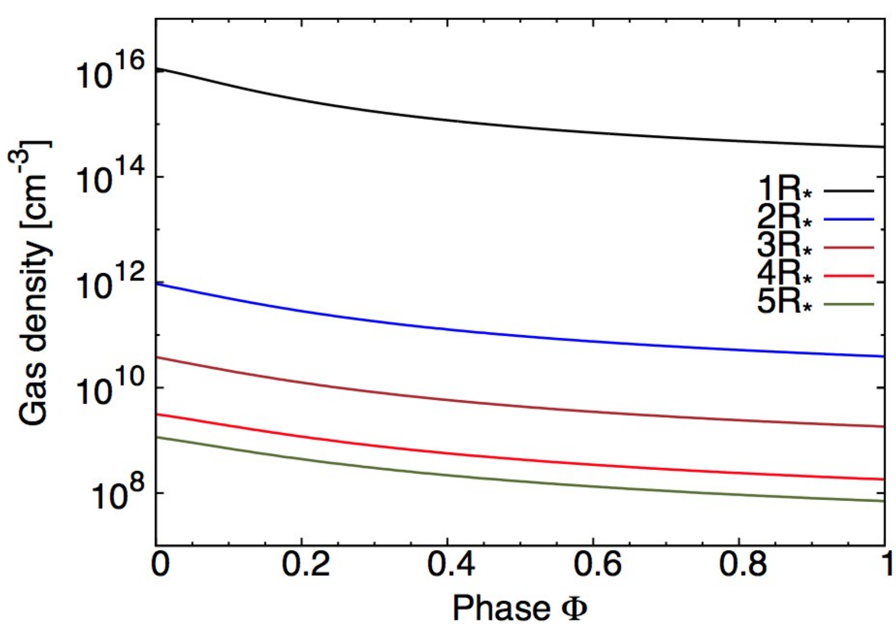
Periodic pulsation model for Miras





Fox & Wood 1985
Bertschinger & Chevalier 1985
Cherchneff 1996
Willacy & Cherchneff 1998
Duari et al. 1999
Cherchneff 2006, 2011 & 2012





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Gas-phase chemistry

Molecular detections in inner oxygen-rich AGB winds:

H_2O, OH, SiO, SiS, NaCl, **CO, CO_2, HCN, CS**, SO, SO_2, NH_3

PN, PO *Milam 2007, Justtanont 1998, Decin 2010, Justtanont 2012, Menten 2010, De Beck 2013*

Chemical network contains termolecular & bimolecular (neutral-neutral, collisional fragmentation, radiative association) processes – no ions

Reaction type	Reaction	formulation	Gas conditions
Unimolecular			
Thermal decomposition	AB	$\rightarrow$ A + B	High T
Bimolecular			
Neutral-exchange	AB + C	$\rightarrow$ A + CB	T dependent
Collisional dissociation	AB + M	$\rightarrow$ A + B + M	High T
Radiative association	A + B	$\rightarrow$ AB + γ	T independent
Termolecular			
Termolecular formation	A + B + M	$\rightarrow$ AB + M	(Very) high n

17 elements
105 molecules
426 reactions

GOAL: Reproduce these molecules in the observed amounts

Chemical network

Bimolecular reaction: A + B → C + D

Change in number density of species C:

$$\frac{dn(C)}{dt} = k_{AB}\, n(A)\, n(B) \qquad k_{AB} = \alpha \left(\frac{T}{298\ \mathrm{K}}\right)^{\beta} \exp\left(\frac{-E_a}{RT}\right)$$

Set of reactions :

Arrhenius reaction rate

$$\frac{dn_i}{dt} = \sum_{j,k} k_{jk} n_j n_k + \sum_{j,k} k_{jkM} n_j n_k n_M - n_i \sum_{l} k_{il} n_l - n_i \sum_{n} k_n$$

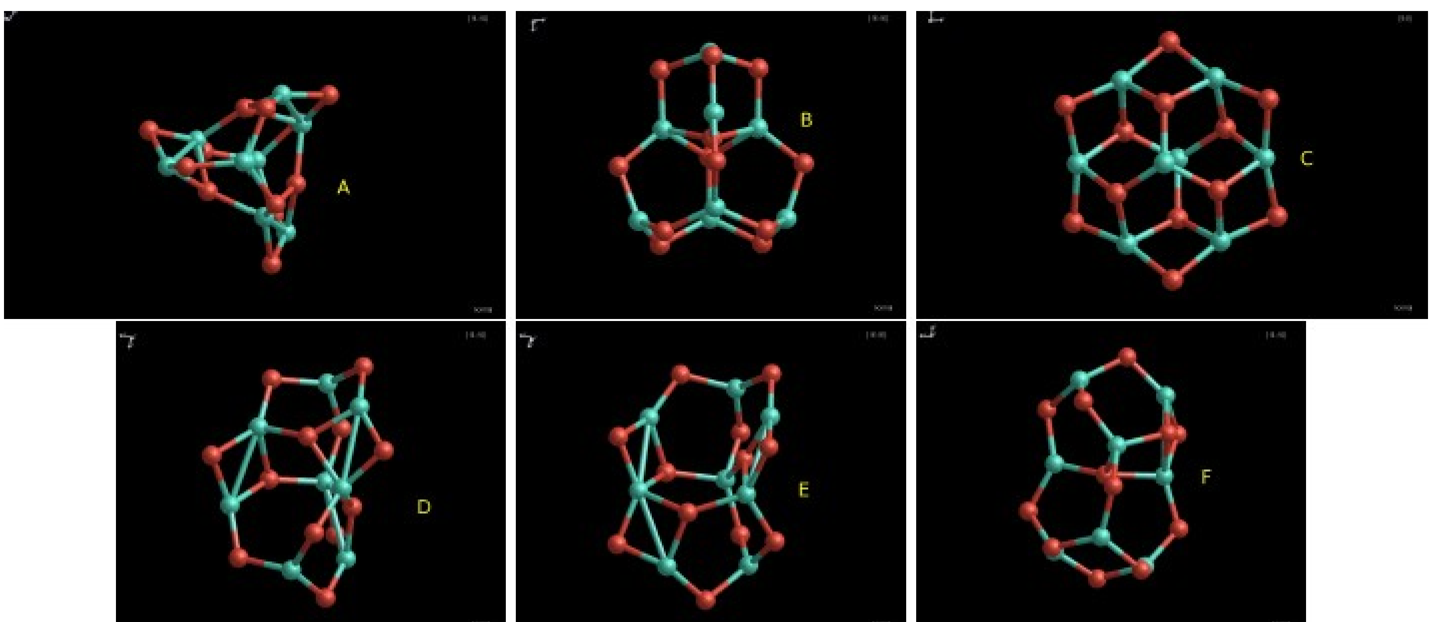
→ set of stiff, coupled, non-linear ordinary differential equations (ODEs)

→ ODEs subject to varying temperature and densities

Cluster nucleation routes

Chemical network involves formation pathways to dimers of alumina (Al_2O_3) & forsterite (Mg_2SiO_4), enstatite ($MgSiO_3$) of metal oxides (SiO, MgO, FeO, TiO), and pure metal clusters (Fe, Al, Si)

- Structure determination by a semi-classical Monte-Carlo-based candidate search & subsequent quantum Density Functional Theory (DFT) calculations
- DFT analysis yields thermochemical properties, which indicate trends for reaction mechanisms and kinetics



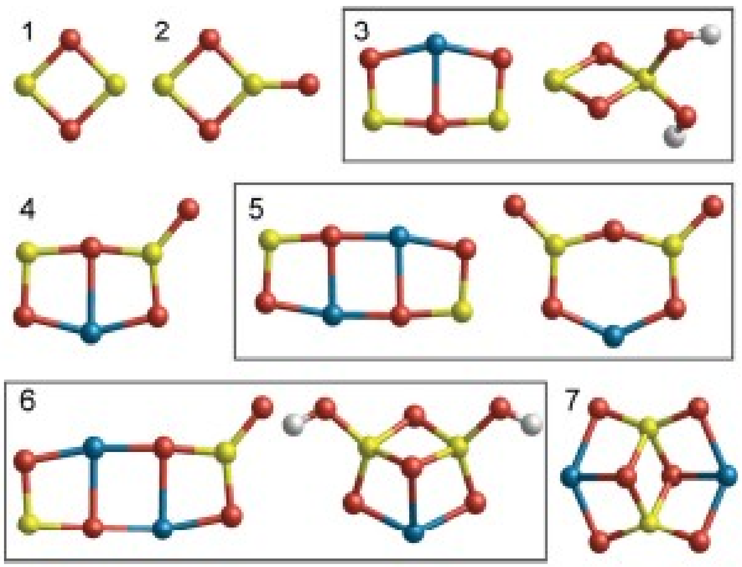
$$\Delta G = \Delta H - T\Delta S$$

Al_8O_{12}

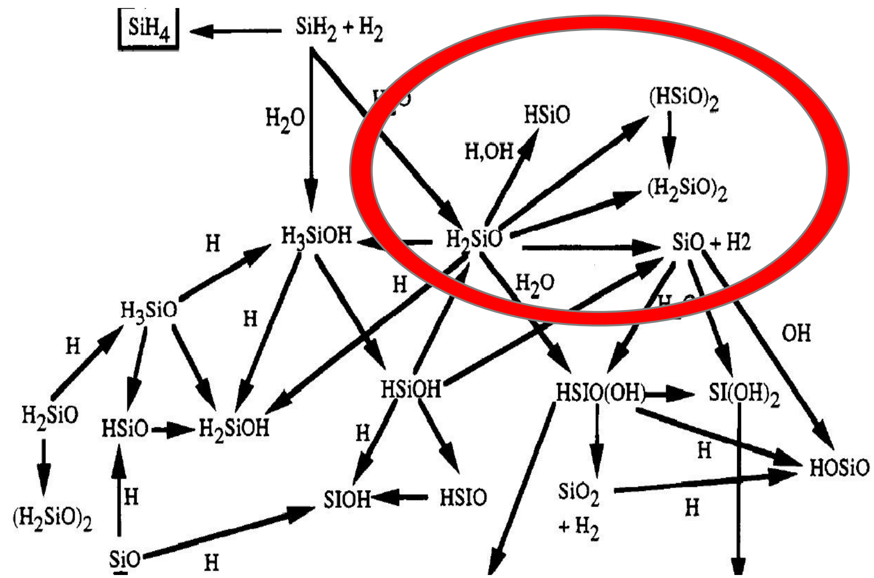
Energetically favoured alumina tetramers

Cluster nucleation routes

Silicates: forsterite dimers $Mg_4Si_2O_8$



Goumans & Bromley 2012
Enstatite formation pathway



Zachariah & Tsang 1995
Formation of hydrogenated silicon oxides
in silane-rich flame

- SiO dimerisation <u>too slow</u> to start silicate nucleation
- Nucleation proceeds via HSiO, $H_2Si_2O_2$ & $H_2Si_2O_3$ formation
- Growth via successive oxidation & Mg inclusion steps
- Efficient mechanism to synthesise silicate dimers (enstatite and forsterite) between ~ 4 R_* and 6 R_*

Dust grain condensation

Formalism based on Brownian thermal motion, which accounts for the scattering, fragmentation, and coagulation of the grains *Plane 2013, Sarangi & Cherchneff 2014*

→ Grains size distributions are derived for silicates of forsterite and enstatite stoichiometry, and alumina.

→ Grains are assumed to be spherical, volume conserving and stable to (stellar) radiation

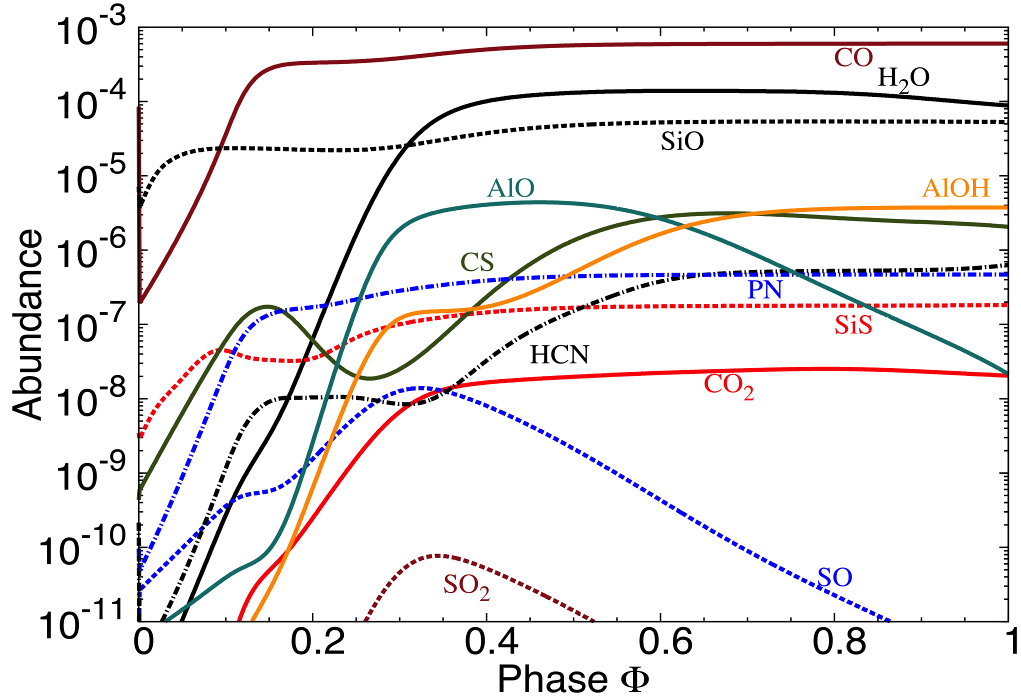
Timescales for dust condensation ?

Consider from hydro models *Bowen 1988, Nowotny 2010*

Dust grains keep growing over several pulsation periods, whereas gas phase molecules reform within one period.

- Drift velocities at $r > 3\ R_*$ for silicates – 1.5 kms^{-1} correspond to two pulsations to cover 0.5 R_*

Results: Molecules in IK Tau



1 R*

CO, H_2O, SiO, SiS, HCl, AlOH & PN form close to the star as soon as gas relaxes and cools down.

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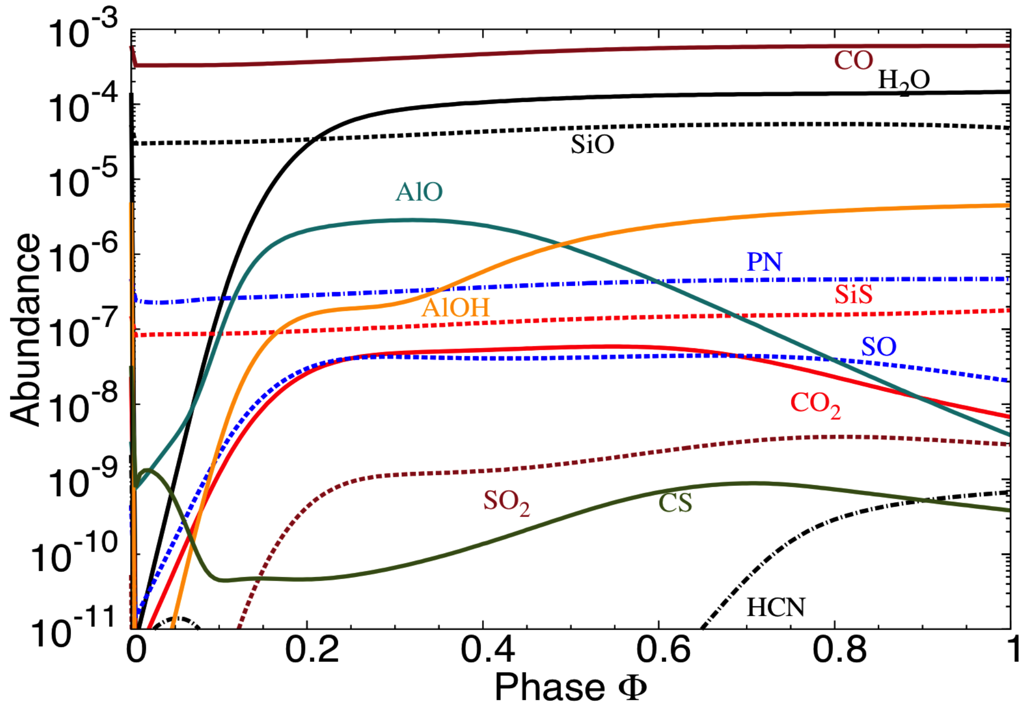
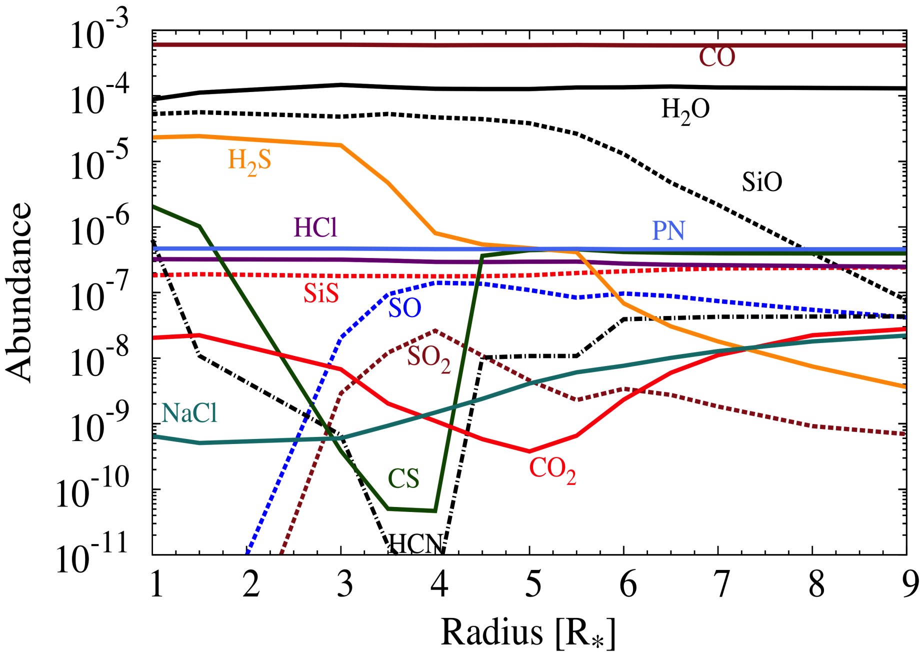


3 R*

Some molecules are more shock chemistry-dependent. C-bearing species form from CO breaking by shocks SO, HCN, CS, CO_2

Results: Molecules in IK Tau



Our parent species include

CO, H_2O, SiO, SiS, PN, SO, HCN, CS, CO_2, $AlOH$, TiO, HCl & $NaCl$

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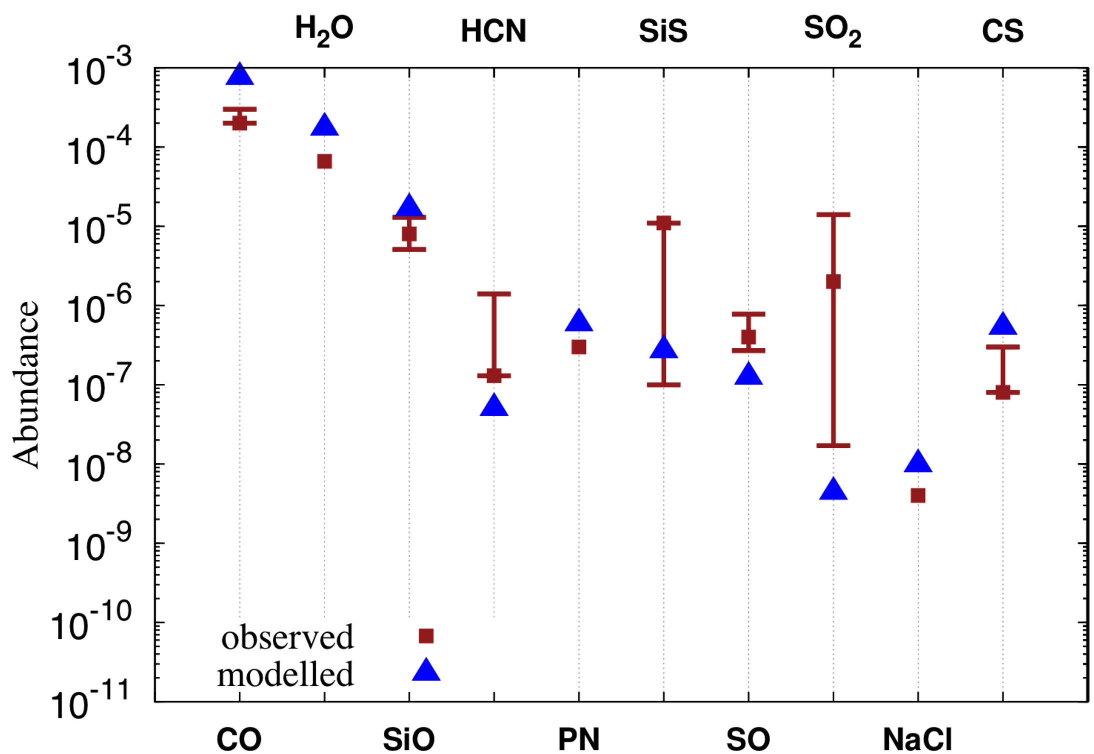
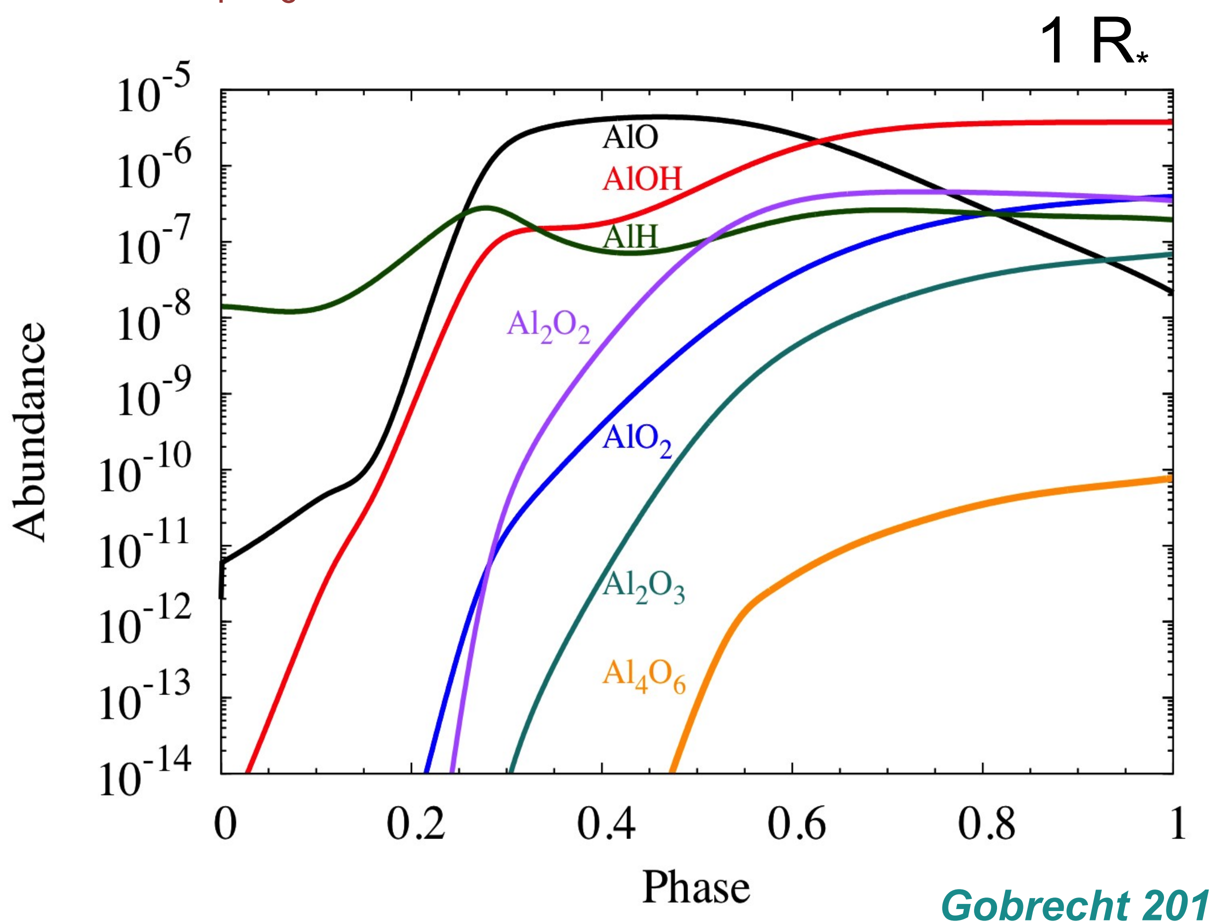
- Modelled abundances for 12 molecules at 6 R* agree well with observations
- Validate shock chemistry scenario → strong impact of shocks on the gas and solid phases of the inner wind
- Discrepancy for SO_2



Results: Dust clusters in IK Tau

Alumina dimers Al_4O_6:



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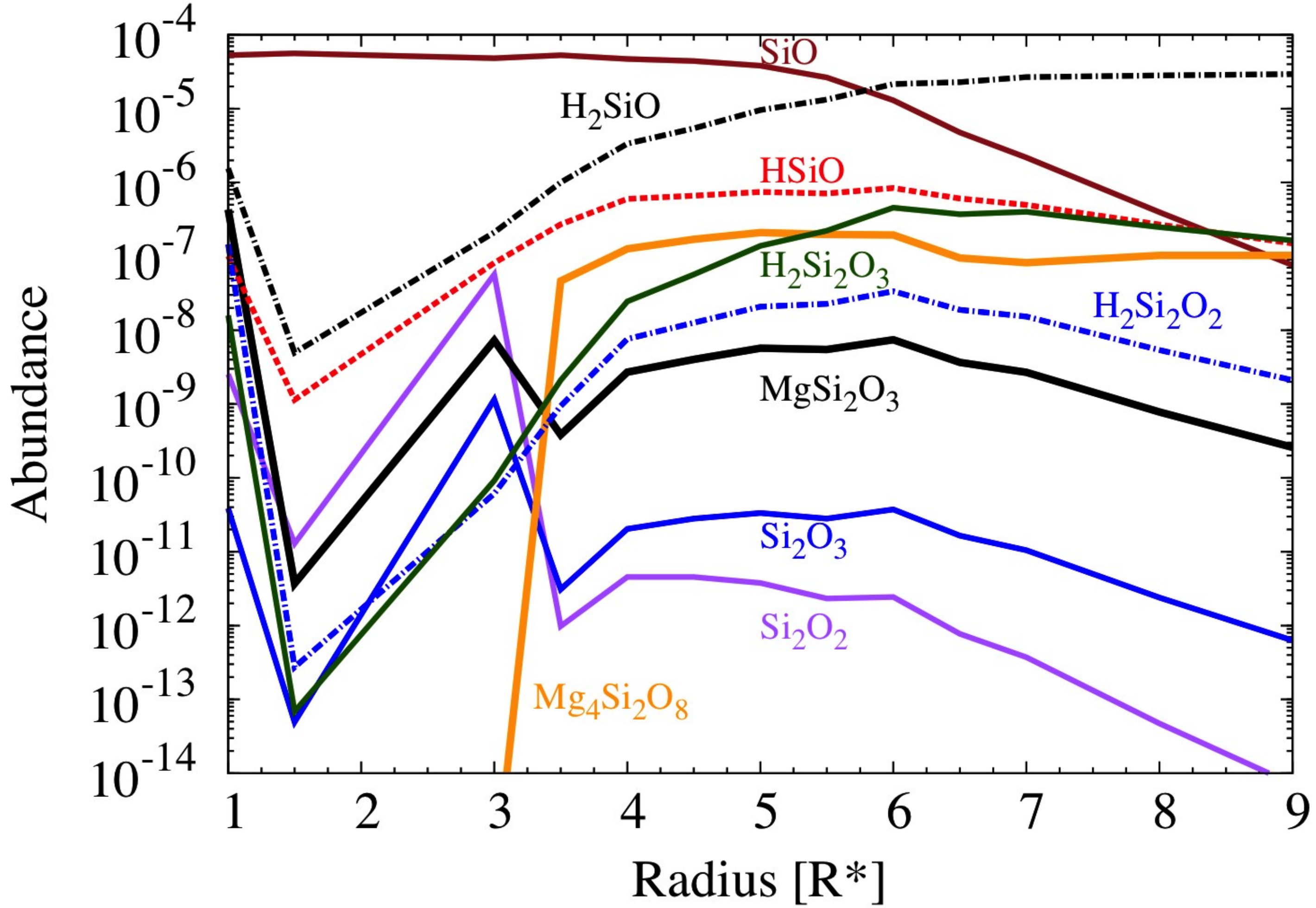
Form at 1 R* when T_{gas}< 2000 K

Abundance of dimers on the low side

Other formation channels, which deplete AlOH ?

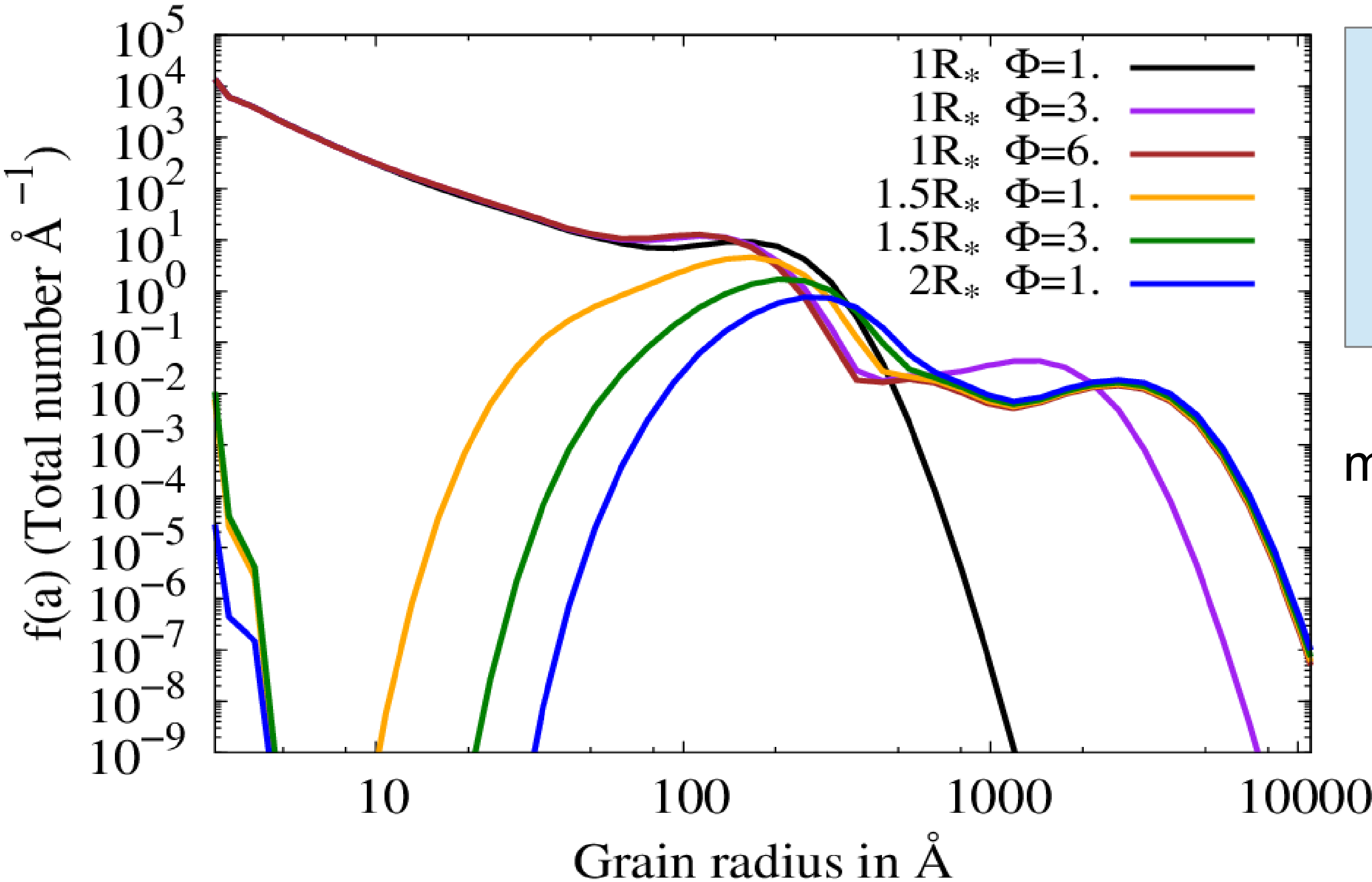
Results: Dust clusters in IK Tau

Silicates: forsterite dimers $Mg_4Si_2O_8$



Start forming at 3.5 R_* from HSiO dimerisation

Grain size distributions: alumina

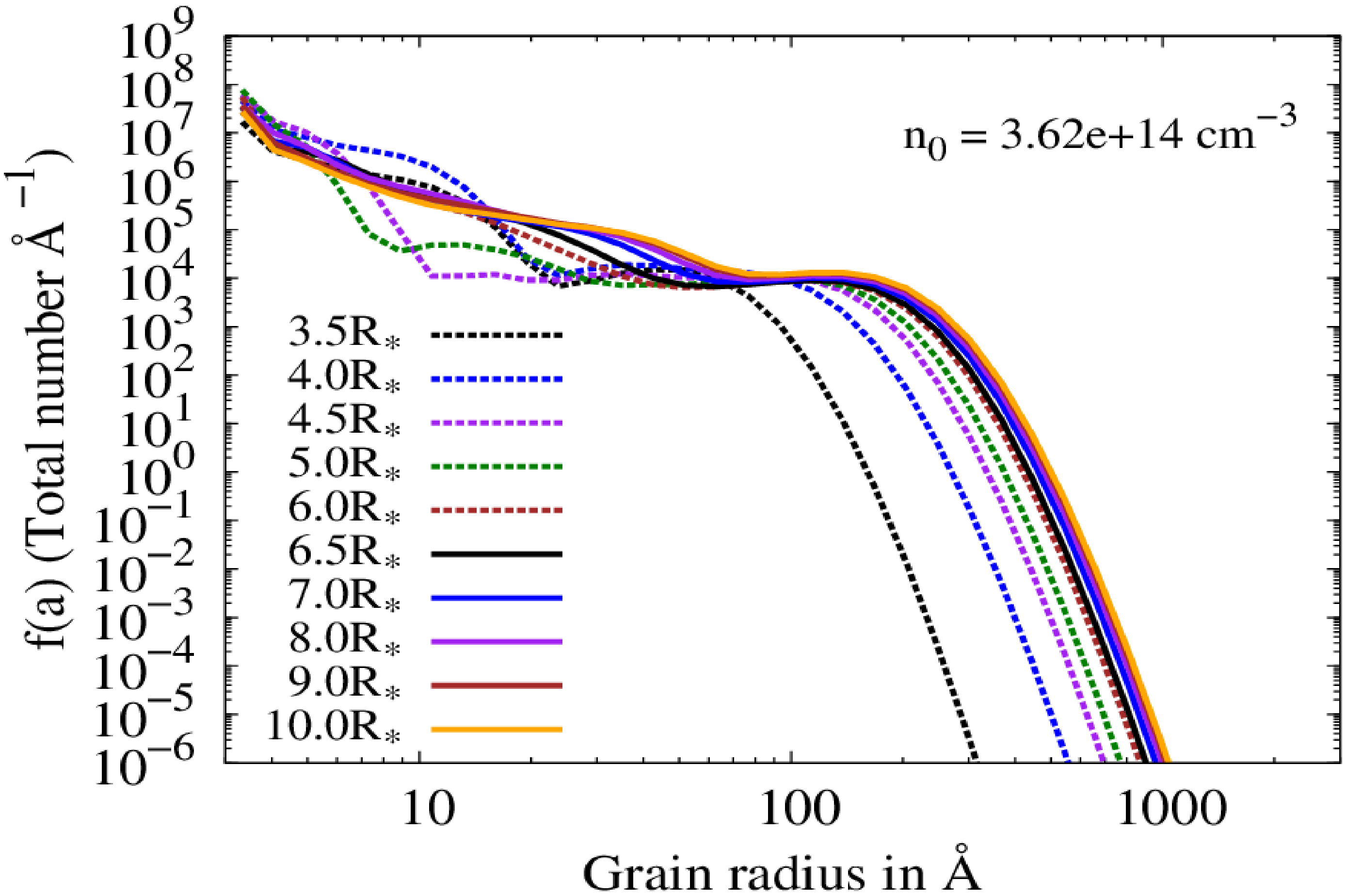


3.3 E-06
1.0 E-05
2.1 E-05
2.2 E-05
2.4 E-05
2.8 E-05

Dust/gas mass ratio

Large grains > 0.02 µm are already formed at 1, because gas densities are high in the postshock gas

Grain size distribution: forsterite

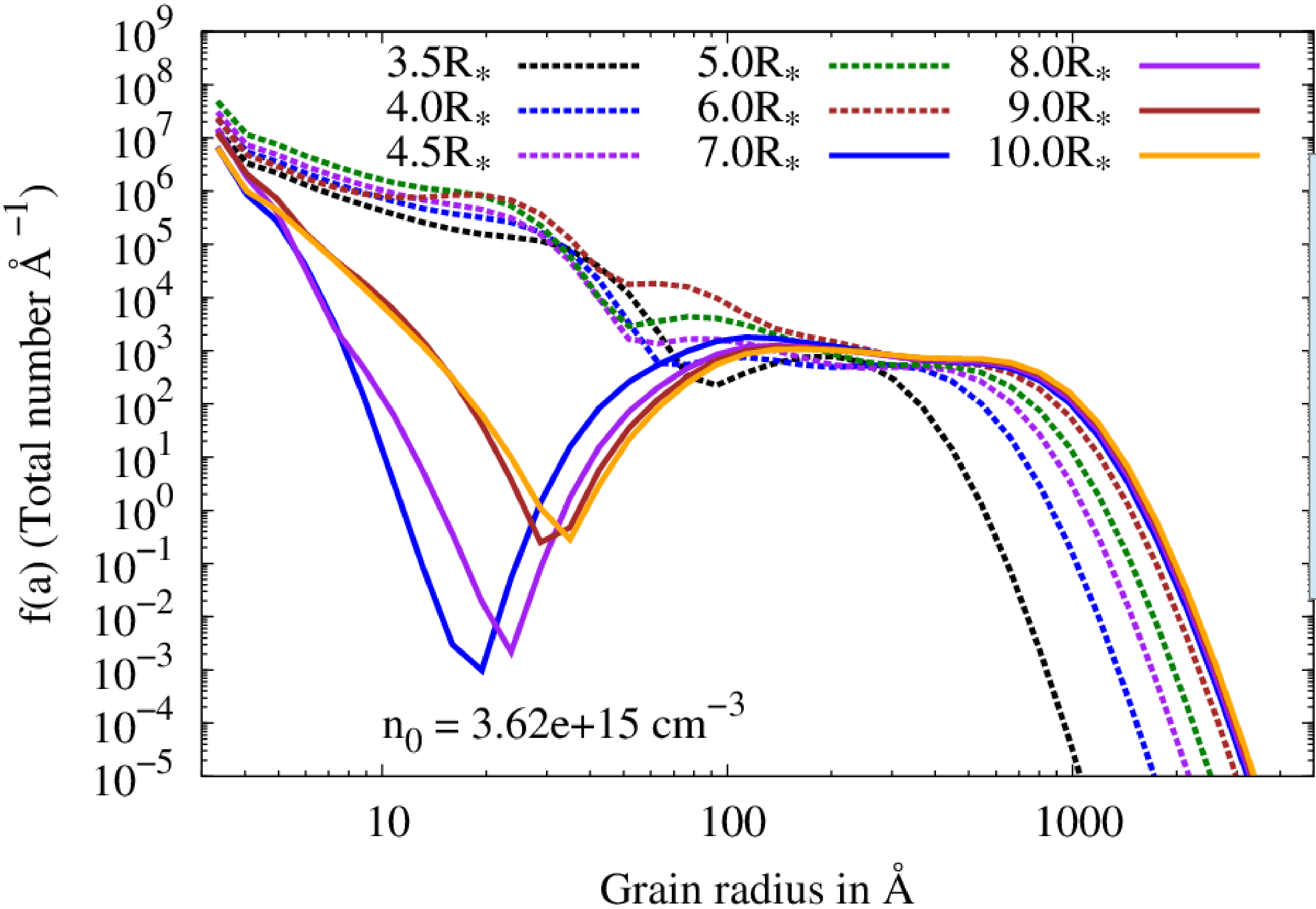


Dust/gas mass ratios

3.5R*	1.3 E-04
4.0R*	4.6 E-04
4.5R*	6.0 E-04
5.0R*	7.3 E-04
6.0R*	1.0 E-03
7.0R*	1.3 E-03
8.0R*	1.6 E-03
9.0R*	2.0 E-03
10.0R*	**2.3 E-03**

- Forsterite grains grow to larger sizes with increasing number of pulsations and radius
- Dust/gas mass ratio after 8 R_* agrees with observations
- Grain size peaks at 0.02 μm, which is a bit low (from obs. a = 0.1 μm)

Enhanced density: forsterite



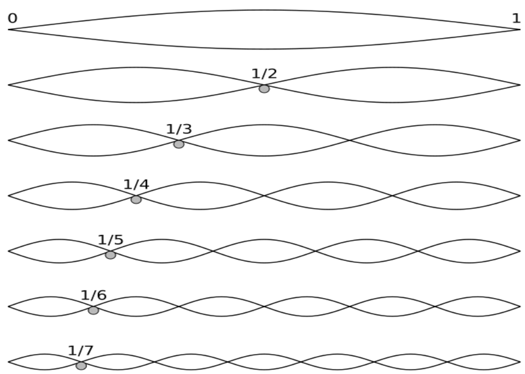
Dust/gas mass ratios

3.5R*	4.7 E-04
4.0R*	1.1 E-03
4.5R*	1.9 E-03
5.0R*	3.0 E-03
6.0R*	5.3 E-03
7.0R*	6.1 E-03
8.0R*	6.7 E-03
9.0R*	7.5 E-03
10.0R*	**8.0 E-03**

A factor x10 in gas density results in grain size distributions peaking at ~ 0.1 μm → inhomogeneous wind will help!

Semiregular variables

Regularity classes (Mira, Sra, Srb and Irregular) are rather loosely defined in GCVS



Mira: M_v > 2.5 mag, P > 100 d

Sra: Mixture of Miras and Srbs

Srb: T_* > 3200 K, P < 150 d

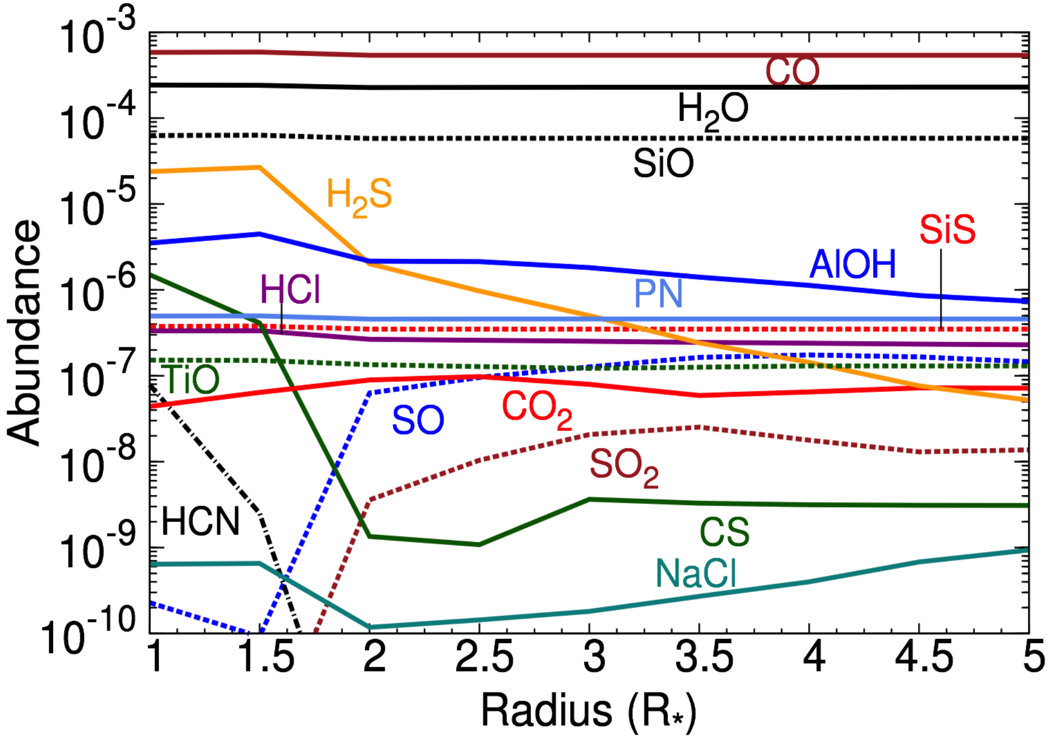
Stellar parameters of SRVs compared to Mira variables:

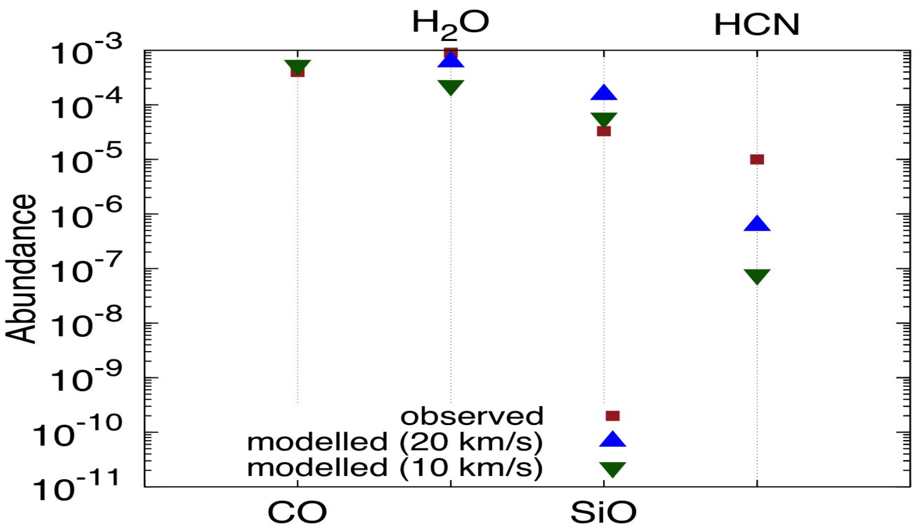
T_*, M_* are higher

P, R_*, C/O, v_{term}, $\dot{M}$ are lower

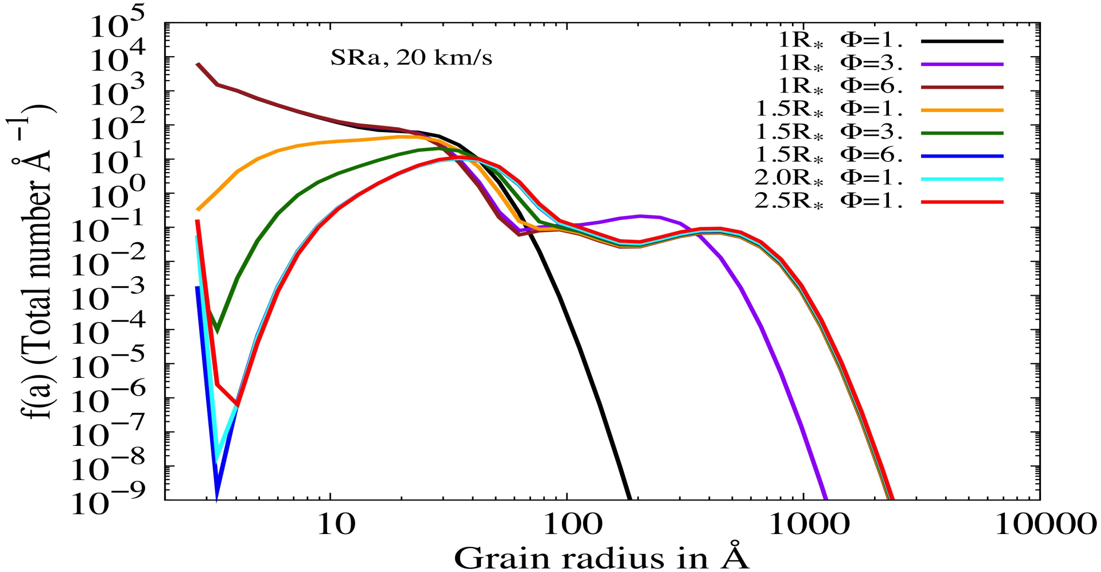
=> interpreted as stars on the early AGB

Results for W Hydrae (SRa)



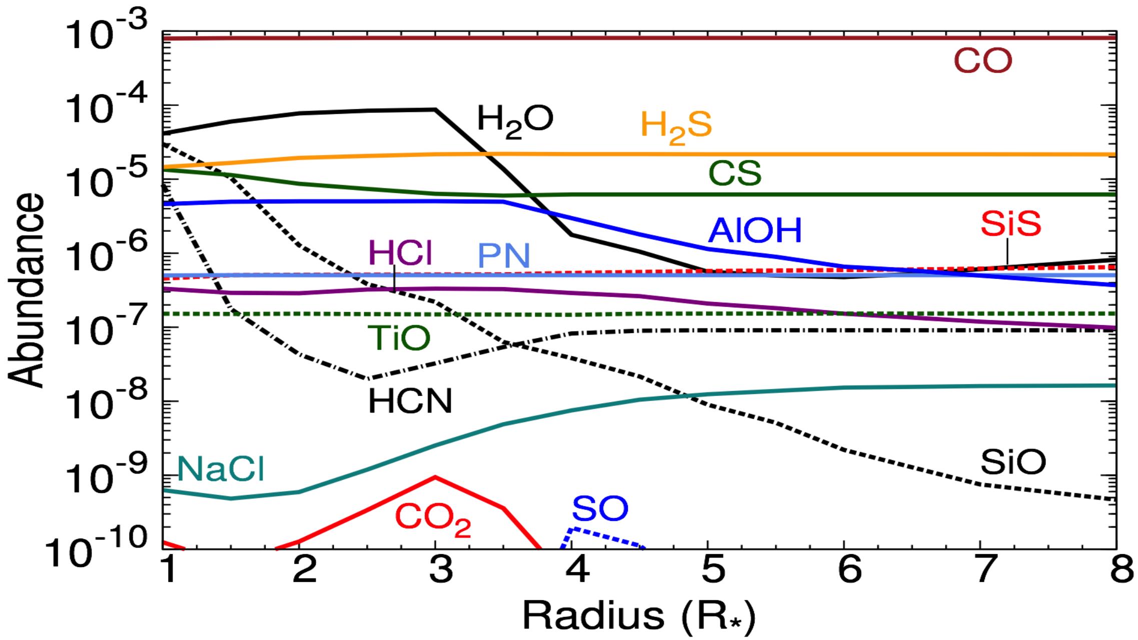


Khouri 2014



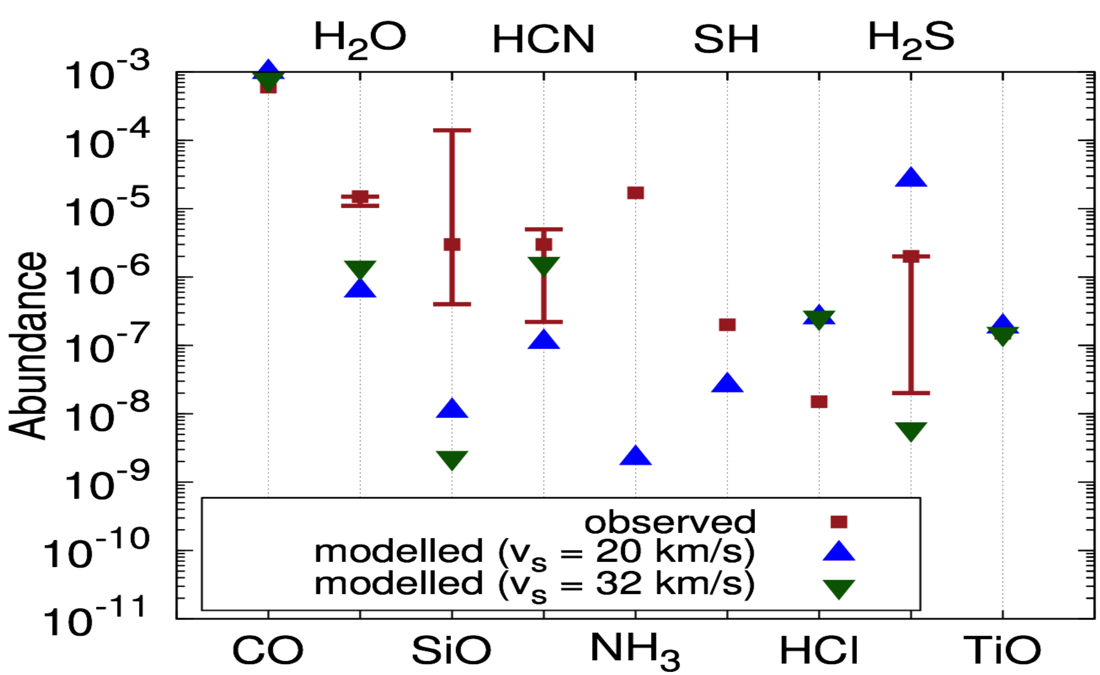
Alumina grains form, Silicate clusters form, but at too low gas density to efficiently condense

Results: S-type star



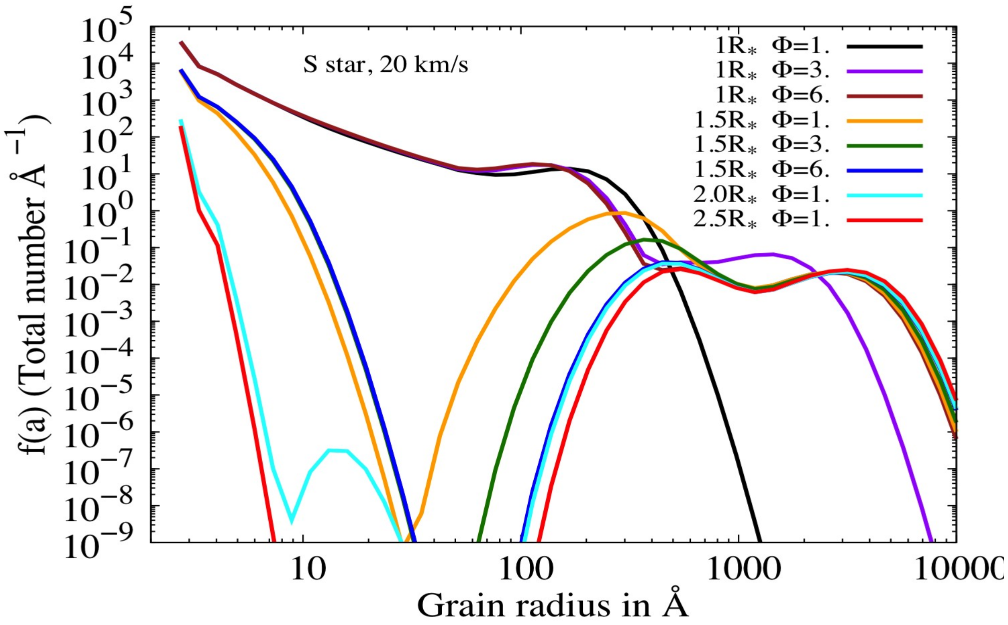
Molecular abundances vs. Radius for a 20 km/s shock and parameters for W Aquilae

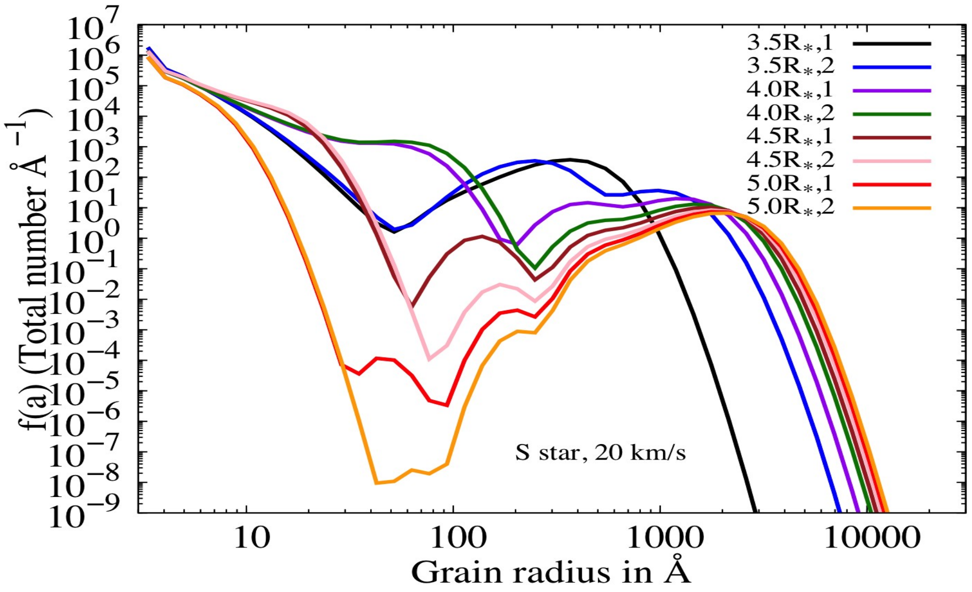
Danilovich 2014



Comparison of modelled abundances with the most recent Herrschel/HIFI and previous observations

Results: S-type star

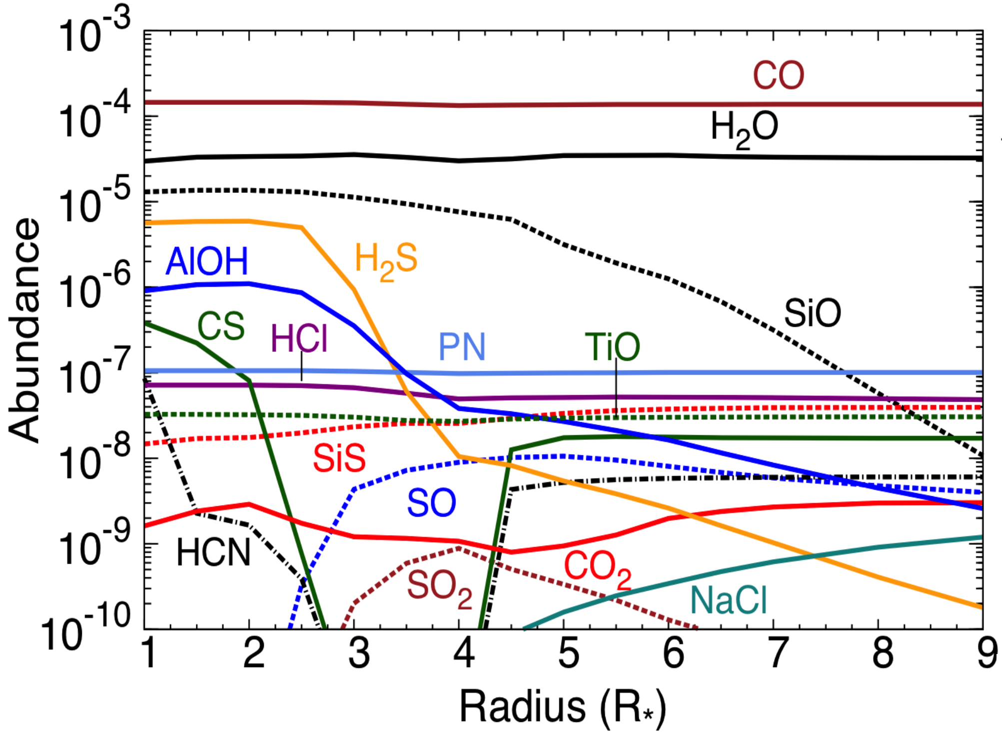


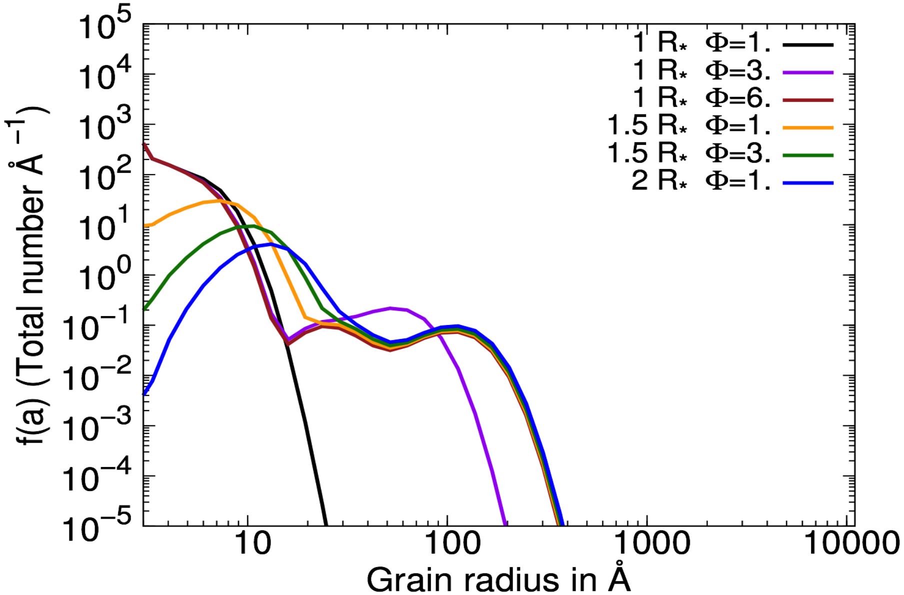


Alumina and forsterite grains form in quantity and large sizes, despite the comparable high C/O = 0.95. Observations predict a mass loss rate of $3 \cdot 10^{-6}$ M_{sun} /yr and a dust-to-gas mass ratio of $5 \cdot 10^{-3}$. This is consistent with our dust-to-gas mass ratio at 8 R_* :

$\Psi = 4 \cdot 10^{-3}$ for a 20 km/s shock and $\Psi = 6 \cdot 10^{-3}$ for a 32 km/s shock

Miras in the SMC





Alumina dust:

$\Psi = 1.3 \cdot 10^{-8}$

$A_{grain} = 13$ Å

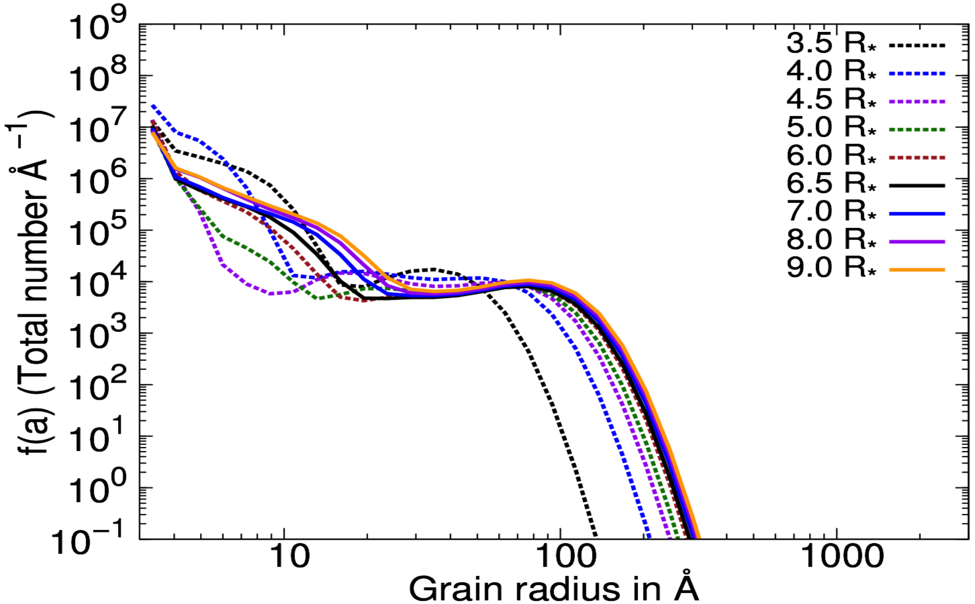
Z = 0.003

D = 61 kpc

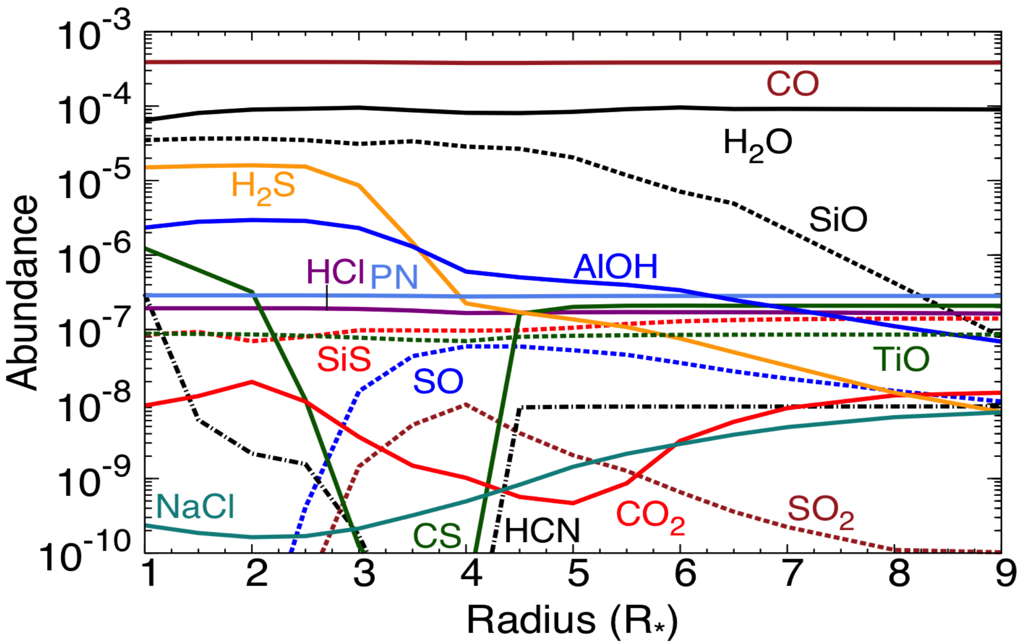
Forsterite dust:

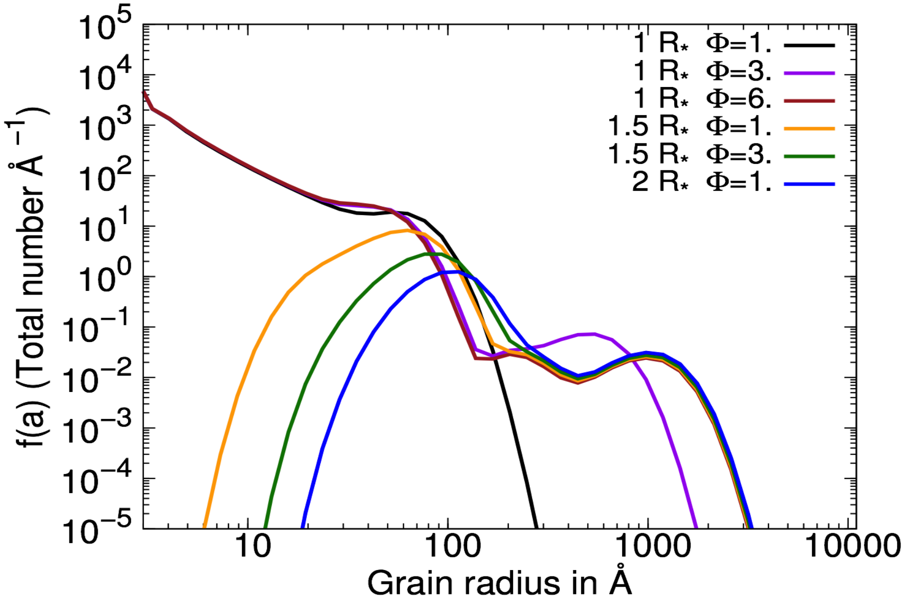
$\Psi = 3.1 \cdot 10^{-4}$

$A_{grain} = 75$ Å



Miras in the LMC

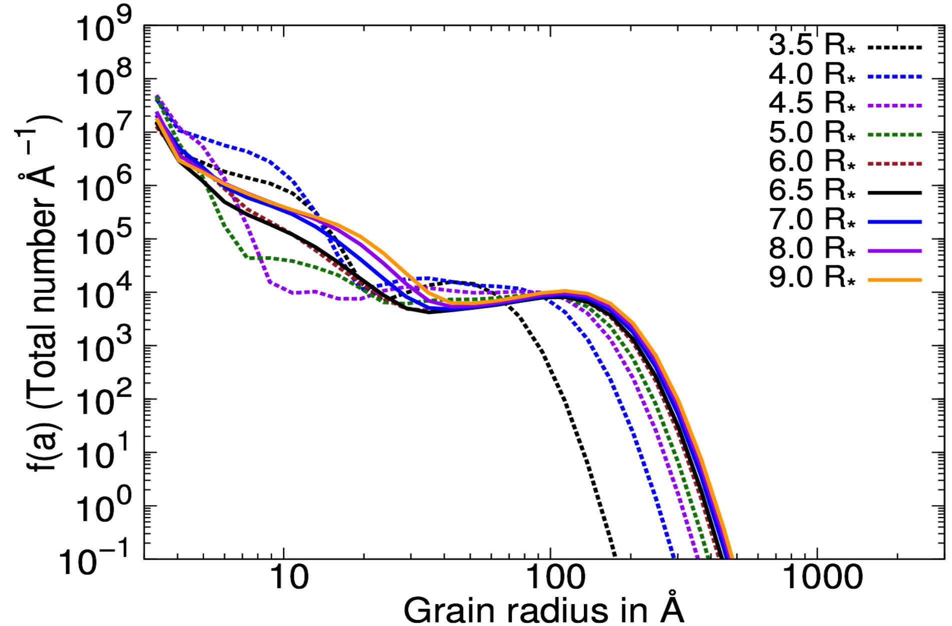




Alumina dust:
$\Psi = 3.2 \cdot 10^{-6}$
$A_{grain} = 115$ Å

Forsterite dust:
$\Psi = 1.1 \cdot 10^{-3}$
$A_{grain} = 110$ Å

Z = 0.008
D = 50 kpc



Conclusions

- Pulsation models of the inner wind of Mira stars well explain observed molecular abundances of H_2O, OH, SiO, SiS, **CO, CO_2, HCN, CS**, SO ,PN and HCl
- NH_3, SO_2 and PO cannot not reproduced by the models. Observations indicate that these species

  - are located outside the inner envelope or

  - synthesized by processes not considered here (photo-chemistry, grain surface reaction)
- Alumina grains (> 0.1 μm) form close to the star at $r \leq 1.5\ R_*$
- Silicate (forsterite) grains form between 4 R_* and 6 R_* from a new nucleation route involving HSiO

→ Consistent with recent MIDI/VLT observations

Karovicova 2013

Conclusions

Semi-regular (SRV) model: Molecular abundances agree with observations (CO, SiO, HCN). Alumina dust forms, but silicates can hardly be synthesized, owing to low densities.

S-type star model: Models predict large amounts of alumina and silicate dust. Modelled abundances (in particular SiO and H_2O) agree with obervations before the onset of forsterite formation.

Low metallicity model: Smaller amounts of clusters and dust are derived, owing to the lower availability of heavy elements.

For the first time, detailled non-equilibrium chemical models accounting for - gas phase,
- cluster nucleation, and
- dust condensation,

are set up for the inner winds of AGB stars (O-rich Miras, semi-regular, S-type, and Miras in the SMC/LMC)

and explains the prevalent molecules and dust condensates.

Questions

Any questions?

Suggestions for improvement ?

Looking for experts in Hydrodynamics!