

CHEMICAL MODELING OF INTERSTELLAR MgS

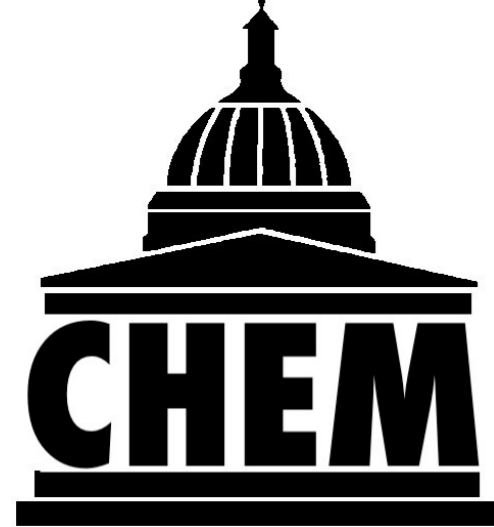
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1. Introduction

The Galactic Centre molecular cloud G+0.693-0.027 (hereafter G+0.693) is distinguished by its chemically-rich environment attributed to low-velocity shocks that release significant amounts of material from dust grains into the gas phase through sputtering. Recently, we have reported the discovery of the metal-sulfides MgS and NaS in this cloud (Rey-Montejo et al. 2024) but we ignore the chemical processes involved in their formation. In this work, we model the chemistry of the previously detected MgS towards this cloud, and analyse the dominant reactions involved in the formation and destruction of this molecule, their associated time-scales, and the depletion factor needed to recover the observed abundances, representing the first analysis of the chemistry of the metal-sulfide MgS.

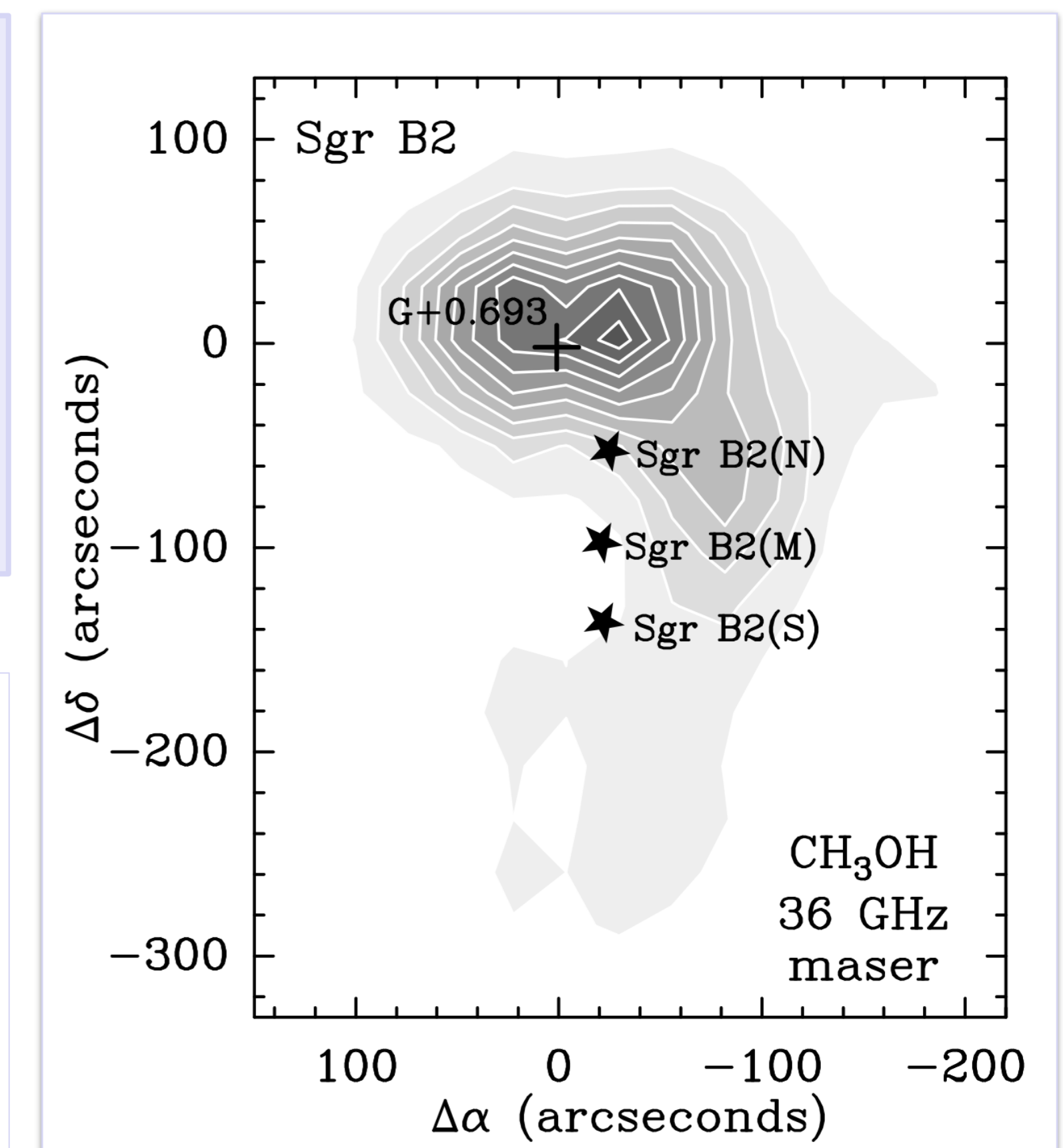
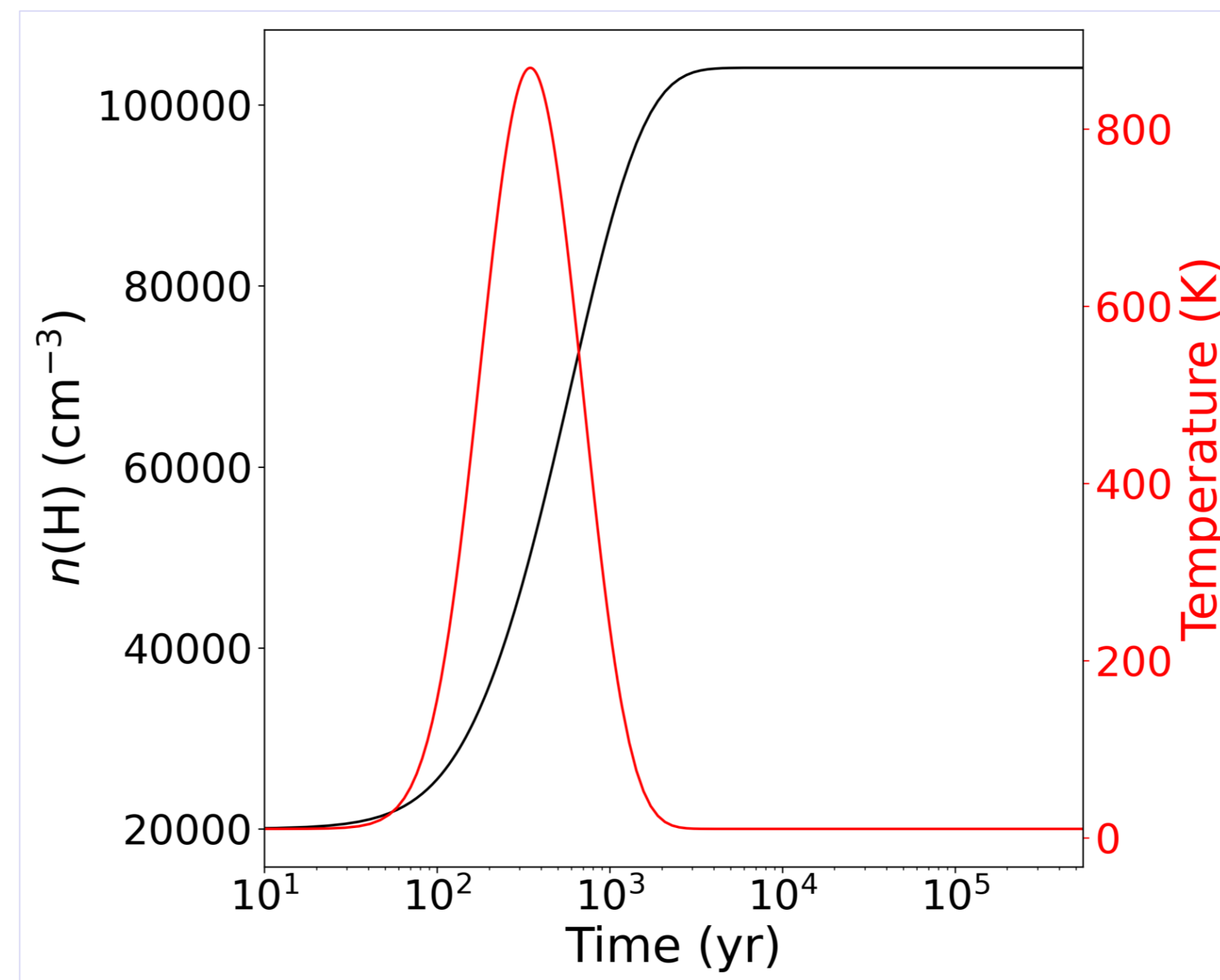
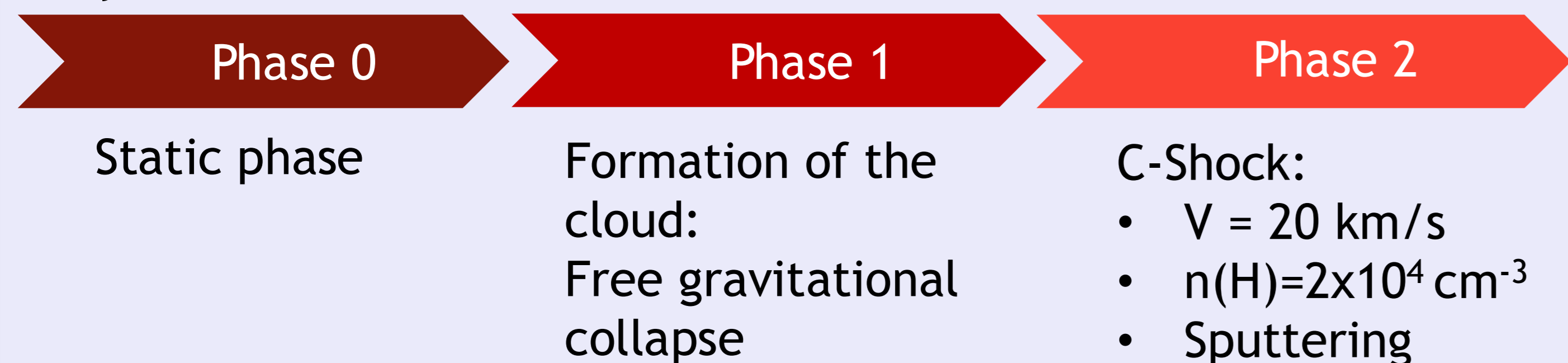
2. UCLCHEM v3.5.3



New Chemical network for MgS:

- SiS as a proxy.
- Study of the endothermicity of the proposed reactions with MgS using quantum chemical computations.

Physical conditions of G+0.693:



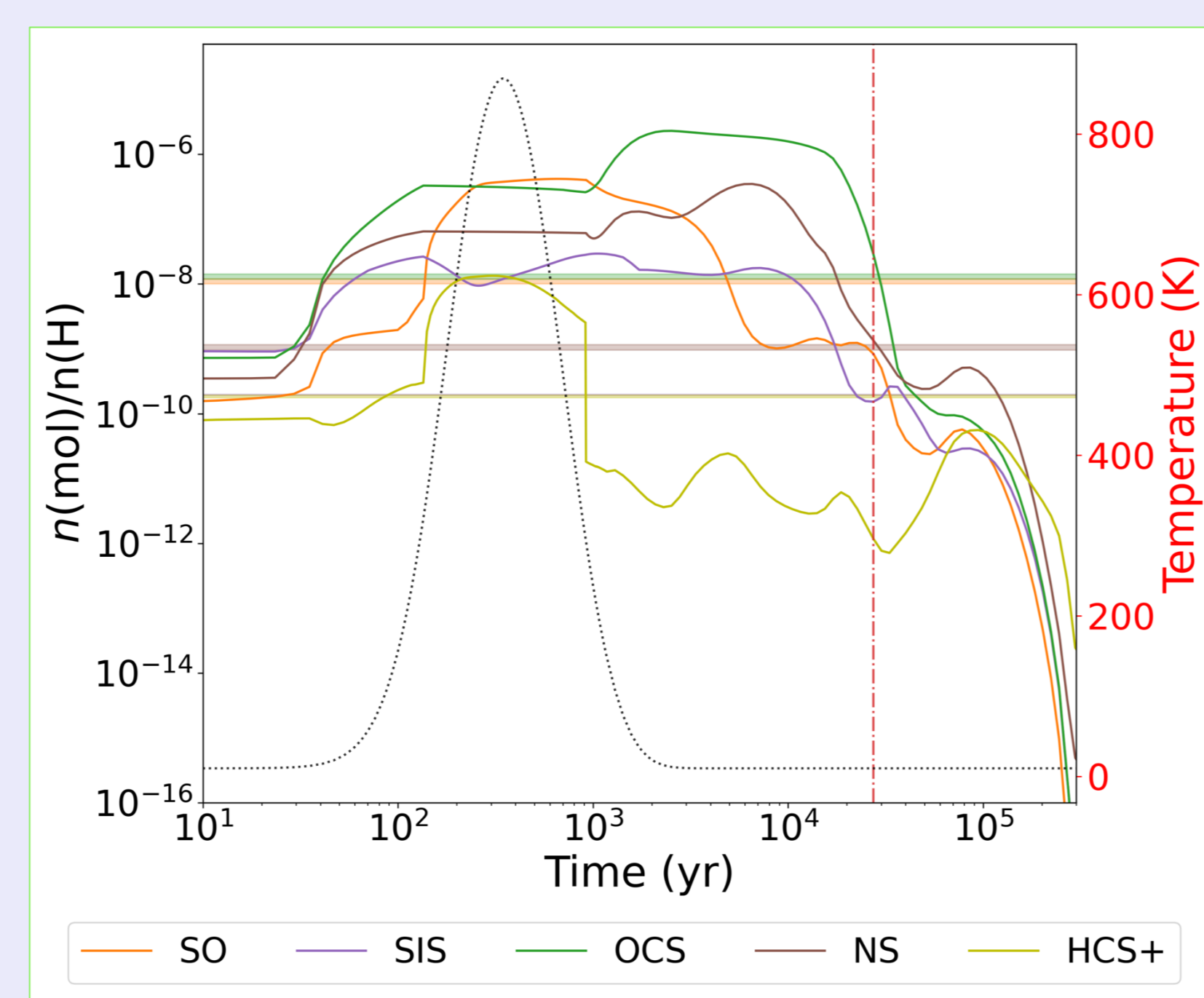
Jiménez-Serra (2025)

3. Constraining initial parameters for S

Grid of models

$\zeta \backslash D$	$D_1=0$	$D_2=10$	$D_3=100$
$\zeta_1=1$	(ζ_1, D_1)	(ζ_1, D_2)	(ζ_1, D_3)
$\zeta_2=100$	(ζ_2, D_1)	(ζ_2, D_2)	(ζ_2, D_3)
$\zeta_3=1000$	(ζ_3, D_1)	(ζ_3, D_2)	(ζ_3, D_3)

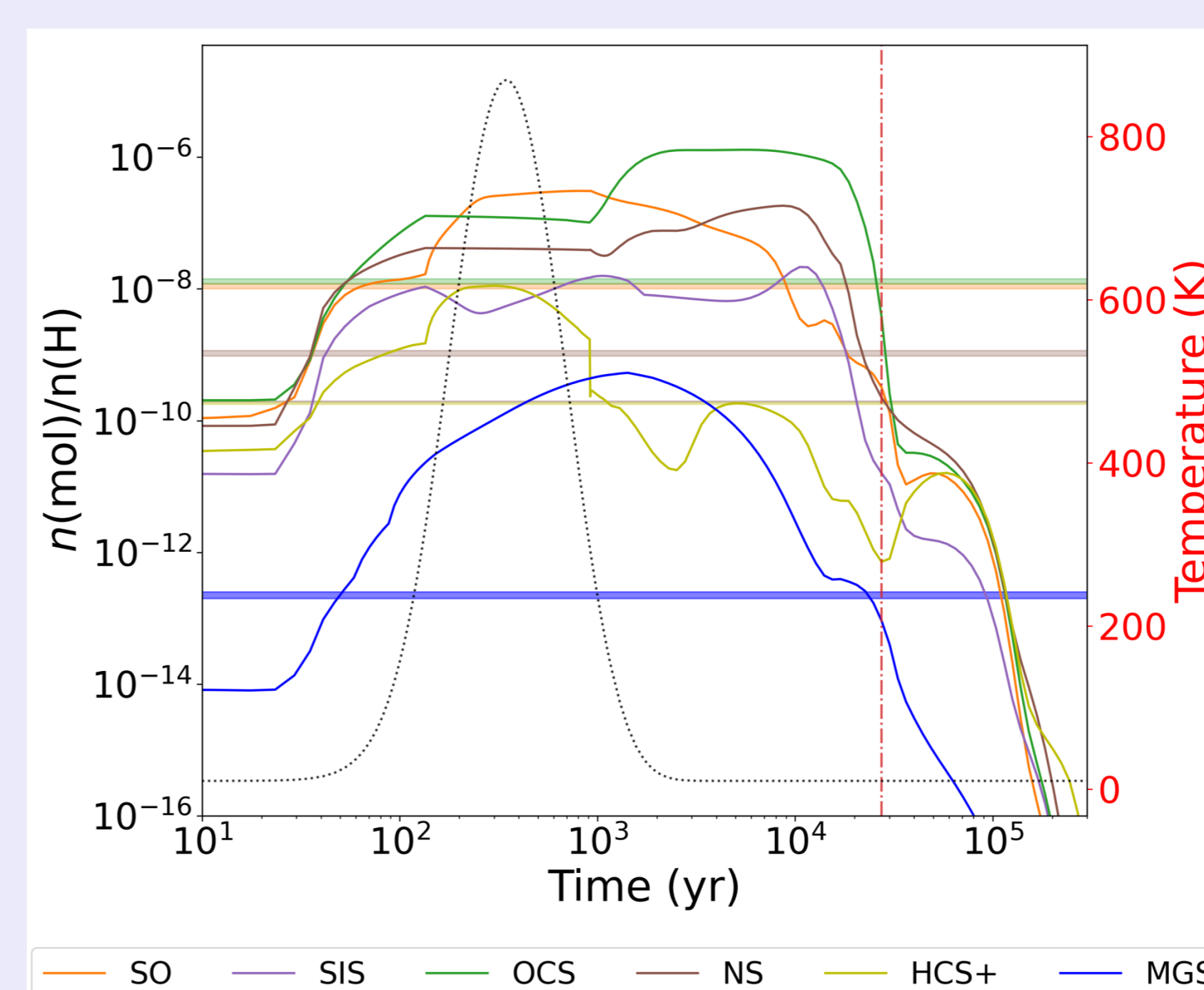
Solar abundance: $S = 1.32 \times 10^{-5}$
Standard value: $\zeta = 1.3 \times 10^{-17} \text{ s}^{-1}$



Best MAE
 $S = 1.32 \times 10^{-5}$
 $\zeta = 1.3 \times 10^{-15} \text{ s}^{-1}$

4. Constraining Mg Depletion factor

With fixed S depletion and ζ value, we constrain the depletion factor of Mg by running UCLCHEM for D_1 , D_2 and D_3



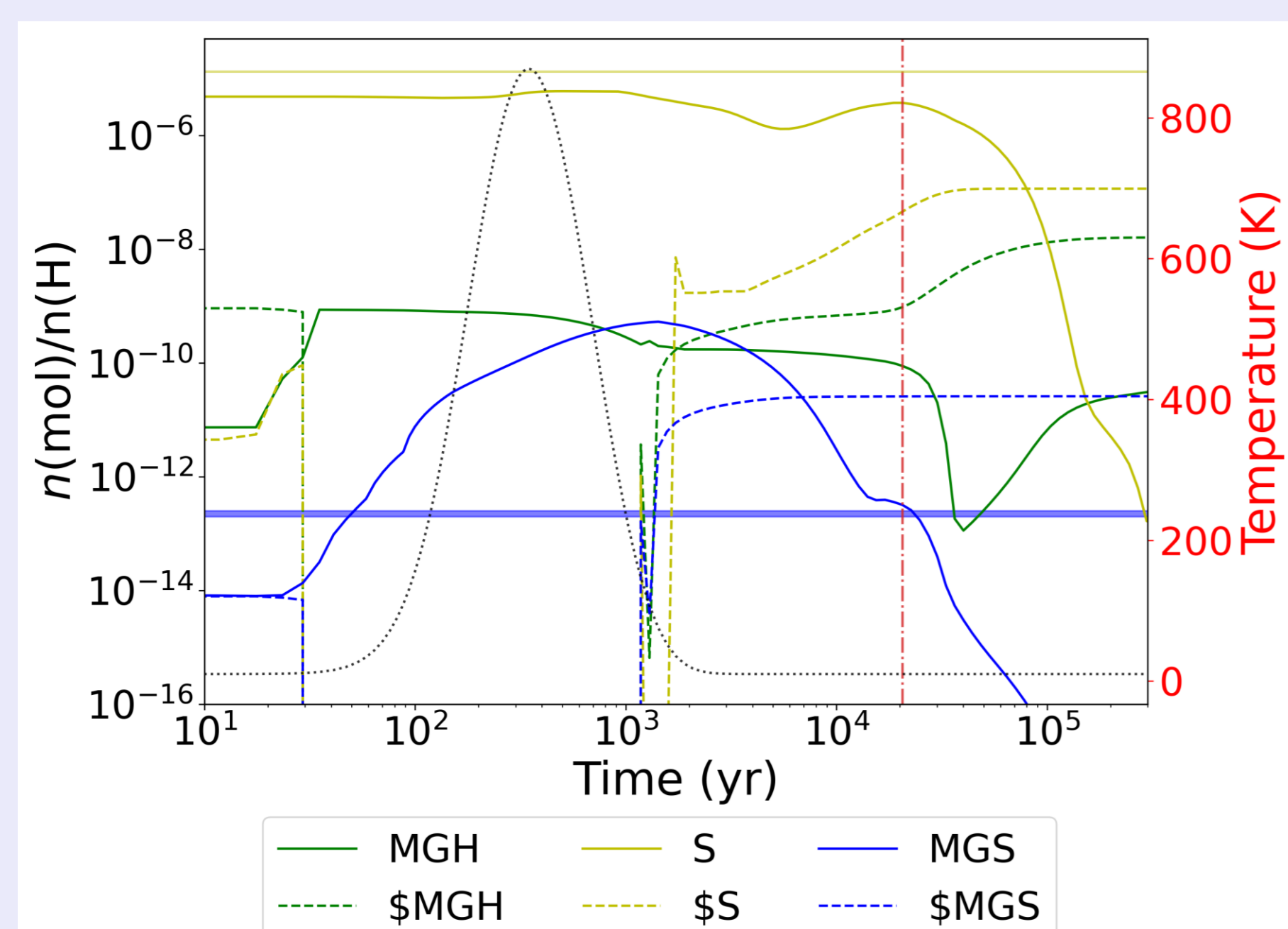
Best MAE
 $\text{Mg} = 3.98 \times 10^{-8}$

99.9% of Mg locked into the core of dust grains

5. Main formation pathway to MgS

Gas phase reaction: $\text{MgH} + \text{S} \rightarrow \text{MgS} + \text{H}$

High abundance of S makes the reaction very efficient.



- 1) MgH is frozen on ices at the beginning of the simulation.
- 2) Shock frees MgH into the gas phase.
- 3) Gas phase MgH reacts with S to form MgS.
- 4) The destruction of MgS is dominated by the reactions:
 $\text{H}_3^+ + \text{MgS} \rightarrow \text{HMgS}^+ + \text{H}_2$

6. Take home messages

- This study represents the first analysis of the chemistry of MgS in the ISM.
- To reproduce the observed abundance of MgS, a Mg depletion factor of 1000 is required, indicating that 99.9% of this element is locked onto dust grains, likely in the form of silicates. Thus, with only 0.1% of Mg available in the gas phase, we can recover the observed abundances of MgS.
- The formation of MgS occurs in the gas phase primarily through the reaction $\text{MgH} + \text{S}$. Thanks to quantum chemical calculations, other formation pathways have been found to present large energy barriers. Future detections of MgH would provide a critical test of this formation pathway.

