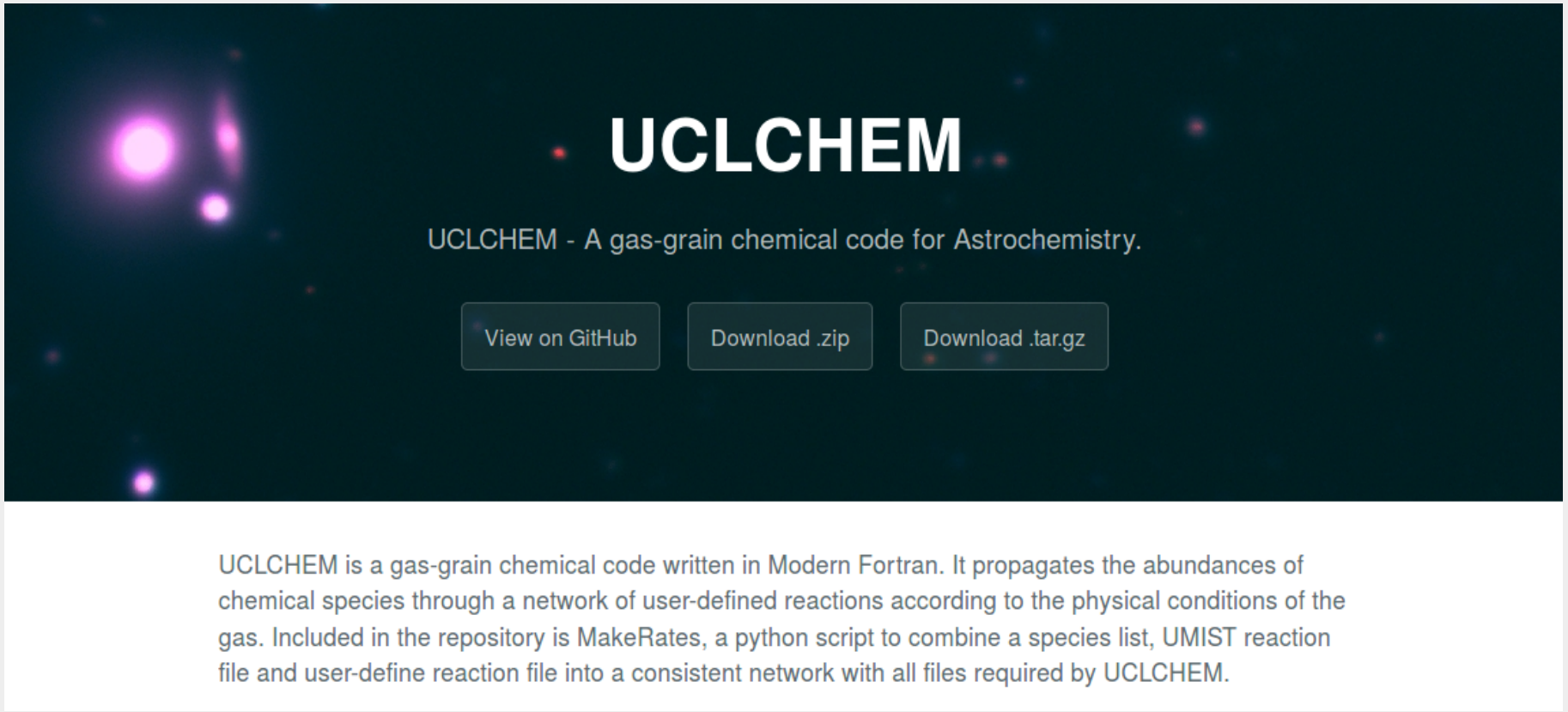
UCLCHEM

Jon Holdship, Serena Viti, Izaskun Jimenez-Serra, Felix Priestley, Antonios Makrymallis

UCLCHEM – Overview

- Time dependent gas-grain chemical model, available on uclchem.github.io



Chemistry Module

- Calculates rates and integrates chemical network
- Handles gas phase reactions, freeze out on to grain surfaces, non-thermal desorption and grain surface reactions via a diffusion treatment or with modified rate equations
- Post-processing script for analysing important formation and destruction routes through time

Networks

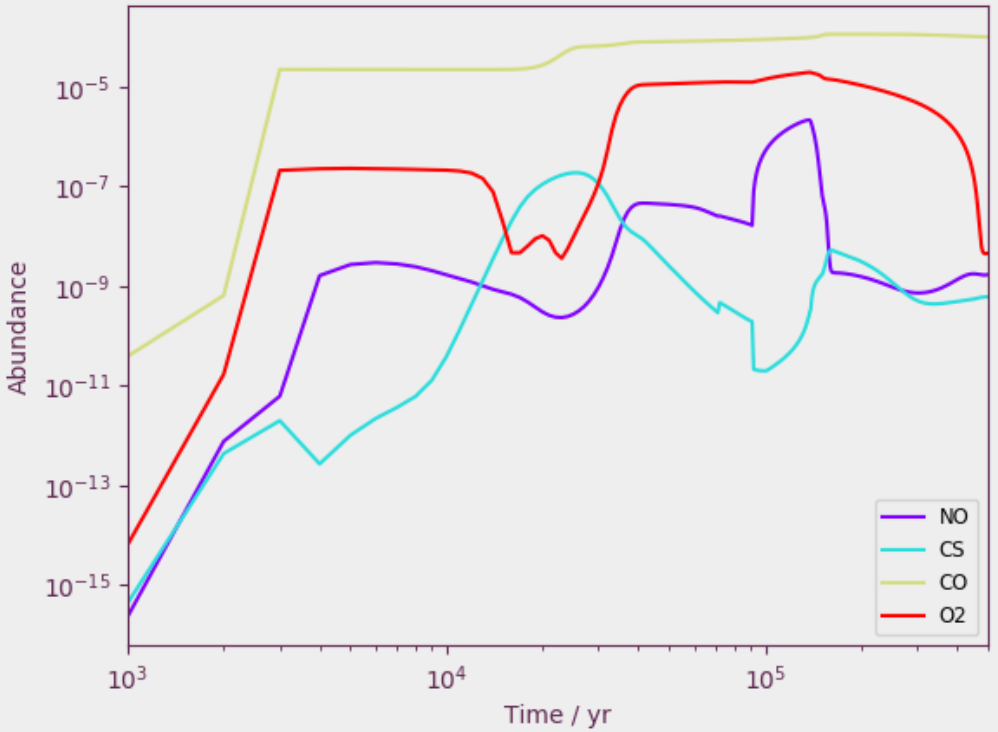
- Gas phase network from UMIST or KIDA
- Grain network is user created, simple network provided with repository
- Network related code generated by python routine

UCLCHEM – Physics Modules

- Physical parameters controlled by interchangable modules
- Two well developed models used to describe many observations: hot core and C-shock modules
- Post-processing and prestellar core models are also in repository

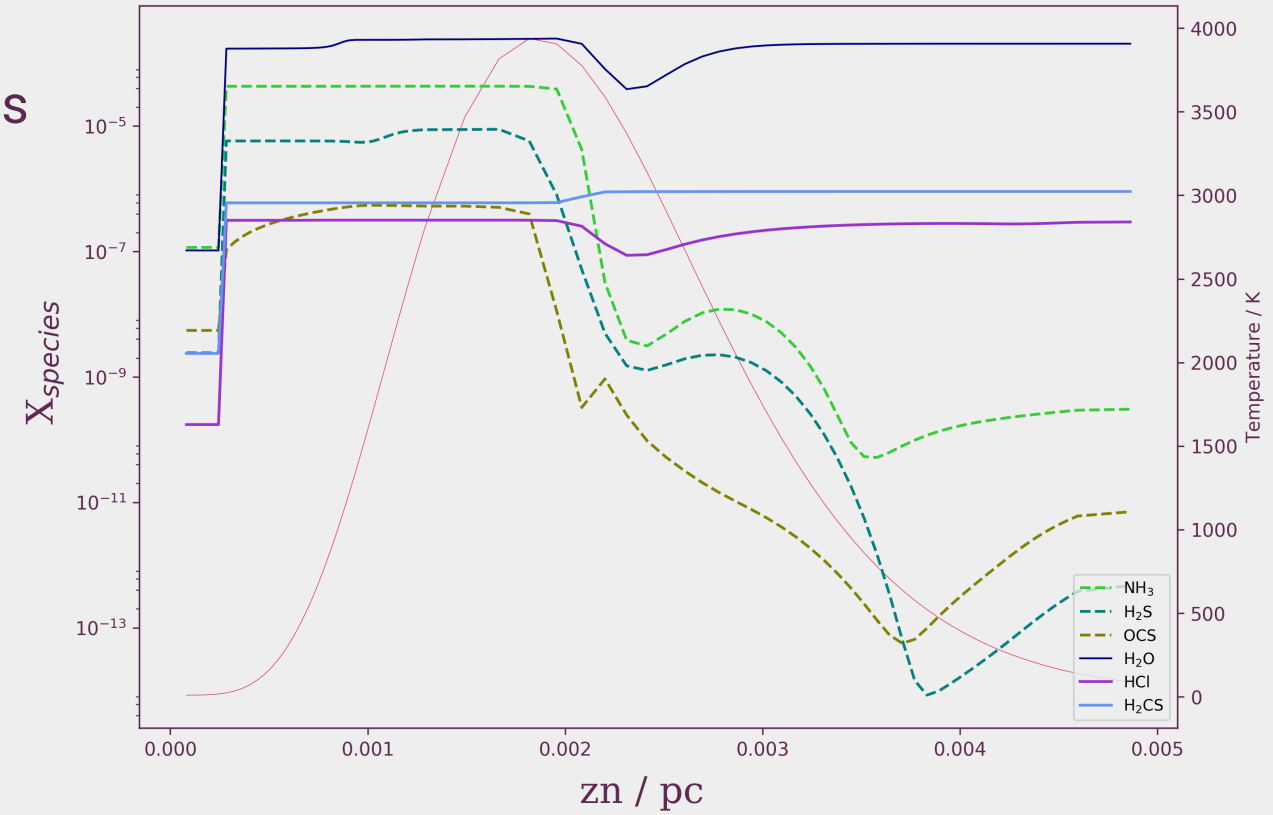
Hot Core Model

- Hot core model has time dependent, radial temperature profiles for a variety of stellar masses
- Thermal desorption in multiple events: mono-layer evaporation at each species' binding energy, volcanic desorption, and co-desorption with the ices at given temperatures



C-shock Model

- C-shock model changes gas density and temperature and includes simple sputtering treatment for grain surface species
- User only needs to specifiy shock velocity and pre-shock gas density



UCLCHEM - Summary

- UCLCHEM is available at uclchem.github.io
- A gas-grain chemical code with modular physics, easy to use C-shock, cloud and hot core models
- Code manual and contact details on the website

Grain Rates – Bayesian Sensitivity Analysis

- Rates of reactions on grain surfaces are uncertain
- Experiments take time
- Can we prioritise reaction rates through chemical modelling?

Grain Rates – The Model

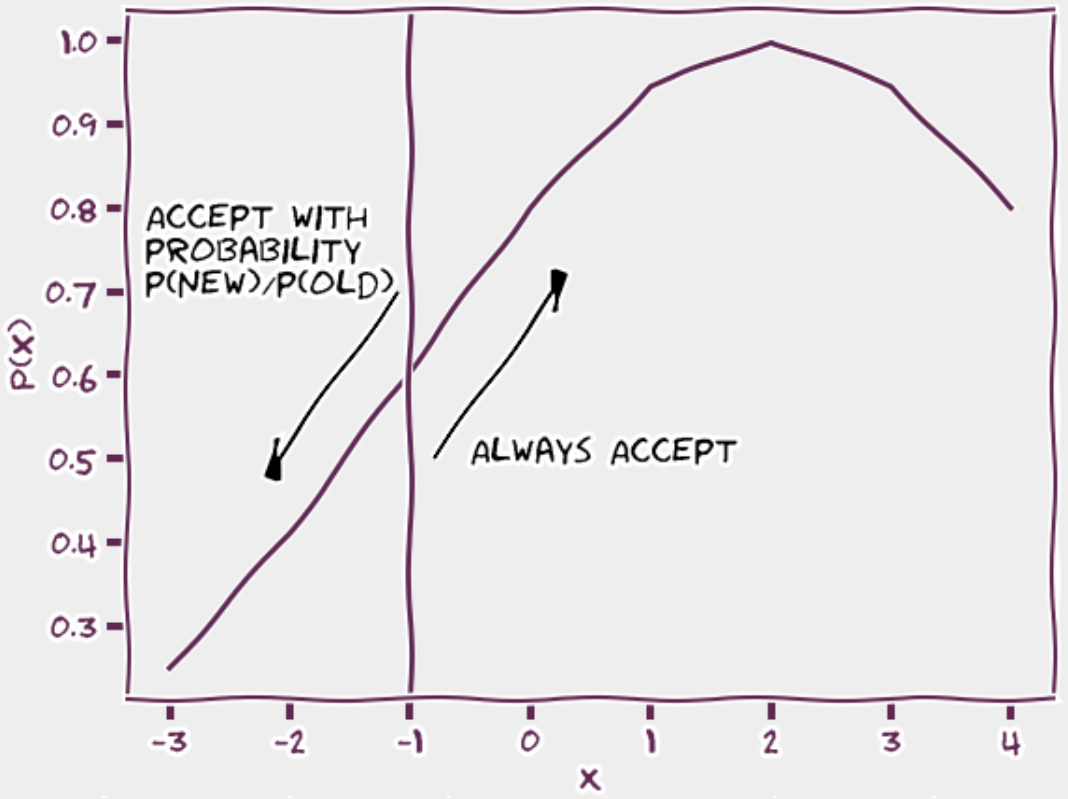
- Reduced chemical model
- 1 Myr collapse from n_H=1000 cm^{-3} to $10^8 cm^{-3}$ at a constant temperature of 10 K
- Pre-calculated freeze out rates for major species
- 23 grain surface reactions and 22 grain species
- Simple rates with constant k values due to constant temperature. For reaction between y_1 and y_2:
  - $dy_1/dt = k\, y_1\, y_2\, n_H$
- Absolute rate values are **not** meaningful

uclchem.github.io

No.	Reactions				
1.	O	+	H	→	OH
2.	OH	+	H	→	H_2O
3.	CO	+	OH	→	CO_2
4.	S	+	H	→	HS
5.	HS	+	H	→	H_2S
6.	H_2S	+	S	→	H_2S_2
7.	CS	+	H	→	HCS
8.	HCS	+	H	→	H_2CS
9.	CO	+	S	→	OCS
10.	OCS	+	H	→	HOCS
11.	H_2S	+	CO	→	OCS
12.	H_2S	+	H_2S	→	H_2S_2
13.	H_2S_2	+	CO	→	CS2 + O
14.	H_2S	+	O	→	SO_2
15.	CS_2	+	O	→	OCS + S
16.	CO	+	HS	→	OCS
17.	S	+	O	→	SO
18.	SO	+	O	→	SO_2
19.	SO	+	H	→	HSO
20.	HSO	+	H	→	SO
21.	CO	+	H	→	HCO
22.	HCO	+	H	→	H_2CO
23.	H_2CO	+	H	→	CH_3OH

Grain Rates - MCMC

- MCMC parameter estimation used to generate probability distributions for each rate's value
- This gives the model's sensitivity to each reaction rate.
- Flat probability distributions imply a rate is not important, peaked implies it is.



Grain Rates – Scoring Models

- MCMC procedure requires P(k), where k are our reaction rates.
- We define two sets of species, those abundant enough to be observable and and those that are unobservable:

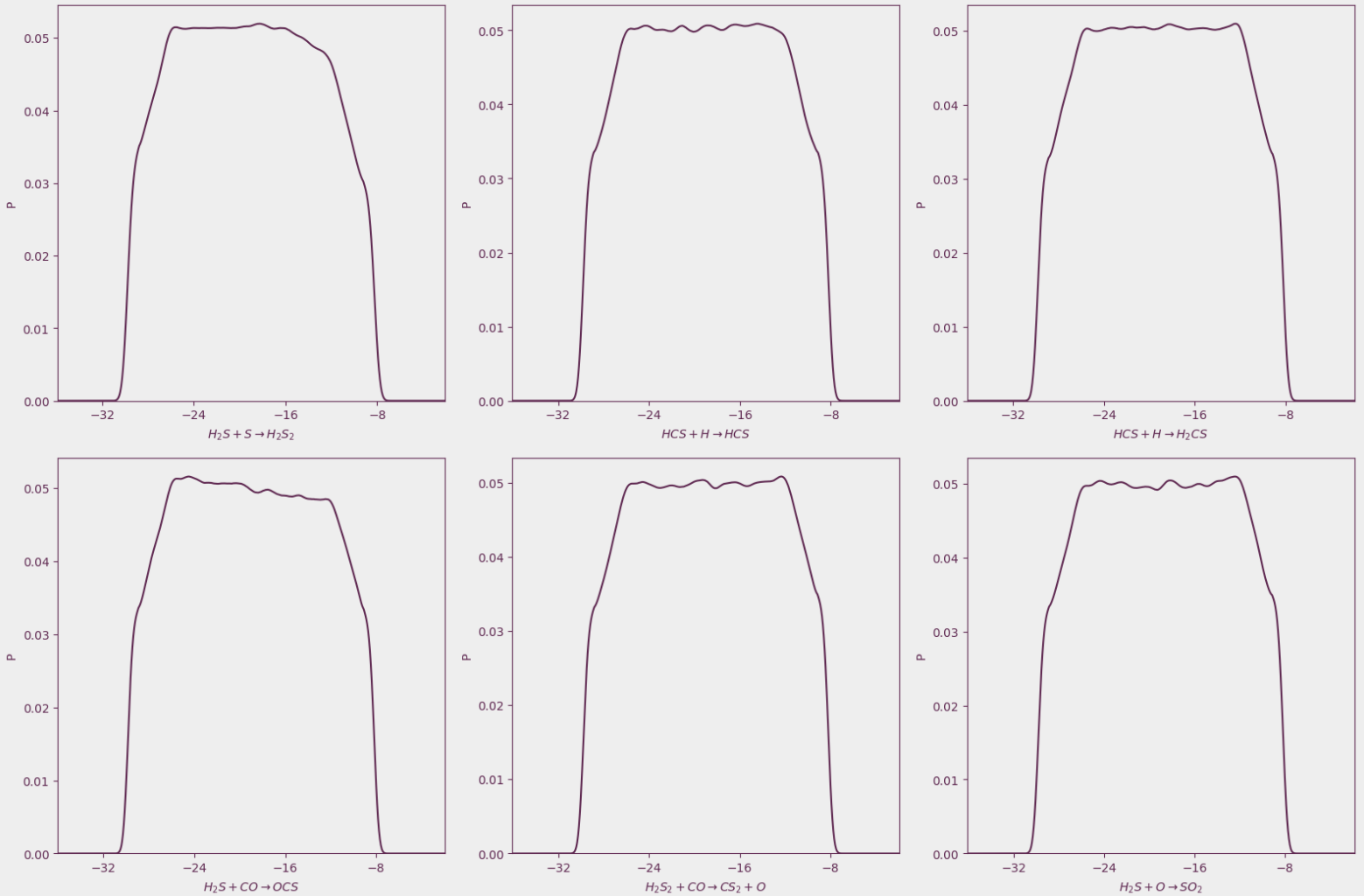
Observable	{CO, CO_2 , H_2O, CH_3OH }	$10^{-8} < X < 10^{-4}$
Unobservable	{HCO, HOCS, HS, O, S, H_2S_2}	$X < 10^{-8}$

- We can then define the probability of a set of rates by the number, n, of species that fall into their correct category

$$P(n) = \frac{\lambda^n e^{-10}}{10!}$$

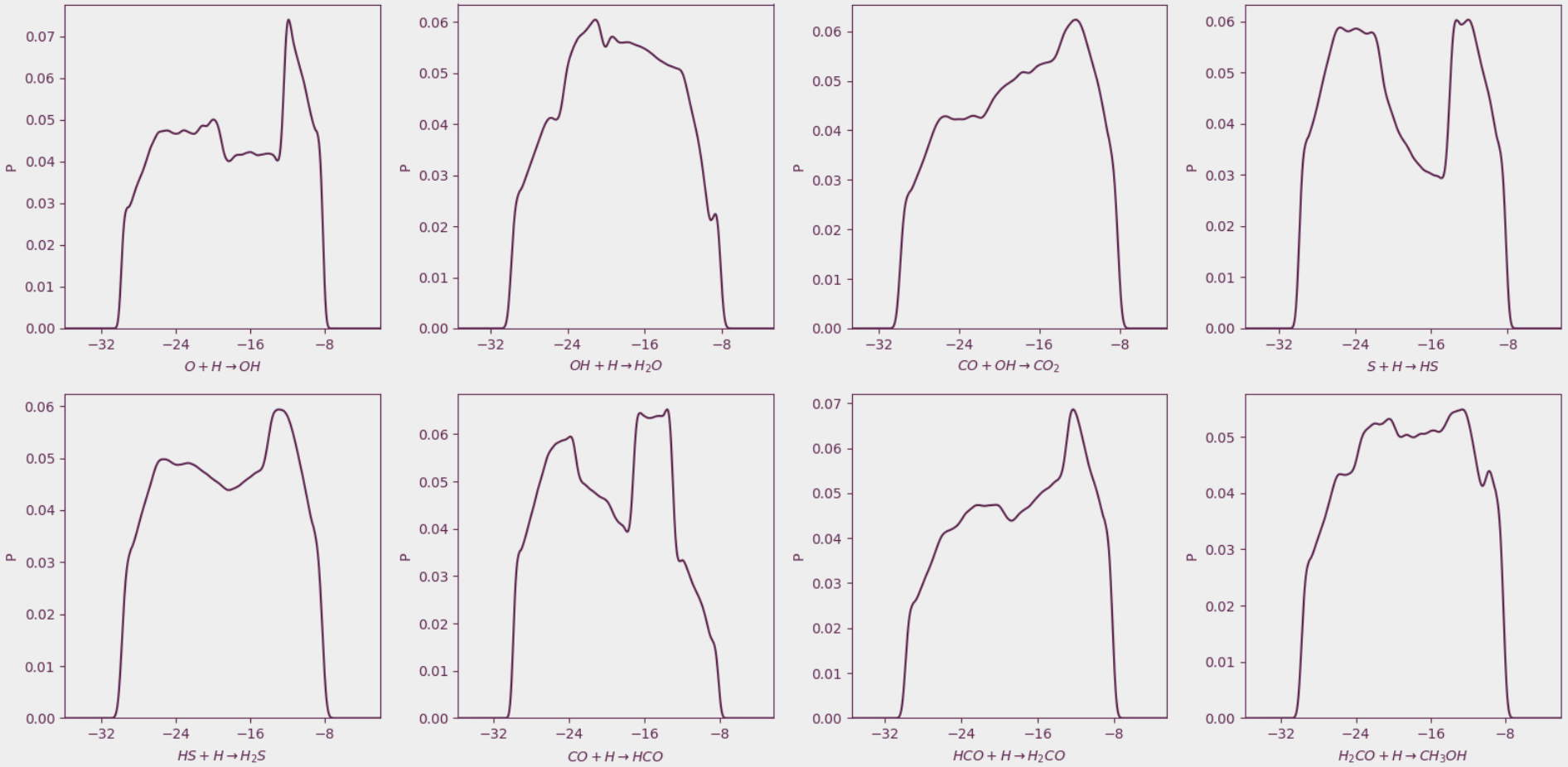
Grain Rates - Results

- The majority of reactions are unimportant



Grain Rates - Results

- But we can conclude these rates are vital



Thank You!