Computational Astrophysics

5a. Micropohysics I: Non-equilibrium chemistry

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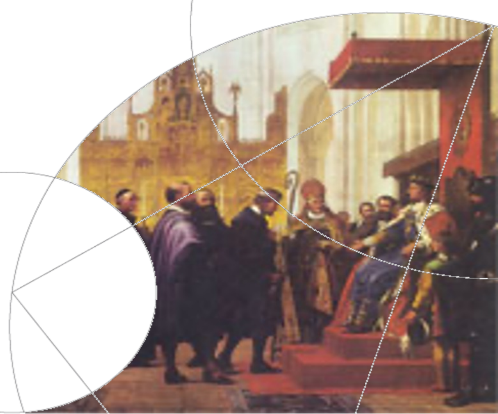
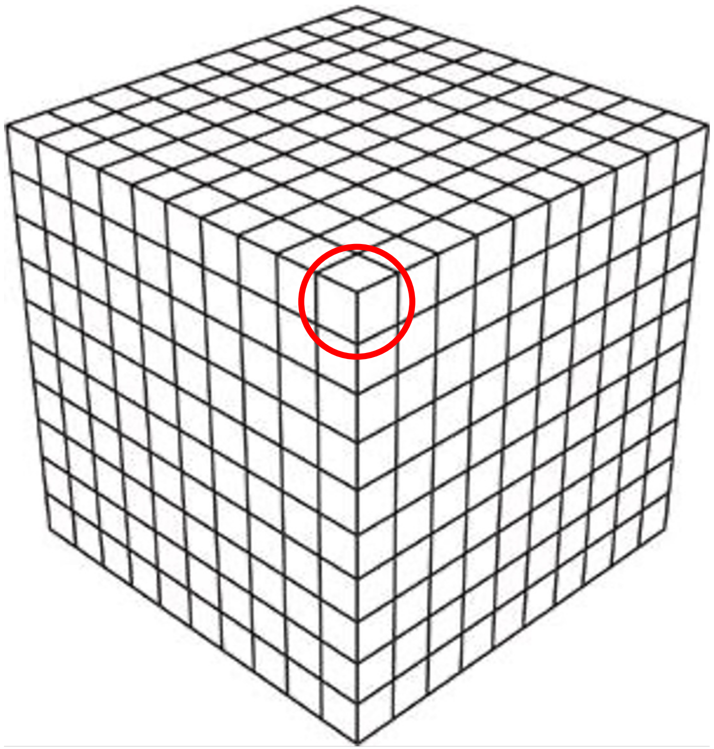
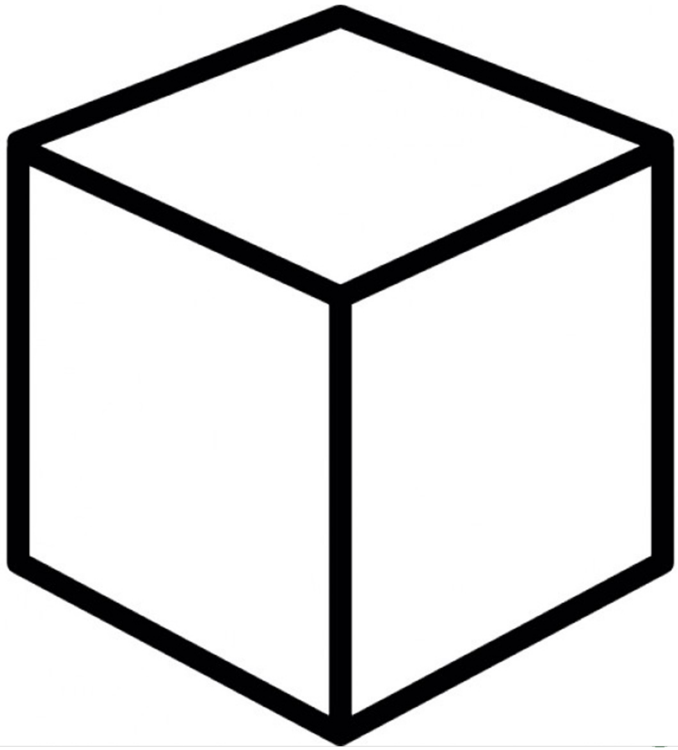


Microphysics

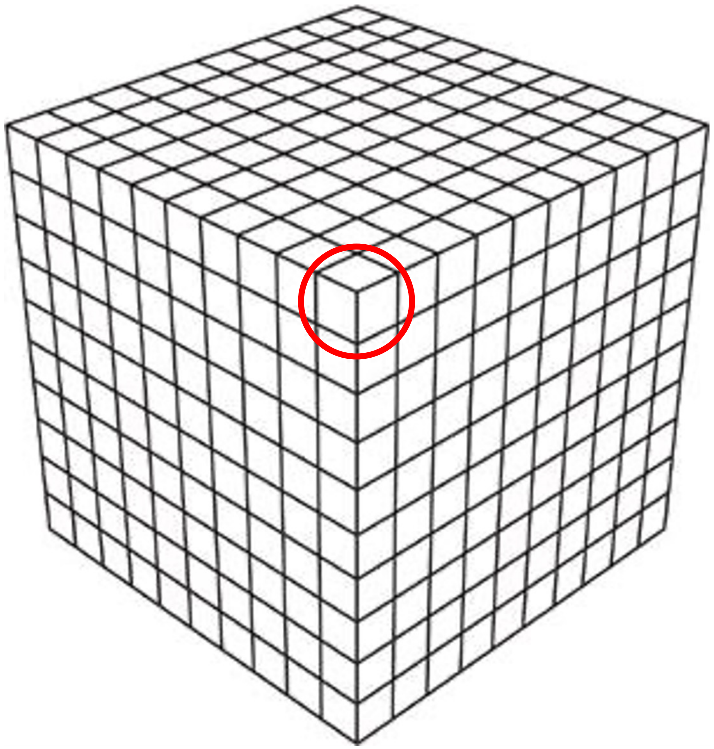
- Basically it’s everything happening inside a cell, on scales below the resolution

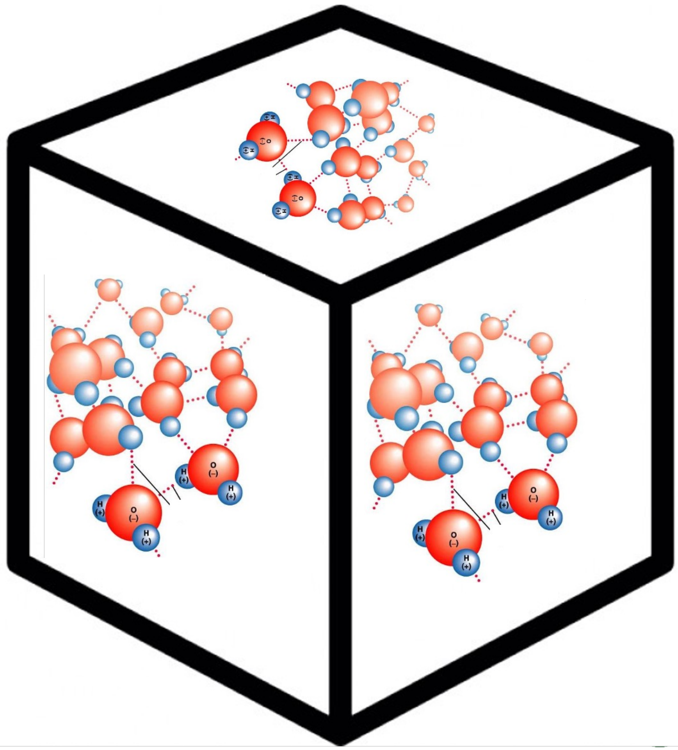




Microphysics

- Basically it’s everything happening inside a cell, on scales below the resolution – today we will start with *astrochemistry*





Why do we need Astrochemistry ?

- As an **observational diagnostic**:
  - H_2, CO, H_2O, O_2, CH are common molecules found in the ISM
  - Molecular ***rotational and vibrational bands*** can be observed at infrared to mm wavelengths
  - The molecular bands trace indirectly the density, temperature, etc ***probing the physical state*** of the gas in the clouds

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  - The molecular bands trace indirectly the density, temperature, etc ***probing the physical state*** of the gas in the clouds
- For **modelling thermal processes**:
  - The ***equation of state*** depends on the chemical abundances
  - ***Heating and cooling*** is directly related to the chemistry
  - ***Ionization and conductivity*** depend on having a reservoir of free electrons and ions

Non-equilibrium chemistry

- Because of the very ***low temperatures*** and (by chemistry standards) also very low densities, ***chemical reactions*** in the interstellar medium (ISM) and proto-planetary disks (PPDs) ***are very slow***
- Consequently, they ***may not reach chemical equilibrium*** (a balance which is computable from a knowledge of the Gibb's free energy of the compounds)
- To investigate and simulate the chemical reactions, we need to ***solve the ordinary differential equations*** (ODEs) that describe the evolution of the *species* (atoms, molecules, dust & ice grains) in the medium

Non-equilibrium chemistry; long story short

$$A+B \xrightarrow{k(T)} C+D$$

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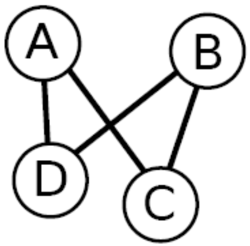

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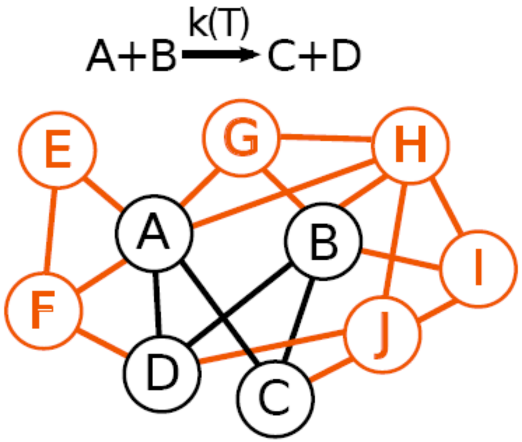

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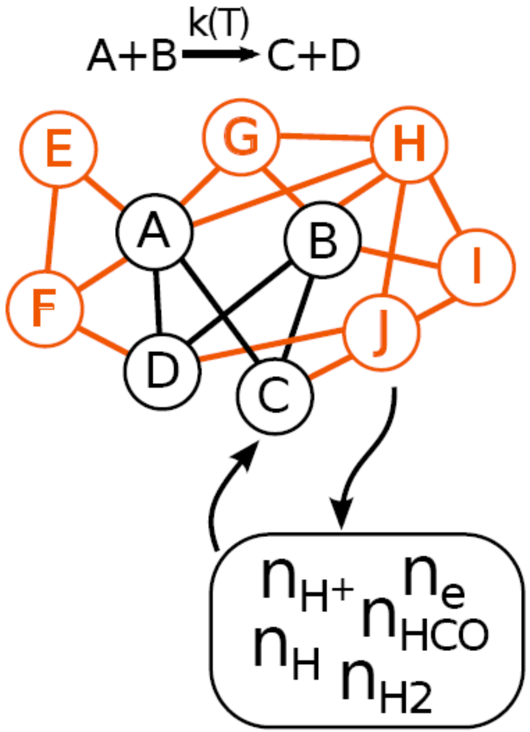

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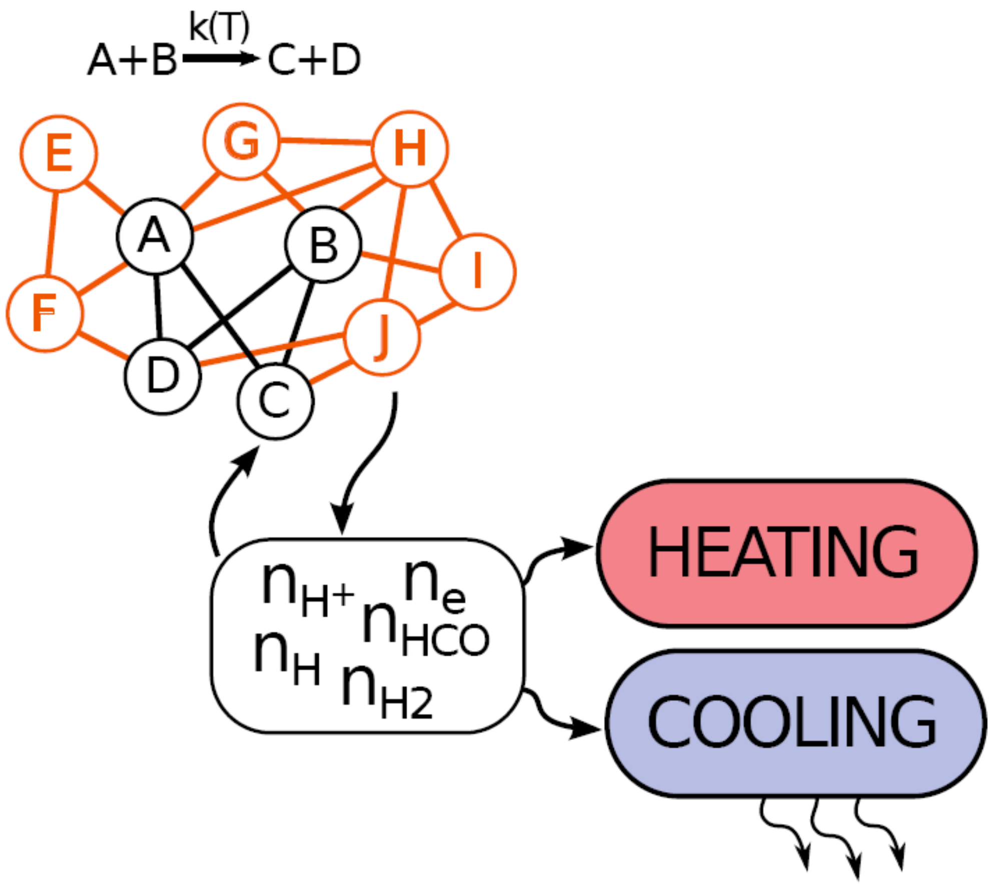

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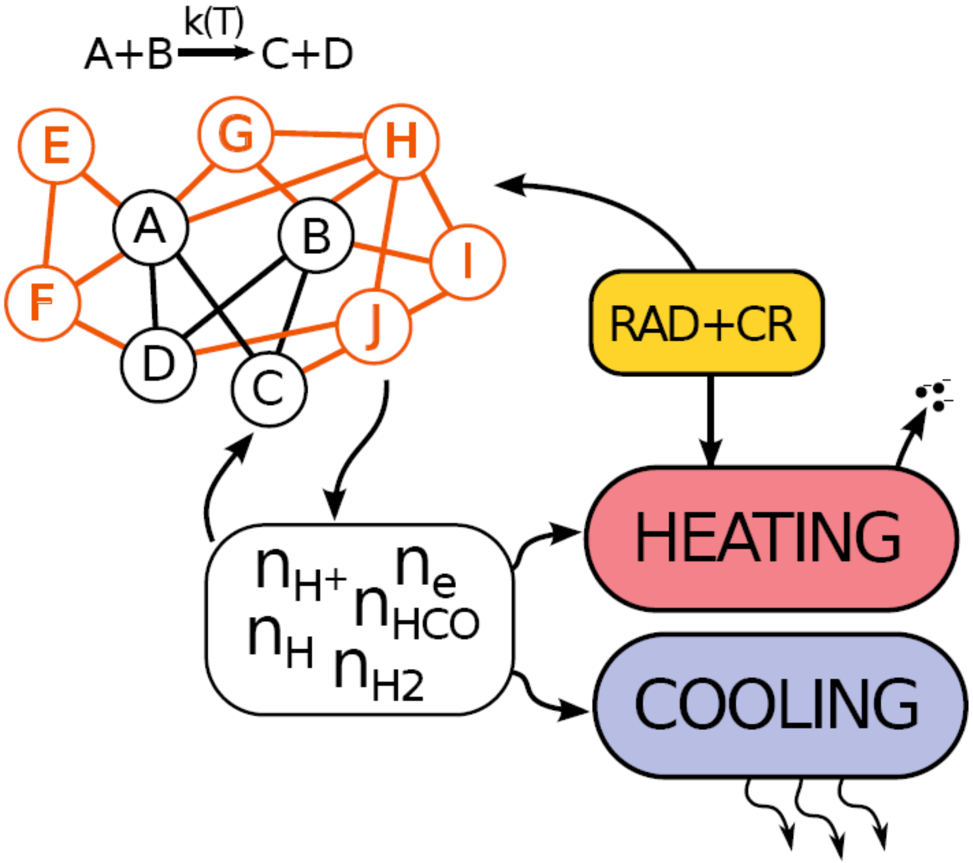

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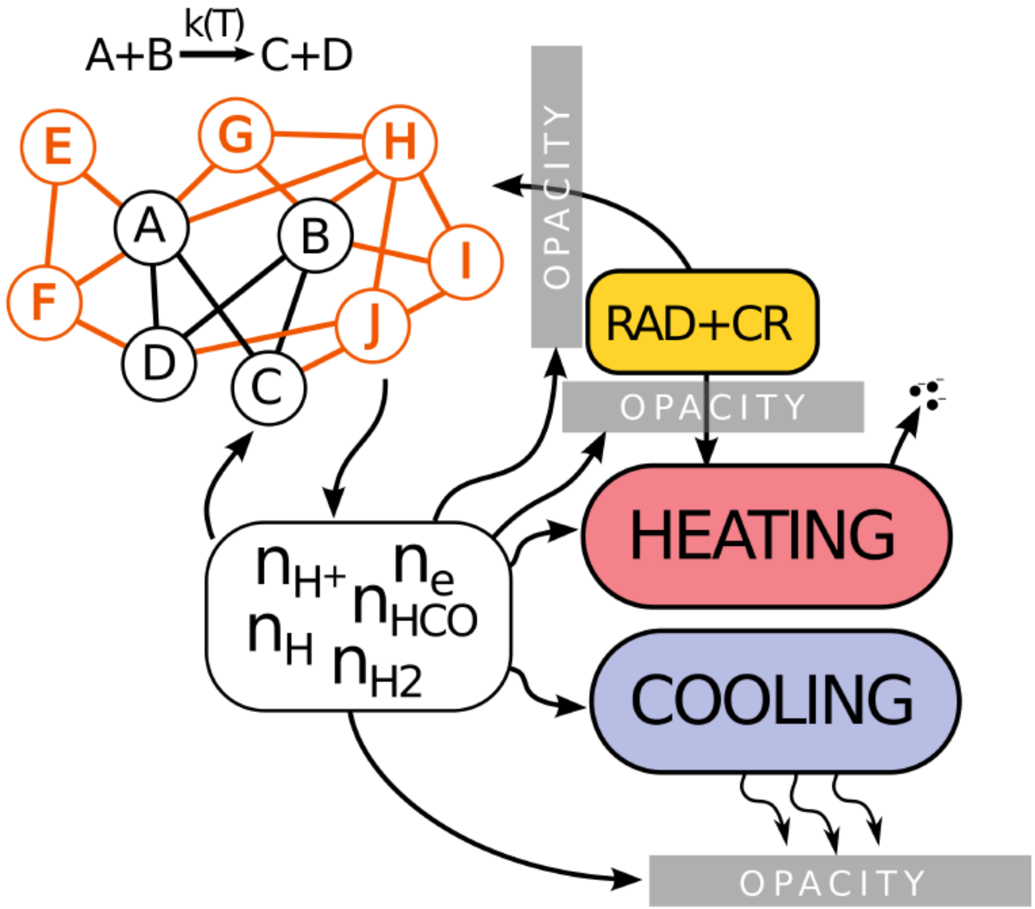

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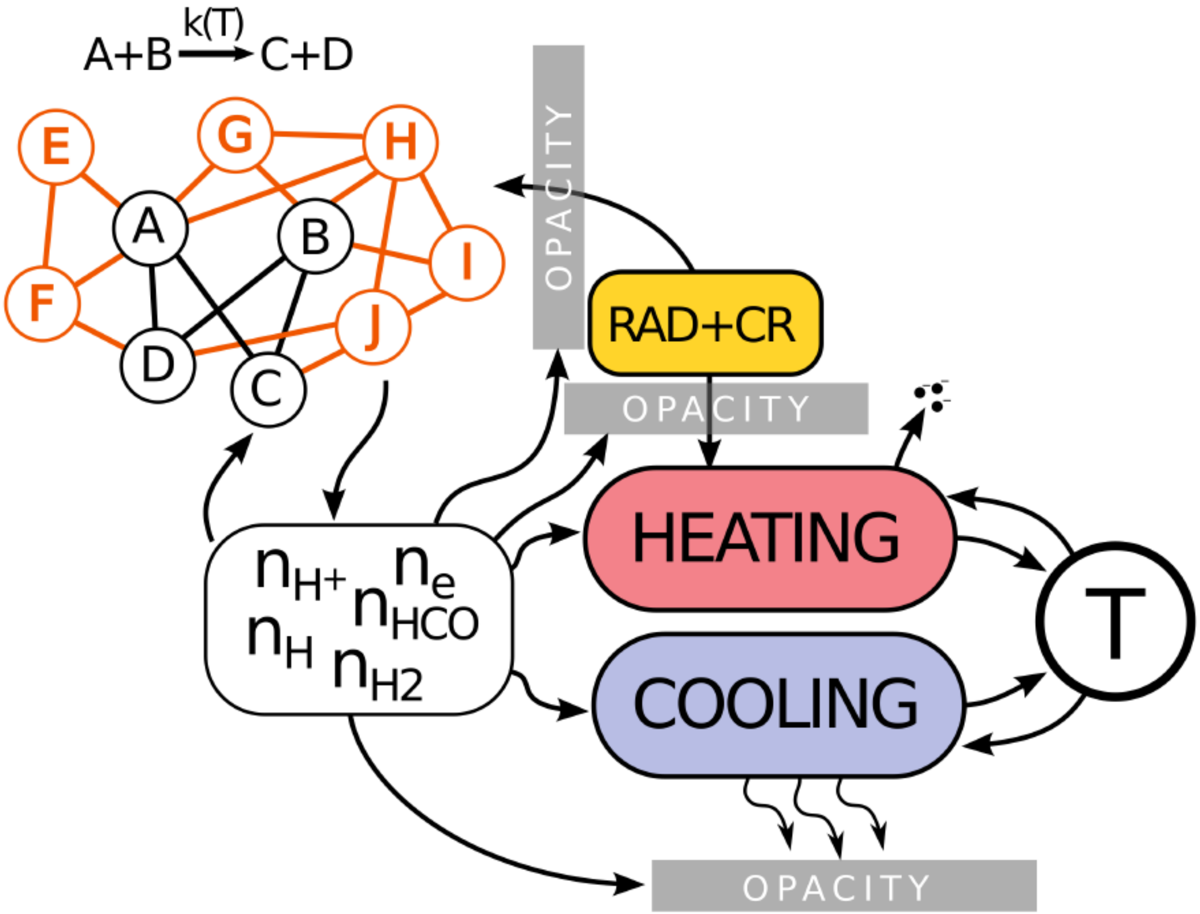

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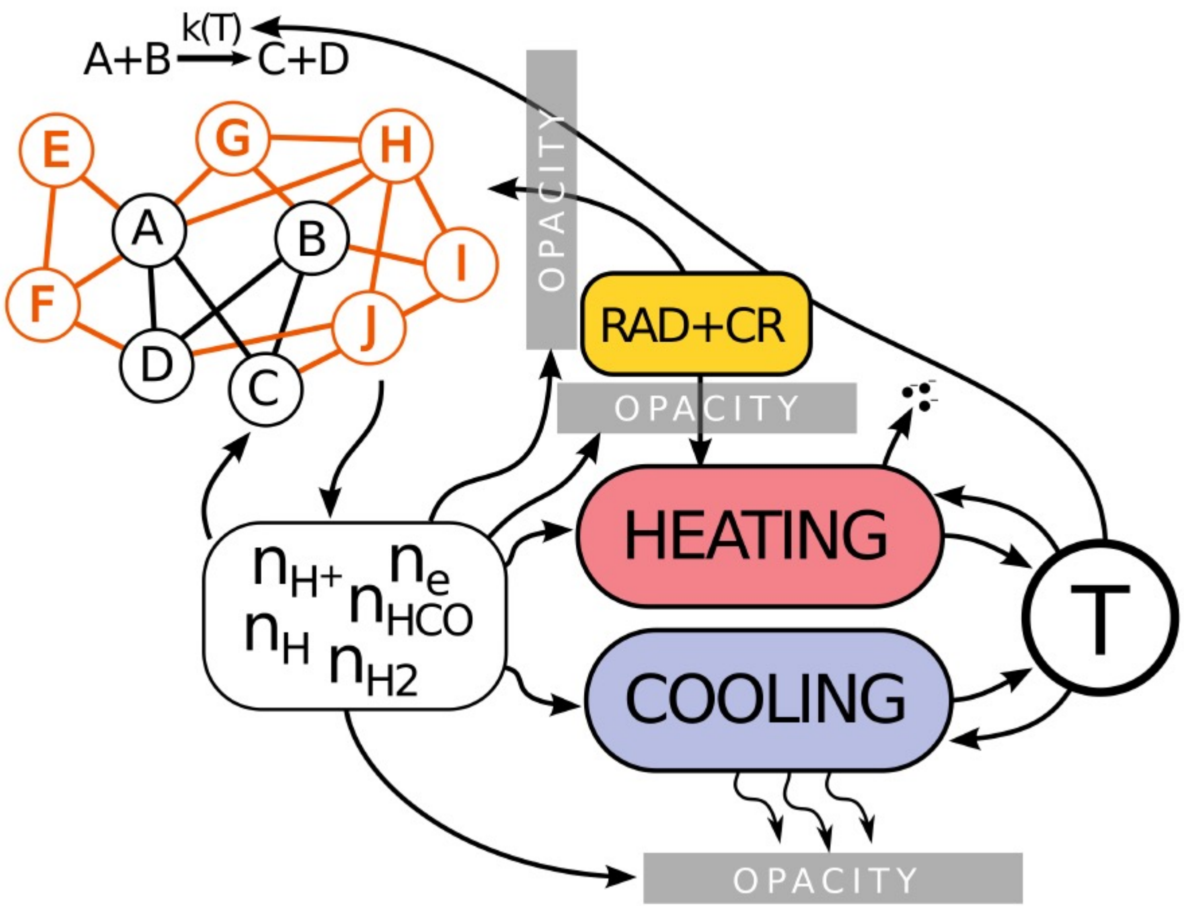

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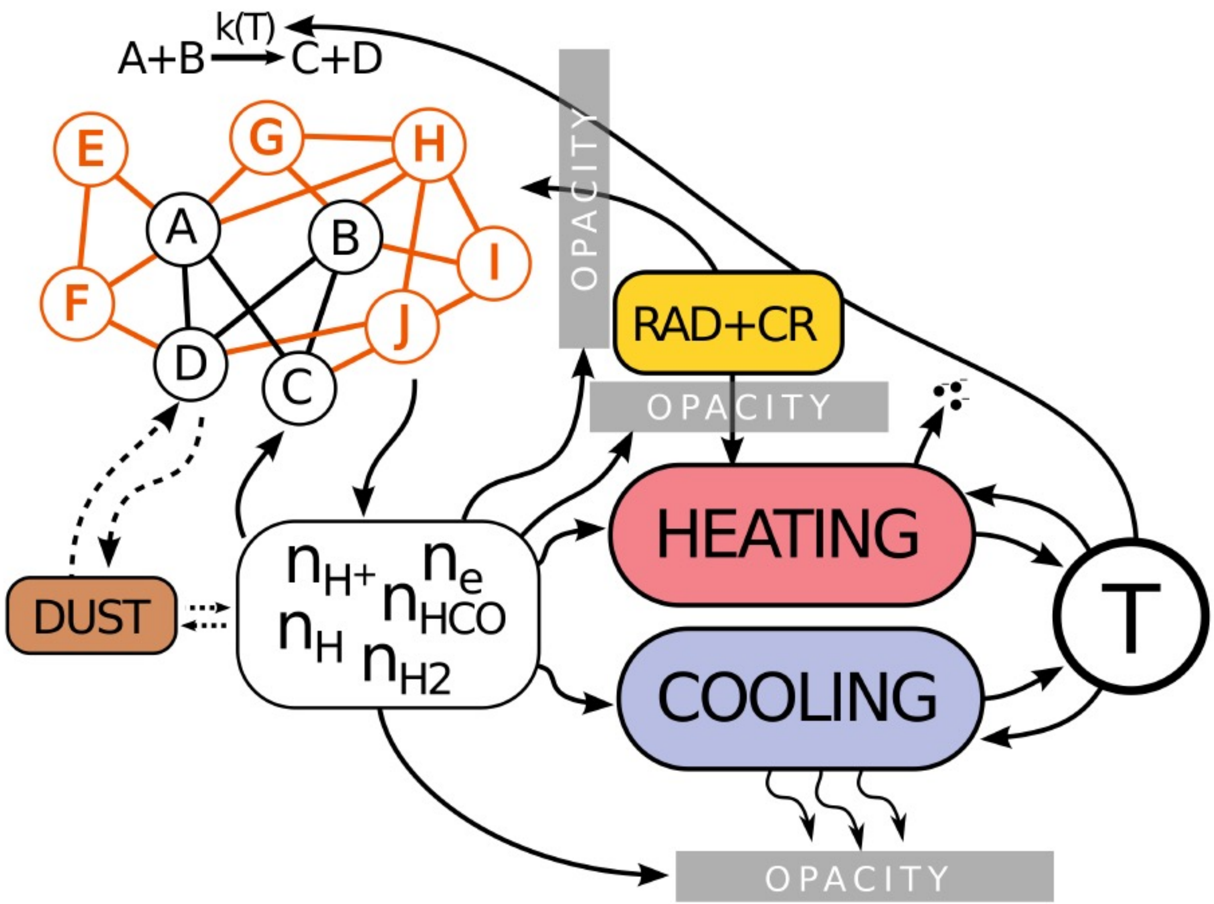

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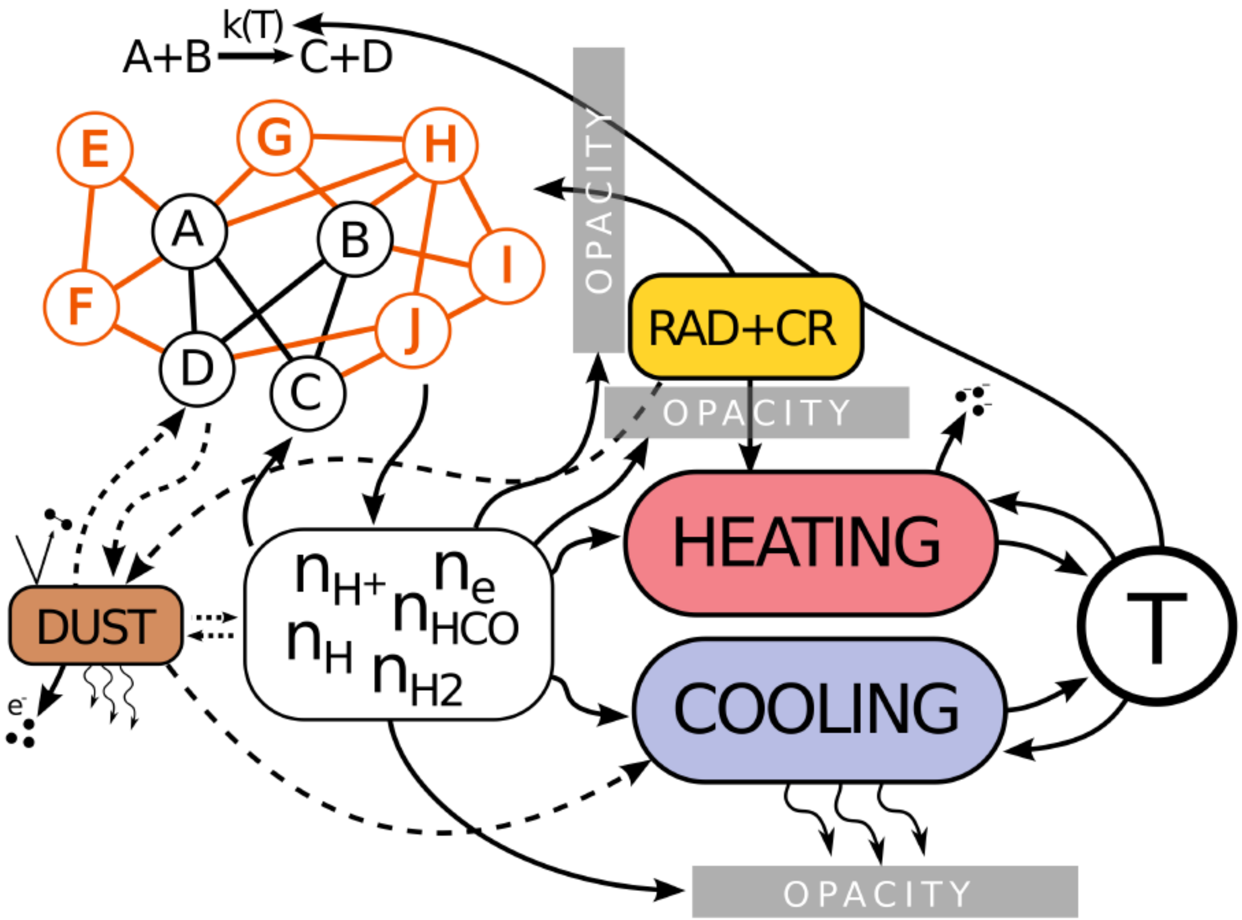

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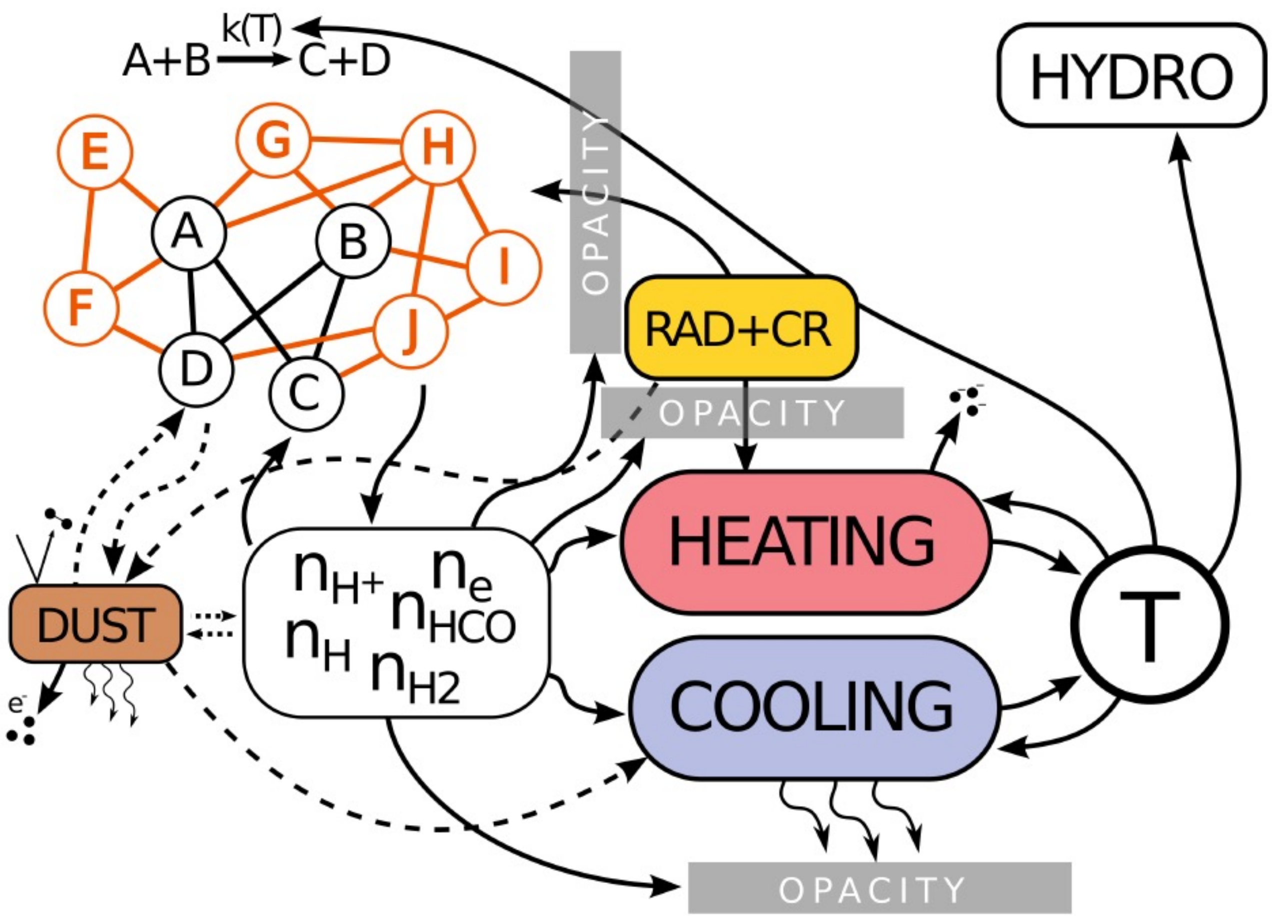

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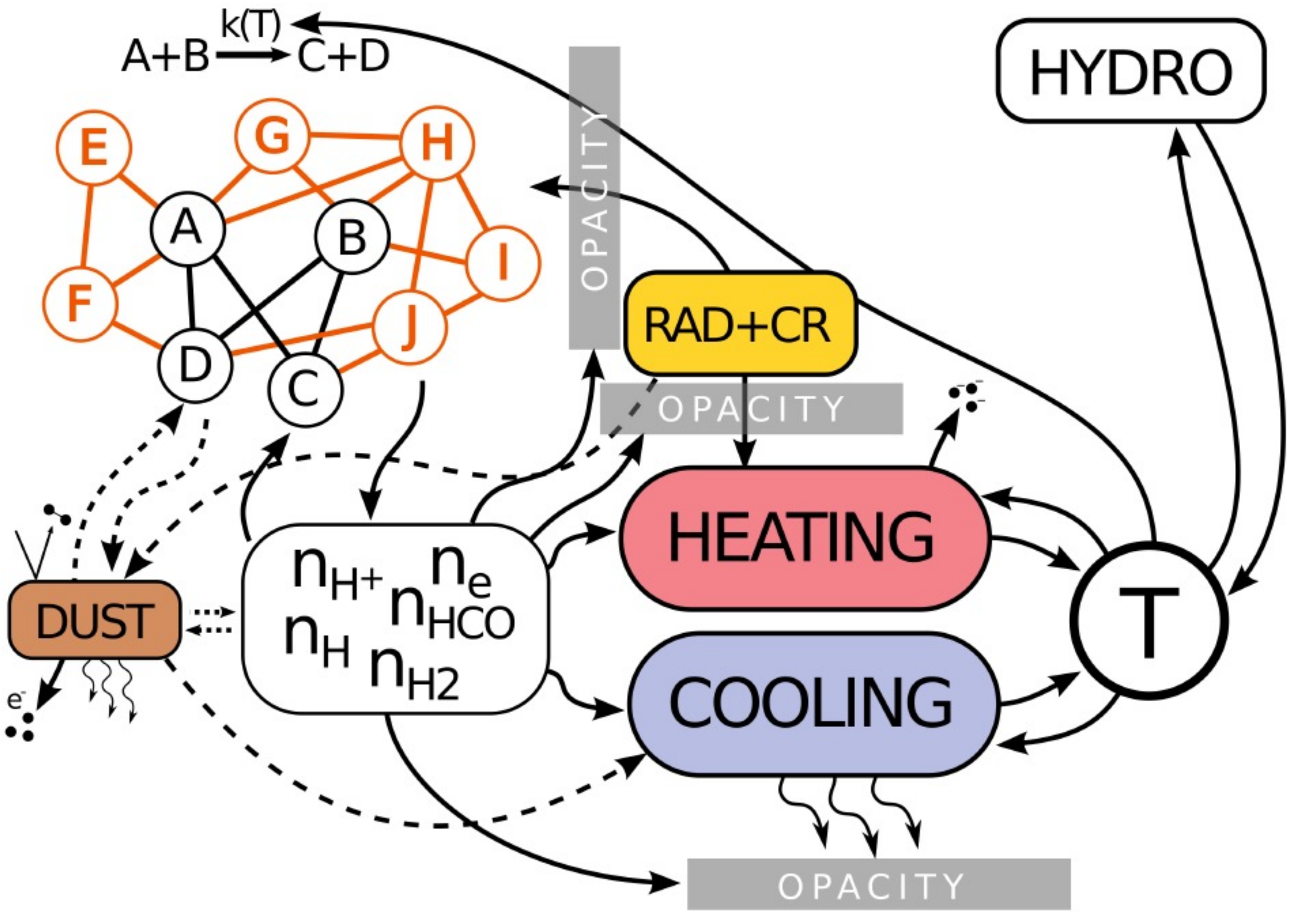

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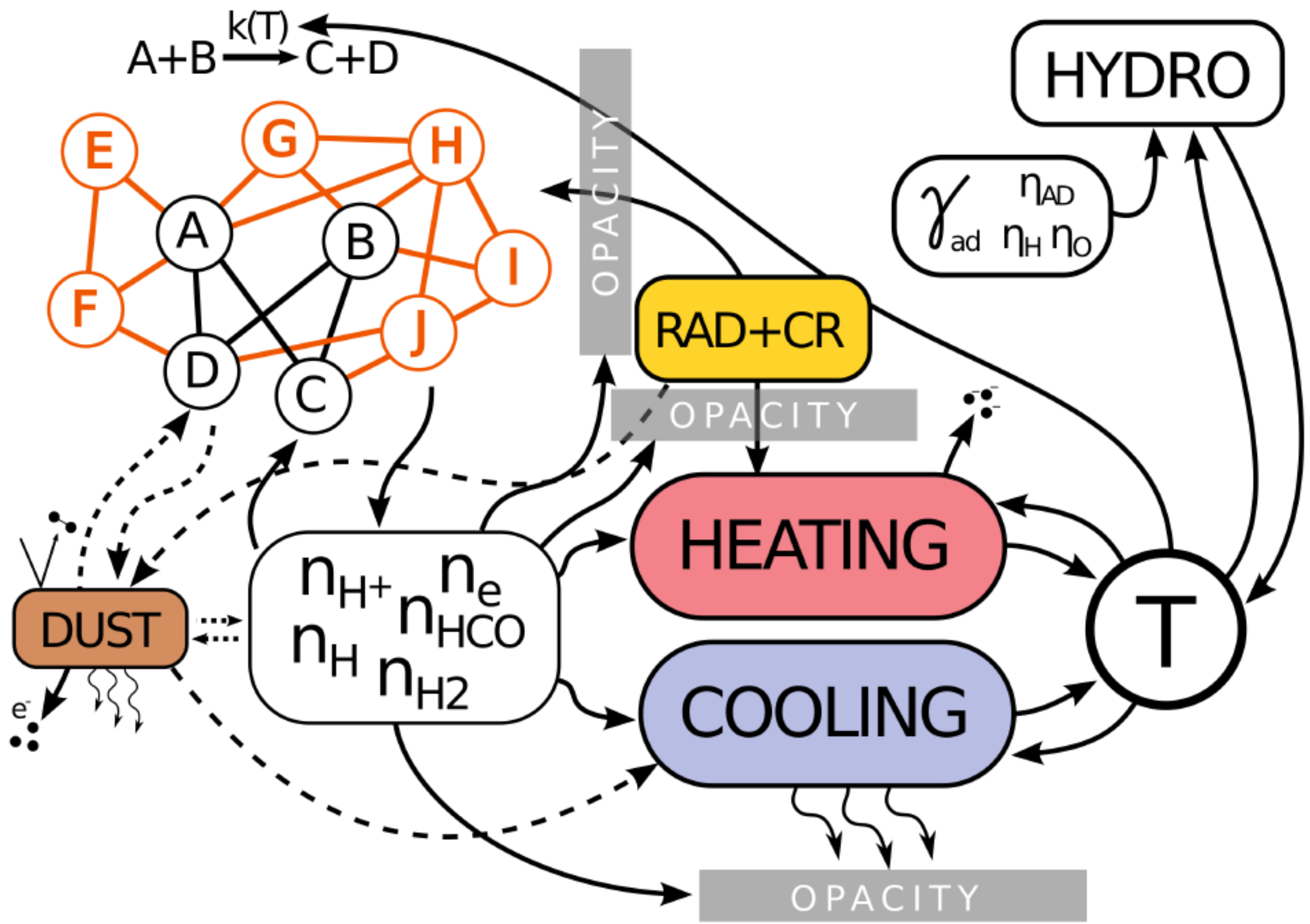

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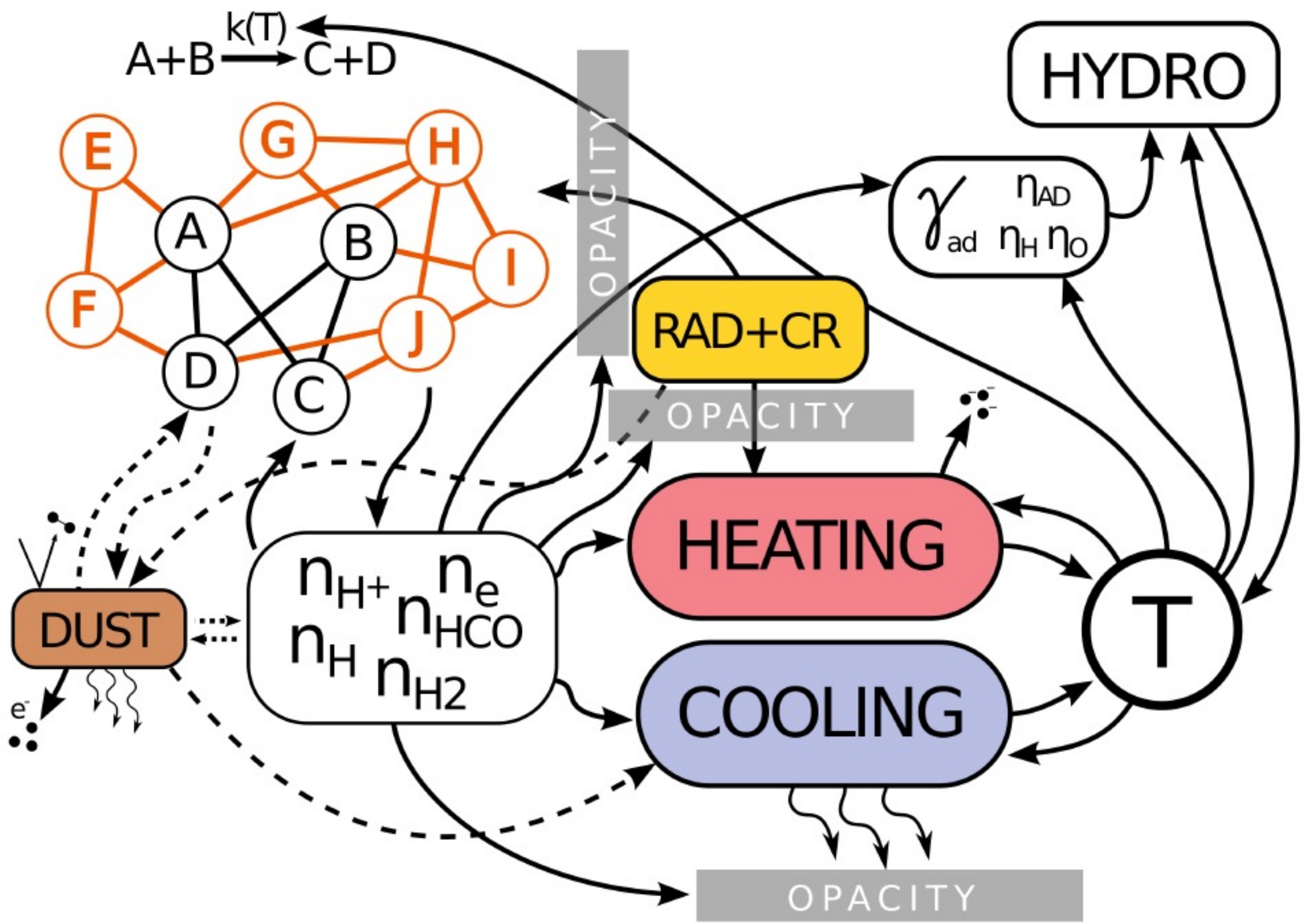

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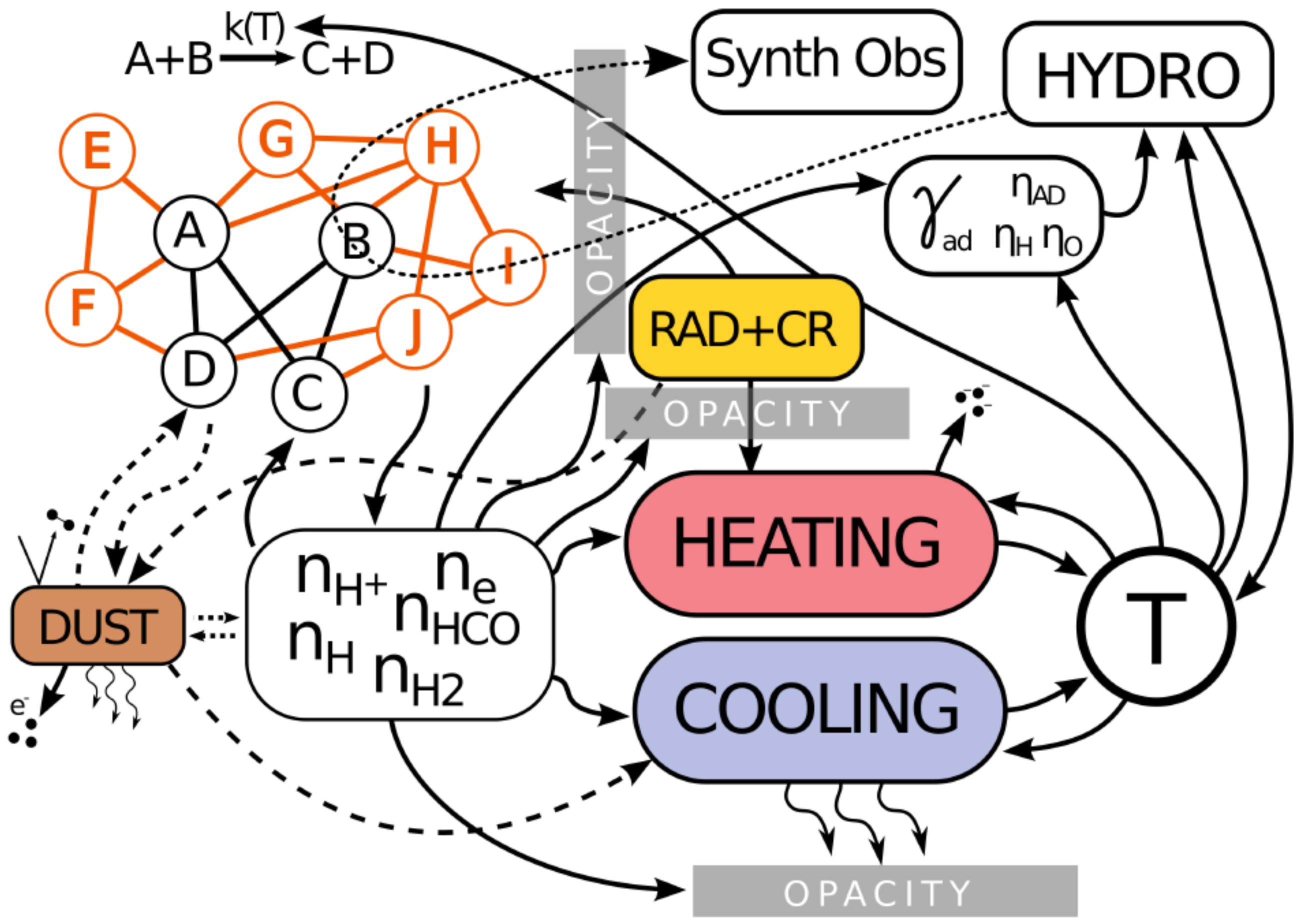
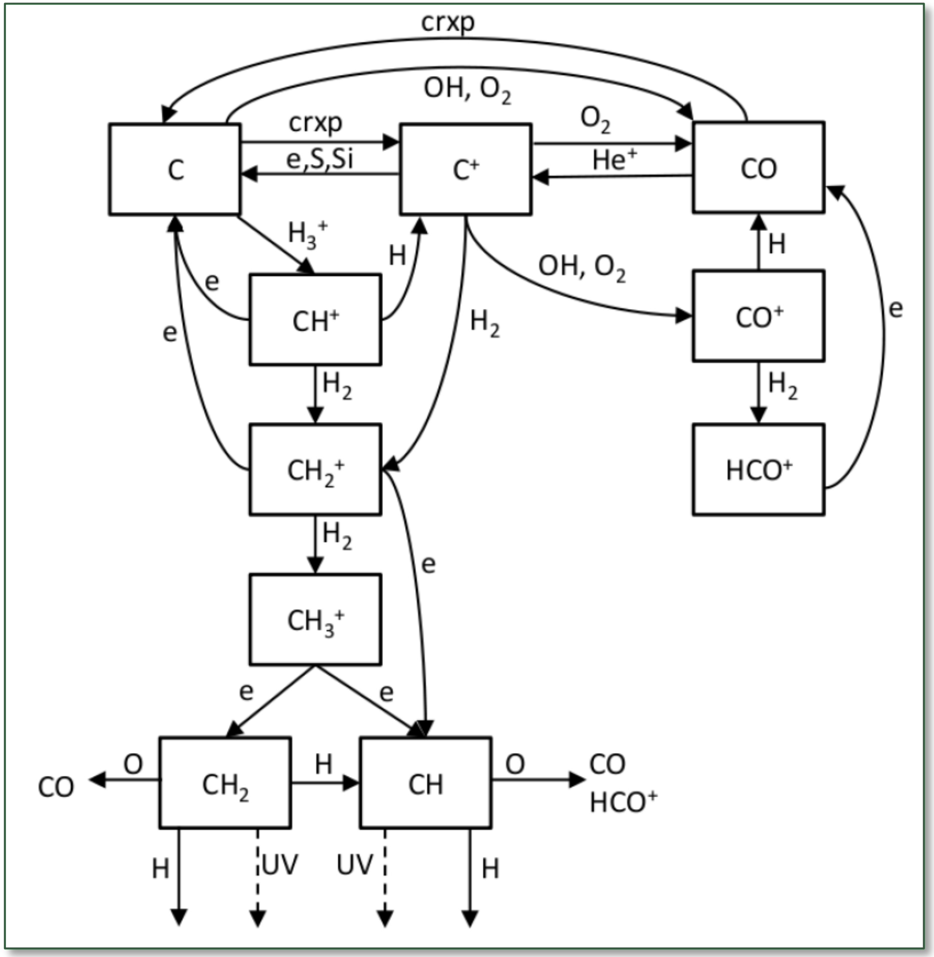


Example CO-network (cf. the ERDA notebook)



[Nelson 99, Langer 76]

Chemical reactions: some definitions

reactants products

$$CO^+ + e^- \rightarrow C + O$$

$$\frac{dn_C}{dt} = R = k \times n_{CO^+} \times n_{e^-}$$

ODE [cm^{-3}/s]

"flux" [cm^{-3}/s]

reaction rate coefficient [(cm^3)$^{N-1}$/s]

reactants abundances [cm^{-3}]

Chemical reactions: Cauchy's problem:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \overbrace{\sum_{lm} k_{lm}(T)n_l(t)n_m(t)}^{formation} - \overbrace{n_i(t)\sum_j k_{ij}n_j(t)}^{destruction} \qquad [\times N_{\mathrm{gas}}]$$

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \sum_{i\in\mathrm{formation}} R_i - \sum_{j\in\mathrm{destruction}} R_j \qquad [\times N_{\mathrm{gas}}]$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} \propto HEAT(T,\bar{n}) - COOL(T,\bar{n})$$

Chemical reactions: A simple example

A simple chemical network

$$\mathrm{H}^+ + \mathrm{e}^- \xrightarrow{k_1} \mathrm{H} + \gamma \tag{1}$$

$$\mathrm{H} + \gamma \xrightarrow{k_2} \mathrm{H}^+ + \mathrm{e}^- \tag{2}$$

ODE and Jacobian (an excerpt)

$$\frac{\mathrm{d}n_\mathrm{H}}{\mathrm{d}t} = k_1 n_{\mathrm{H}^+} n_{\mathrm{e}^-} - k_2 n_\mathrm{H} \tag{3}$$

$$\frac{\partial^2 n_\mathrm{H}}{\partial t \partial n_\mathrm{H}} = k_2 \qquad \frac{\partial^2 n_\mathrm{H}}{\partial t \partial n_{\mathrm{H}^+}} = k_1 n_\mathrm{e} \tag{4}$$

Chemical reactions: A simple example

	H	H^+	H^-	e^-	γ	CR
H						
H^+	x					
H^-	x	x				
e^-	x	x	x			
γ	x	x	x	x		
CR	x	x	x	x	x	

Chemical reactions "commute"

$$H^+ + e^- \rightarrow H + \gamma$$

$$e^- + H^+ \rightarrow H + \gamma$$

Chemical reactions: A simple example

	H	H^+	H^-	e^-	γ	CR
H						
H^+	x	x			x	x
H^-	x	x	x	x		
e^-	x	x	x	x	x	x
γ	x	x	x	x	x	x
CR	x	x	x	x	x	x

Some reactant pairs are impossible
(e.g. $H^- + H^-$ is repulsive)

Chemical reactions: A simple example

	H	H^+	H^-	e^-	γ	CR
H	*x*	*x*				
H^+	x	x	*x*		x	x
H^-	x	x	x	x		
e^-	x	x	x	x	x	x
γ	x	x	x	x	x	x
CR	x	x	x	x	x	x

some reactions lead to species $\notin$ subset (e.g. $H^- + H$ form H_2)

Chemical reactions: A simple example

	H	H^+	H^-	e^-	γ	CR
H	x	x	✓	✓✓	✓	✓
H^+	x	x	x ✓	✓	x	x
H^-	x	x	x	x	✓	✓
e^-	x	x	x	x	x	x
γ	x	x	x	x	x	x
CR	x	x	x	x	x	x

final set of reactions

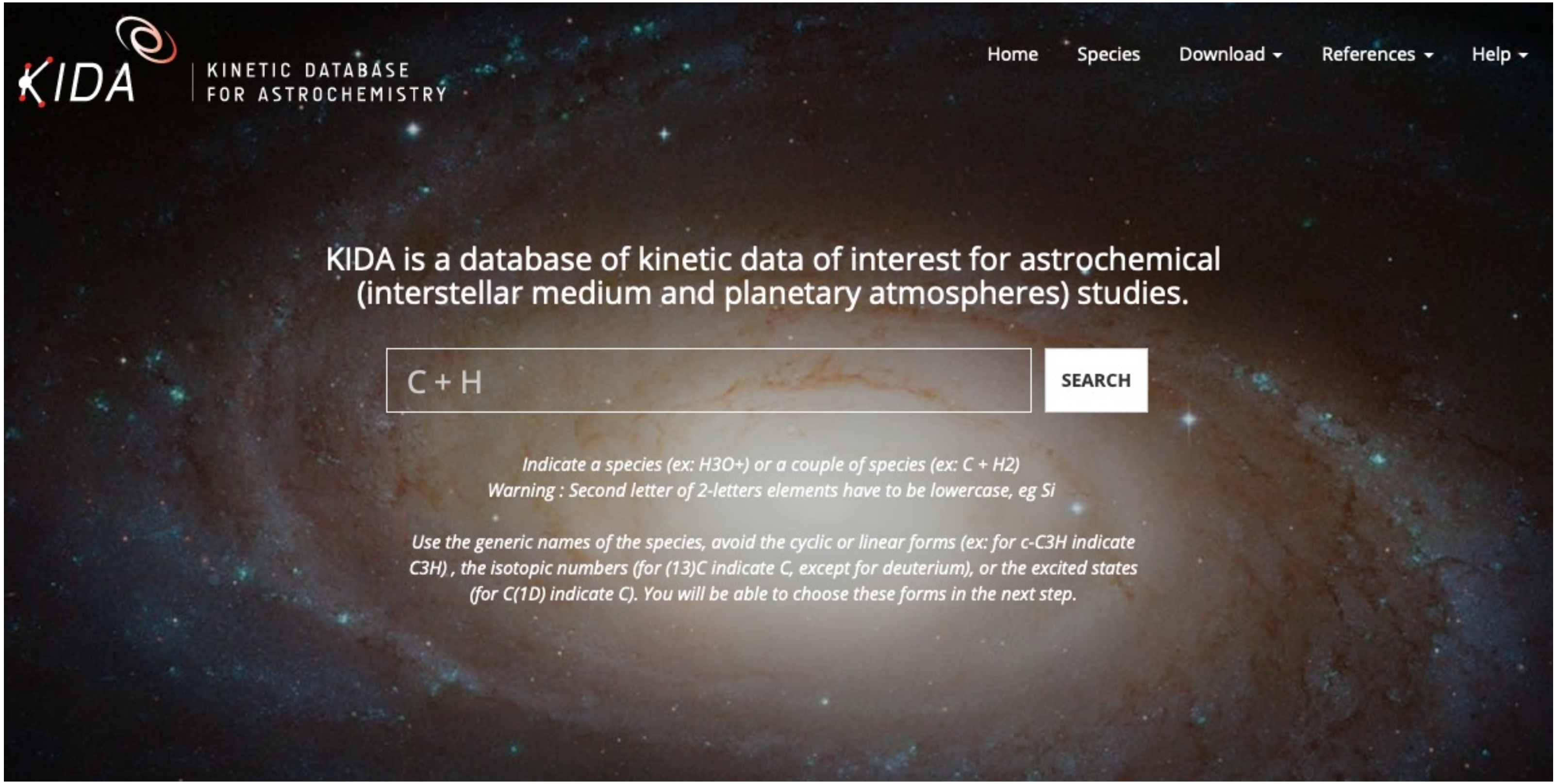
Chemical reactions: A simple example

Final network (4+2 species → 9 reactions)

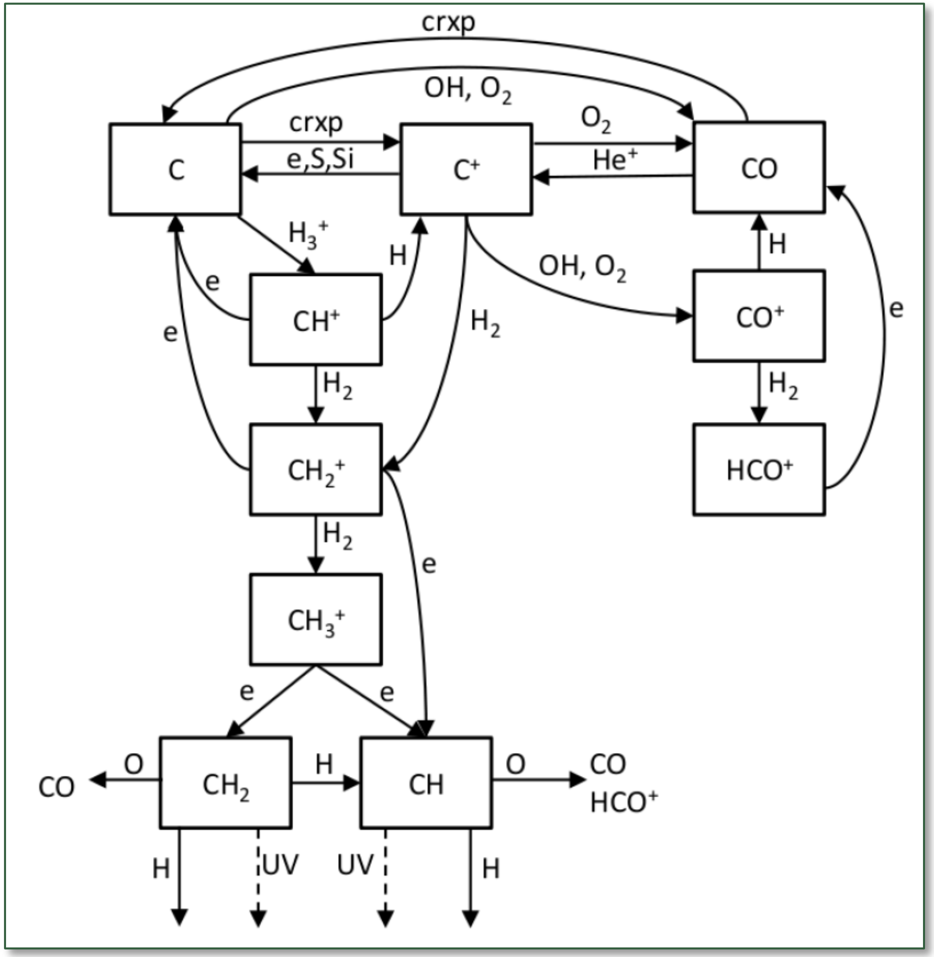
$H + e^-$	$\rightarrow$	$H^+ + 2e^-$	collisional ionization (branch 1)
$H + e^-$	$\rightarrow$	$H^- + \gamma$	radiative attachment (branch 2)
$H + \gamma$	$\rightarrow$	$H^+ + e^-$	photoionization
$H + CR$	$\rightarrow$	$H^+ + e^-$	CR ionization
$H^+ + e^-$	$\rightarrow$	$H + \gamma$	recombination
$H^+ + H^-$	$\rightarrow$	$H + H$	mutual recombination (single branch)
$H^- + \gamma$	$\rightarrow$	$H + e^-$	electron photodetachment
$H^- + H$	$\rightarrow$	$2H + e^-$	collisional detachment
$H^- + CR$	$\rightarrow$	$H + e^-$	CR detachment

Chemical reactions: public domain databases

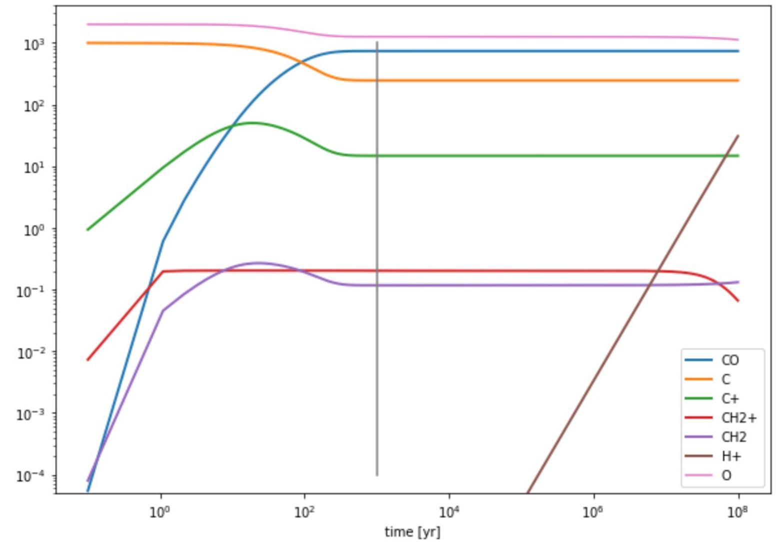
https://kida.astrochem-tools.org



Buffering and stiff equations




```
C+   + H2 -> CH2+ + hv: 5e-16
CH2+ + E  -> CH2  + hv: 2.5e-08
```



Explicit integration: timestep controlled by fast rate, even in equilibrium!

[Nelson 99, Langer 76]

Chemical reactions: Jupyter notebook & tasks

In the **5 Chemistry** notebook we will study the formation of two important molecules:

- Water (H2O) is of central interest in proto-planetary disks, where the water-ice (beyond the "ice-line") may speed up the formation of solid bodies, by condensing onto dust to make fluffy aggregates – dirty "snowballs" perhaps ;-)

- Carbon monoxide (CO) is import both from the modeling and observational point of view. It is a very stable molecule and tends to "steal" all of the carbon and a corresponding amount of oxygen (generally about twice as abundant as carbon), and CO-molecules are key observationally (in different isotopes!)

ERDA Jupyter Notebook !