A PDR code including dust grain chemistry

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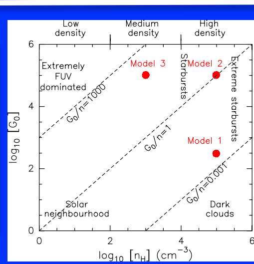
- Aim: to determine the different conditions of the ISM (gas/ice/dust) in regions where the energetic balance is dominated by UV radiation.
- Methods: use of the **PDR_code** (Meijerink et al. 2005) which we improved by implementing **chemistry occurring onto dust grains** and additional reactions in the **gas-phase**. Gas chemistry includes bimolecular, change-exchange, radiative association, associative detachment, dissociative recombination, neutralisation, ion-neutral reactions and ionisation/dissociation by UV photons and cosmic-rays. Dust chemistry includes chemical desorption, freeze out, evaporation, reactivity on surfaces or in the ices and photo-desorption. We consider in total more than **6500 chemical reactions**.

PDR_code

- Stationary code.
- T_{dust} expression from Garrod & Pauli (2011).
- Heating processes: grain heating, carbon ionisation, H_2 photo-dissociation, H_2 collisional de-excitation, gas-grain viscous heating and cosmic-ray heating.
- Cooling processes: fine-structure line, metastable-line, recombination and molecular cooling by H_2, CO and H_2O.



Model 1

$n_H=10^5$ cm^{-3} & $G_o=10^{2.5}$

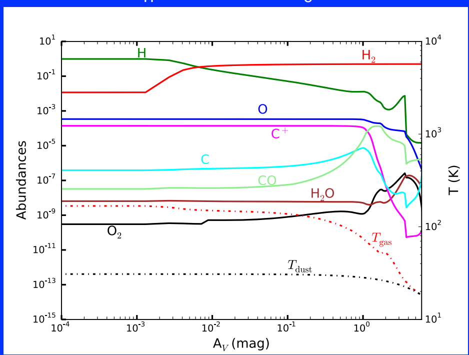
Model 2

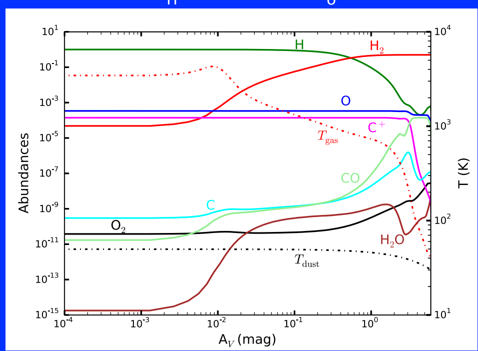
$n_H=10^5$ cm^{-3} & $G_o=10^5$

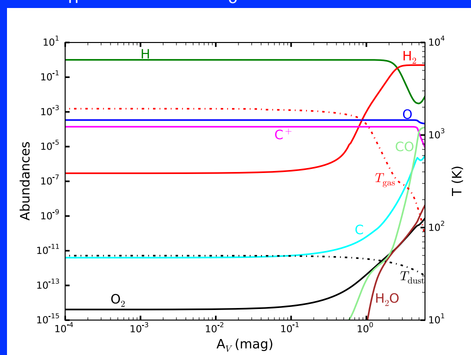
Model 3

$n_H=10^3$ cm^{-3} & $G_o=10^5$

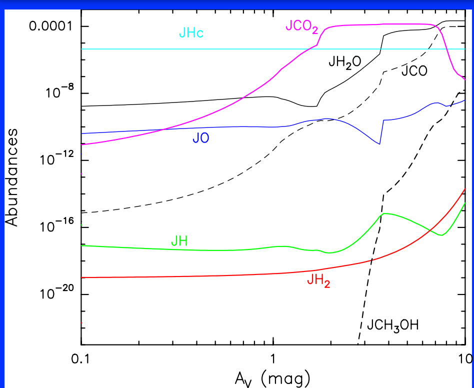
Gas-species

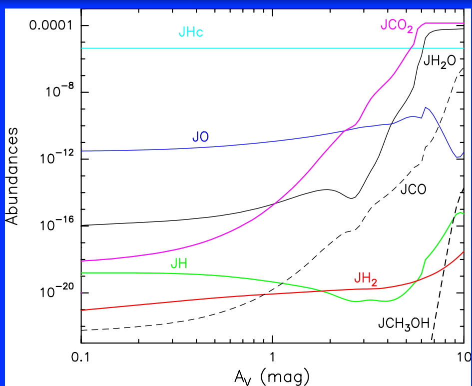


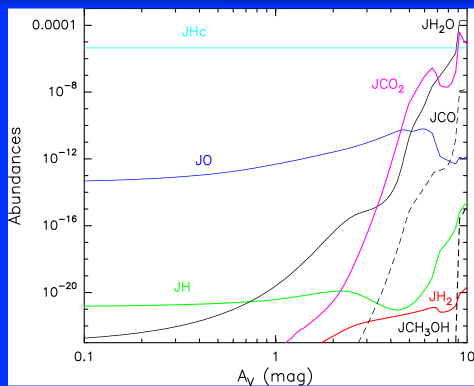




Dust-species







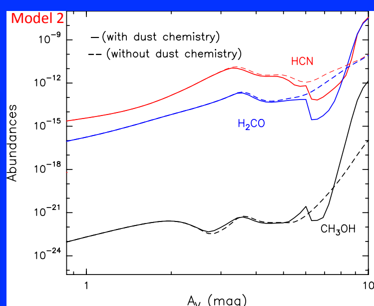
Low G_0 and high n_H

High G_0

Thermal balance:

- Colder dust grains (T_d~12 at A_v=10).
- Heating: dominated by photo-electric emission, H_2 dissociation and carbon ionisation (low A_v), and by gas-grain collisions and cosmic-rays (high A_v).
- Cooling: dominated by recombination and gas-grain collisions (low A_v), and by recombination (high A_v).

- Warmer dust grains (T_d~20 K at A_v=10).
- Heating: dominated by photo-electric emission and H_2 dissociation (low A_v), and by cosmic-rays (high A_v).
- Cooling: gas-grain collisions and recombination (low and high A_v). OI important at low A_v.



Chemistry:

- H ➡ H_2 transition at low A_v (<0.01).
- Formation of CO_2 and H_2CO ices at A_v >1.
- Formation of CO ice at A_v<10.

- H ➡ H_2 transition at A_v > 0.5.
- Formation of CO_2 and H_2O ices at A_v > 5.
- No formation of CO ice at A_v<10.

- **Dust chemistry leads to enrichment of abundances of gas-phase species, such as HCN, CH_3OH and H_2CO, by more than two orders of magnitude at high A_v.**

- **Ice formation depends more strongly on radiation flux than on density.**
- **High G_o leads to formation of CO_2 and H_2O ices at greater depth than low G_o.**
- **Formation of CO ice at A_V<10 only for low G_o.**

- **Low C abundances in the transition C^+→CO are due to the new gas-phase reactions and not to the dust chemistry.**