X-ray photochemistry of planetary atmospheres

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Outline

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- **Introduction**
- **X-rays & Röntgen Spheres**
- **Photochemestry of Toy Atmospheres**
- **Conclusions & next steps**

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Introduction

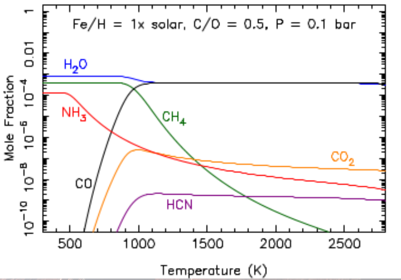
Chemistry

The abundance of elements in atmosphere is governed by chemistry, and depends on:

- Temperature
- Pressure

Disequilibrium processes

- Vertical mixing (eddy & molecular diffusion)
- **Photochemistry**



Mixing ratios as functions of the temperature at the chemical equilibrium. *Moses+13*

X-rays

Ionization rate: primary ionization

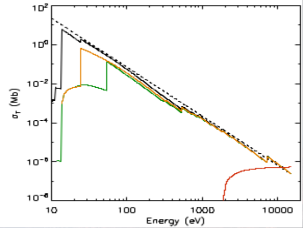
$$\varsigma'_X = \sum_k \int_{E_0}^{\infty} \frac{F_X(E)}{E} x_k \sigma_k(E) dE \qquad (1)$$

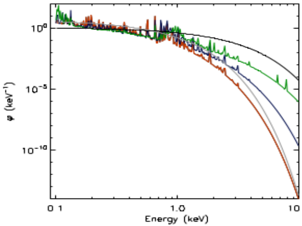
- $F_X(E,r) = \frac{\mathcal{L}_X(E)}{4\pi r^2} \times e^{-\tau(E,r)}$
- $\tau(E,r) = n_{\rm H}\sigma(E)r$
- $\mathcal{L}_X(E) = L_X \times \varphi(E)$

Ionization rate: secondary ionization

$$\varsigma''_X = \sum_{k=1}^{3} \int_{E_0}^{\infty} F_X(E) \frac{x_k \sigma_k(E)}{W} dE \qquad (2)$$

- W is the energy to make a ion pair
- $\varsigma''_{{\rm X},i} = (\sigma_i^{(e)}/\sigma_H^{(e)})\varsigma''_{\rm X}$





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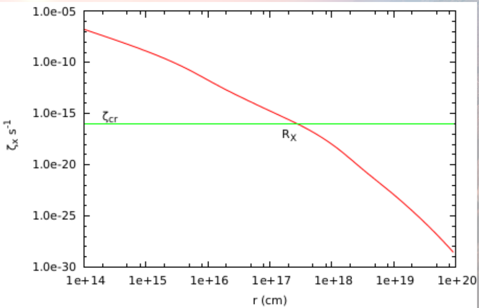
Röntgen sphere

The Röntgen sphere (*Lorenzani & Palla 01*) is defined as circumstellar regions in which the ionization rate due to X-rays exceeds the background level provided by cosmic rays, $\varsigma_{\rm cr}$.

$$\varsigma_X(r\prime) = \varsigma_{\rm cr}$$

then $r\prime \Longrightarrow$ Röntgen radius $R_{\rm X}$



Röntgen sphere of pre-main sequence stars and solar proxies

Röntgen radii for solar proxies

star†	age (Gyr)		R_X (pc)	
K0	0.002	1.9(-1)	4.1(-2)	5.6(-3)
EK Dra	0.1	8.1(-2)	1.6(-2)	3.1(-3)
π^1 UMa + χ^1 Ori	0.3	3.7(-2)	8.3(-3)	1.8(-3)
κ^1 Cet	0.65	2.8(-2)	6.7(-3)	1.5(-3)
β Com	1.6	1.3(-2)	4.2(-3)	9.2(-4)
Sun	4.56	6.7(-3)	2.6(-3)	5.6(-4)
β Hyi	6.7	4.2(-3)	1.9(-3)	4.2(-4)
$\log_{10}(n_H/cm^{-3})$		2	4	6

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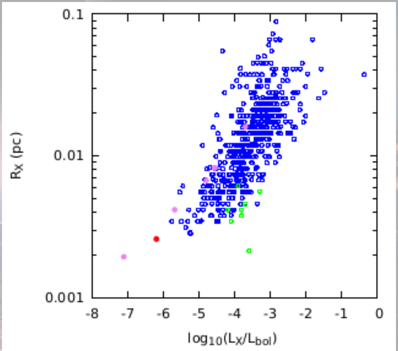


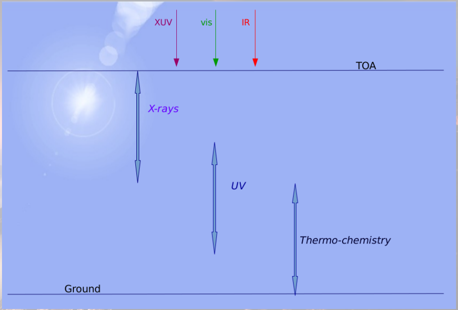
Orion Nebula Cluster

Photochemistry of Toy Atmospheres

Continuity equation

$$\frac{dn_i(z)}{dt} = P_i(z) - n_i(z)L_i(z) \quad (3)$$

- z: altitude
- n_i: number density
- L_i: loss rate coefficient
- P_i: production rate coefficient



An atmosphere of pure Oxygen

Chemical network

$$\mathrm{O} + \mathrm{O_2} + \mathrm{M} \longrightarrow \mathrm{O_3} + \mathrm{M}$$

$$\mathrm{O} + \mathrm{O_3} \longrightarrow \mathrm{O_2} + \mathrm{O_2}$$

$$\mathrm{O_2} + \mathrm{h}\nu \longrightarrow \mathrm{O} + \mathrm{O}$$

$$\mathrm{O_3} + \mathrm{h}\nu \longrightarrow \mathrm{O} + \mathrm{O_2}$$

Photolysis rate

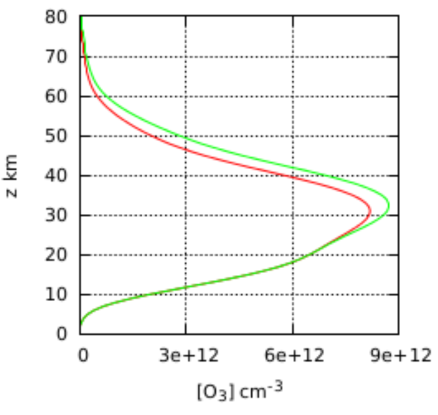
$$J_i(z) = \int \sigma_i(E) F(E,z) dE \qquad (4)$$

- $\sigma_i(E)$ photo-dissociation cross-section of i-th process
- $F(E,z) = F_0 e^{\tau(E,z)}$
- $\tau = \sum_i \sigma_i(E) N_i(z)$

An atmosphere of pure Oxygen

Initial set-up

- $n_l = 80$
- $\Delta z = 1$ km
- $T(z) = 245$ K
- $n_g = 5.48 \cdot 10^{18}$ cm^{-3}
- $[O_2]_m(z) = 1.$



The effects of X-rays on planetary atmospheres

X-ray ionization rate

$$\varsigma_{X,i}(z) = \varsigma'_{X,i}(z) + \varsigma''_{X,i}(z) \qquad (5)$$

- We calculate molecular ionization cross-section as sum of those atomic
- We need to accurately calculate W (*Cecchi-Pestellini+06*)
- We can work into three configuration:
  - H, H_2, He
  - H_2O, O_2, N_2
  - H_2O, CO_2, N_2

X-rays inside toy atmospheres

Density	R_X (km)	
(cm^{-3})	Solar composition	Heavy element rich
10^9	1.6×10^9	3.2×10^7
10^{12}	1.5×10^7	$2. \times 10^5$

$L_X = 1 \times 10^{30}$ erg/s
$\mathcal{Z} = 1 \times 10^{-16}$ s^{-1}

Primary atmosphere

Composition & chemical network

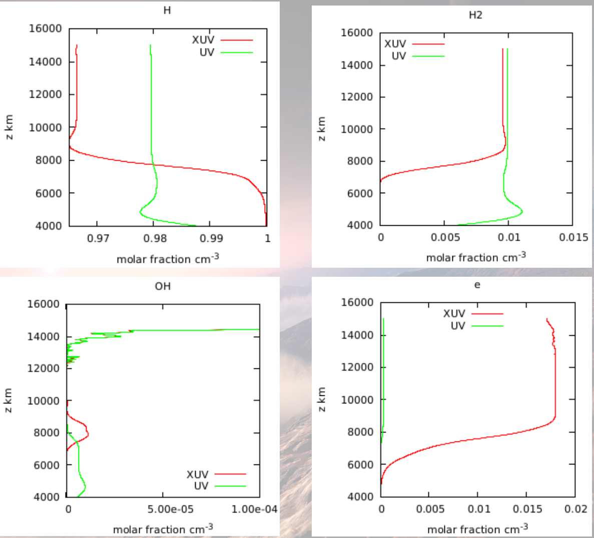
For our toy atmosphere we have considered:

- 6 species: H, H_2, He, O, H_2O, OH (and their ions)
- 22 chemical reactions between bimolecular and recombination reactions
- 4 photo-dissociation reactions (UV)
- 6 photo-ionization reactions (XUV)

Initial conditon & set-up

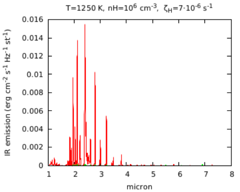
- $n_l = 1.5 \cdot 10^3$
- $\Delta z = 10$ km
- $T(z) = 300$ K
- $n_g = 5.48 \cdot 10^{20}$ cm^{-3}
- $n_{TOA} = 6 \cdot 10^{-6}$ cm^{-3}
- $L_X = 10^{30}$ erg s^{-1}
- $[H]_m(z) = 9.7 \cdot 10^{-1}$
  $[H_2]_m(z) = 1 \cdot 10^{-2}$
  $[He]_m(z) = 1 \cdot 10^{-2}$
  $[O]_m(z) = 3.3 \cdot 10^{-3}$
  $[H_2O]_m(z) = 3.3 \cdot 10^{-3}$
  $[OH]_m(z) = 3.3 \cdot 10^{-3}$

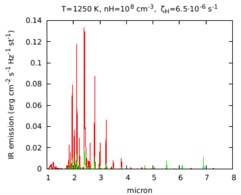
Primary atmosphere

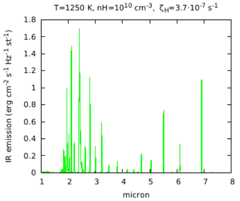


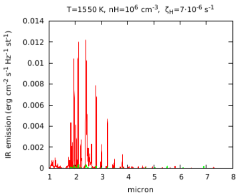
IR induced spectra (The case of HD 189733b)

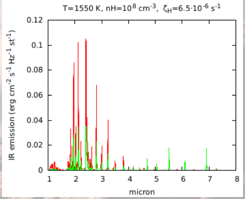
$n_{H_2} = 10^6,\ 10^8,\ 10^{10}\ \mathrm{cm}^{-3} \rightarrow \langle \varsigma_H \rangle = 7\cdot10^{-6},\ 6.5\cdot10^{-6},\ 3.7\cdot10^{-7}\mathrm{s}^{-1}$;
$L_X = 1.5\times10^{28}$ erg s^{-1}; T=1250, 1550 K

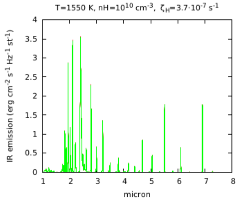












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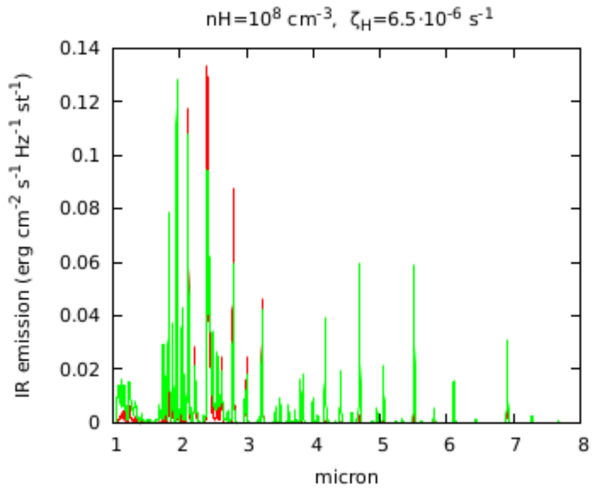

Conclusion & next steps

Conclusion

- X-rays affect the chemistry of upper layers of primordial atmospheres
- High levels of electronic concentration, for instance can enhance the hydrodynamic escape
- H_2 induced infrared emission spectra can be a diagnostic for the stellar high energy planet interaction

Next steps

- Include into continuity equation the vertical transport of particles
- Create a complete chemical network
- Include molecular excitation cross-section for electronic impact for the calculation of W
- Couple the chemical model with a 1D Radiative-Thermo-Convective model