FORMATION AND DESTRUCTION OF ORGANIC MOLECULES IN THE ATMOSPHERE OF TITAN

Aline Ramos Ribeiro, Diana P. P. Andrade, Heloisa M. Boechat-Roberty
Observatório do Valongo, Universidade Federal do Rio de Janeiro

ALLAM: Astrochemistry LLAMA Meeting
IAG/USP, August 9, 2019

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WHAT'S INTERESTING ABOUT TITAN

Shares many similatiries with Earth

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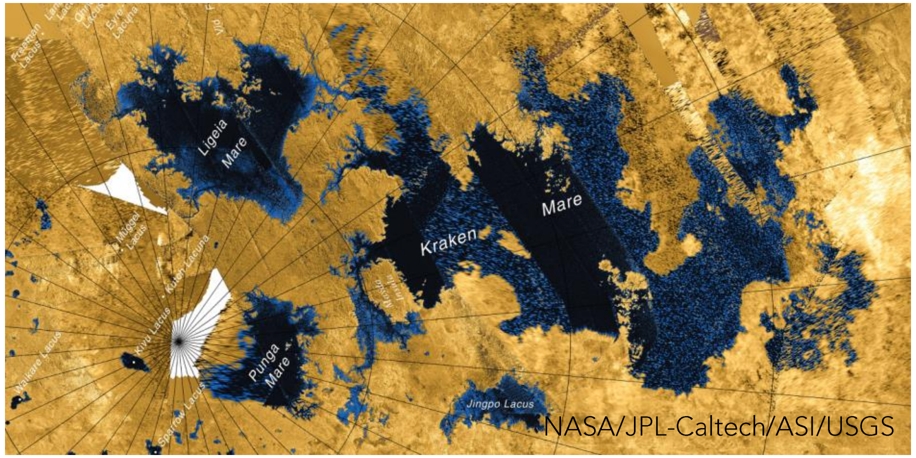
- Lakes



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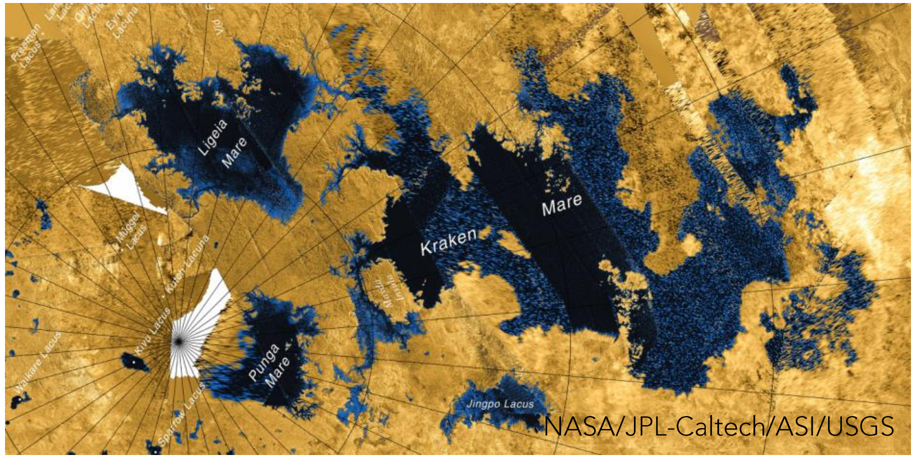

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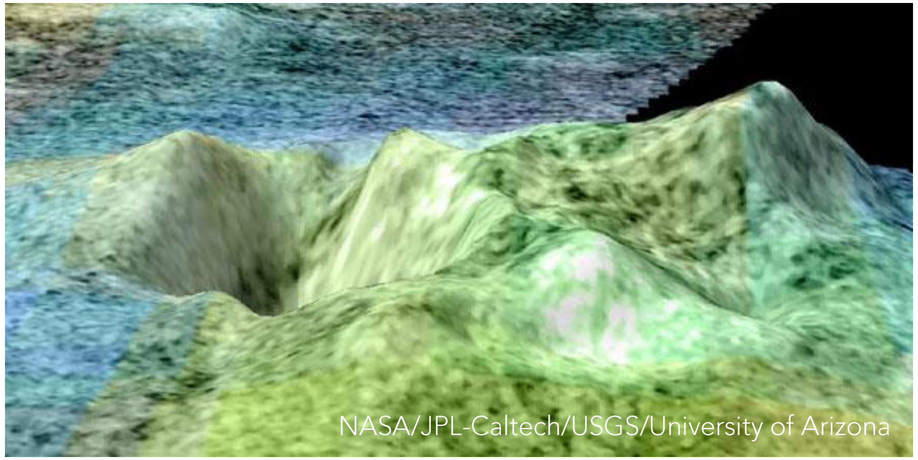
- Cryovolcanism



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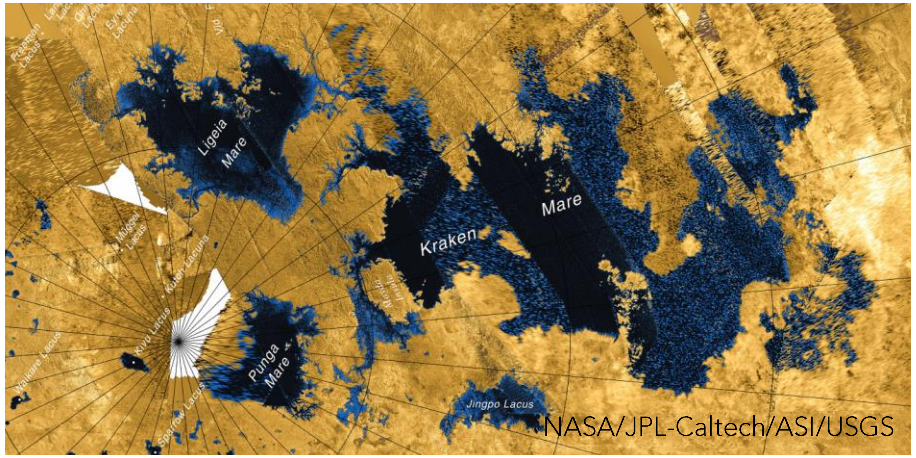

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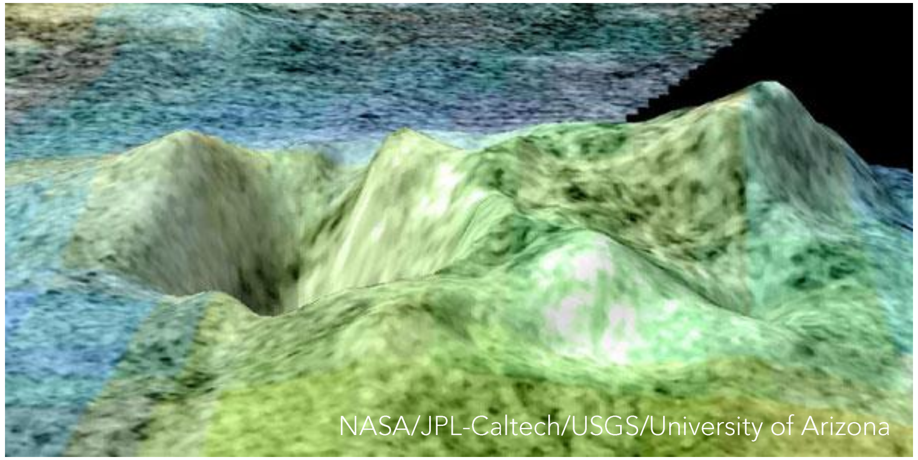

- Dense atmosphere

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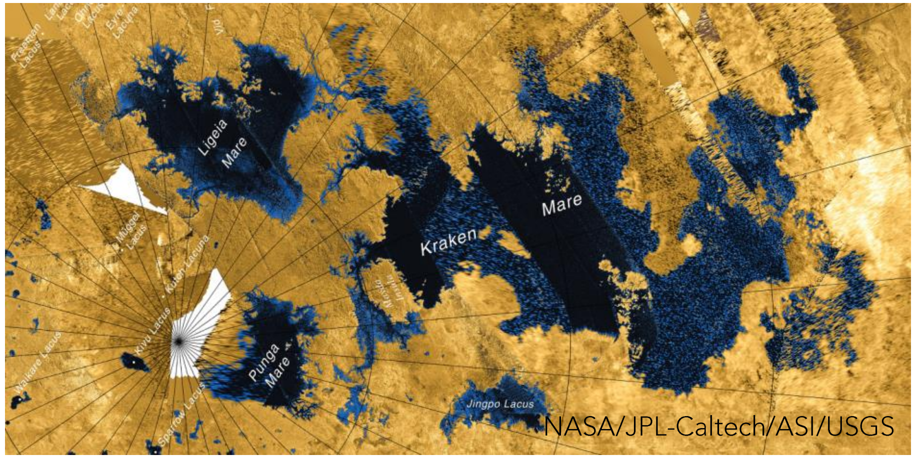

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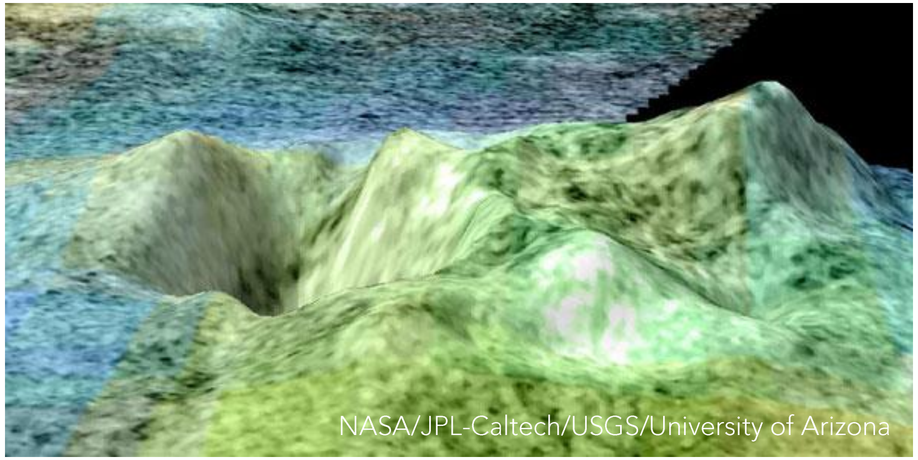
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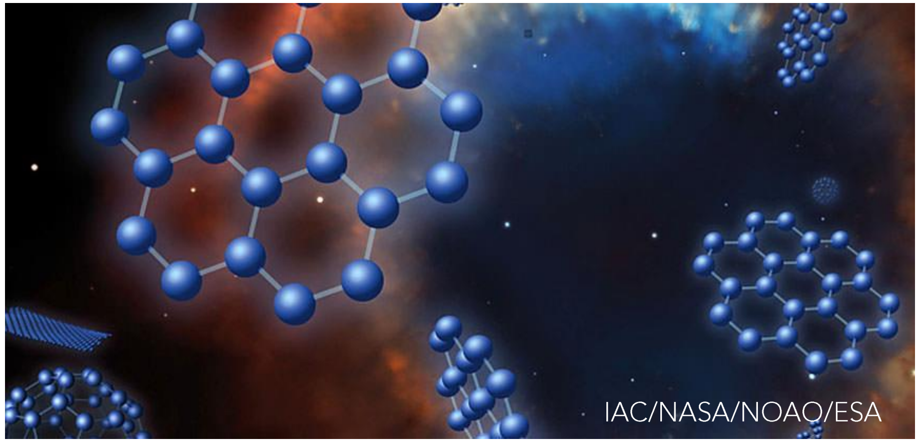
- Dense atmosphere


NASA/JPL

- Complex organic molecules (COMs)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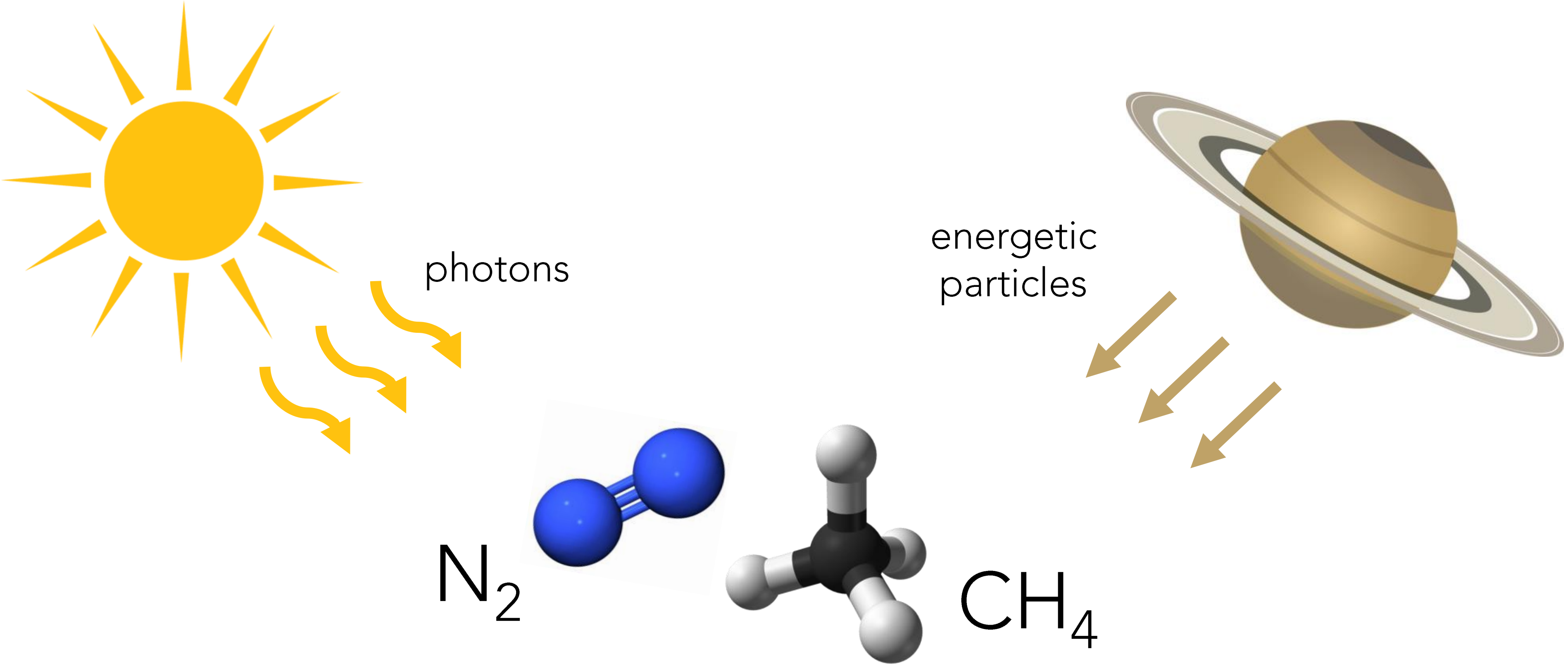
CHEMISTRY IN TITAN



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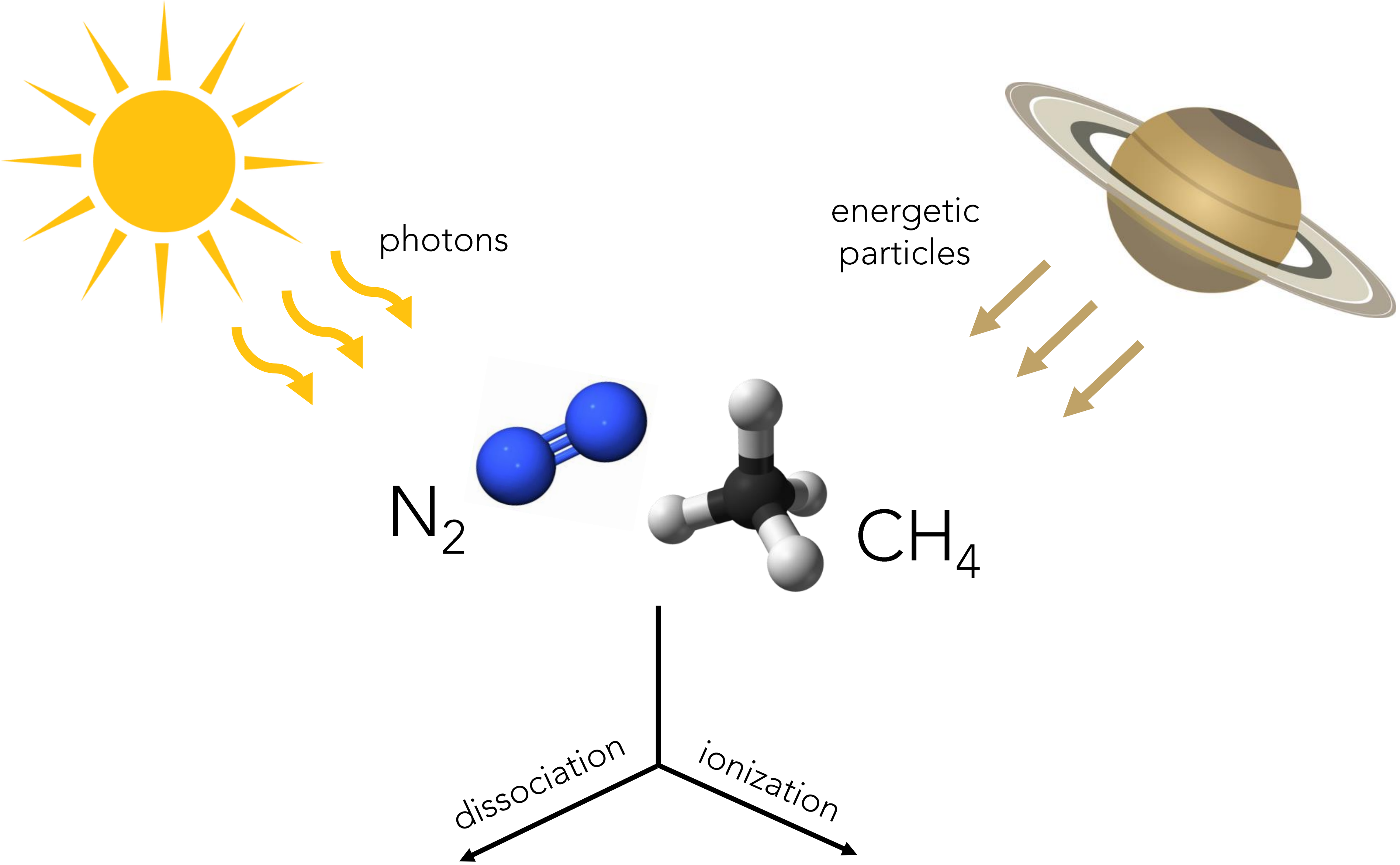

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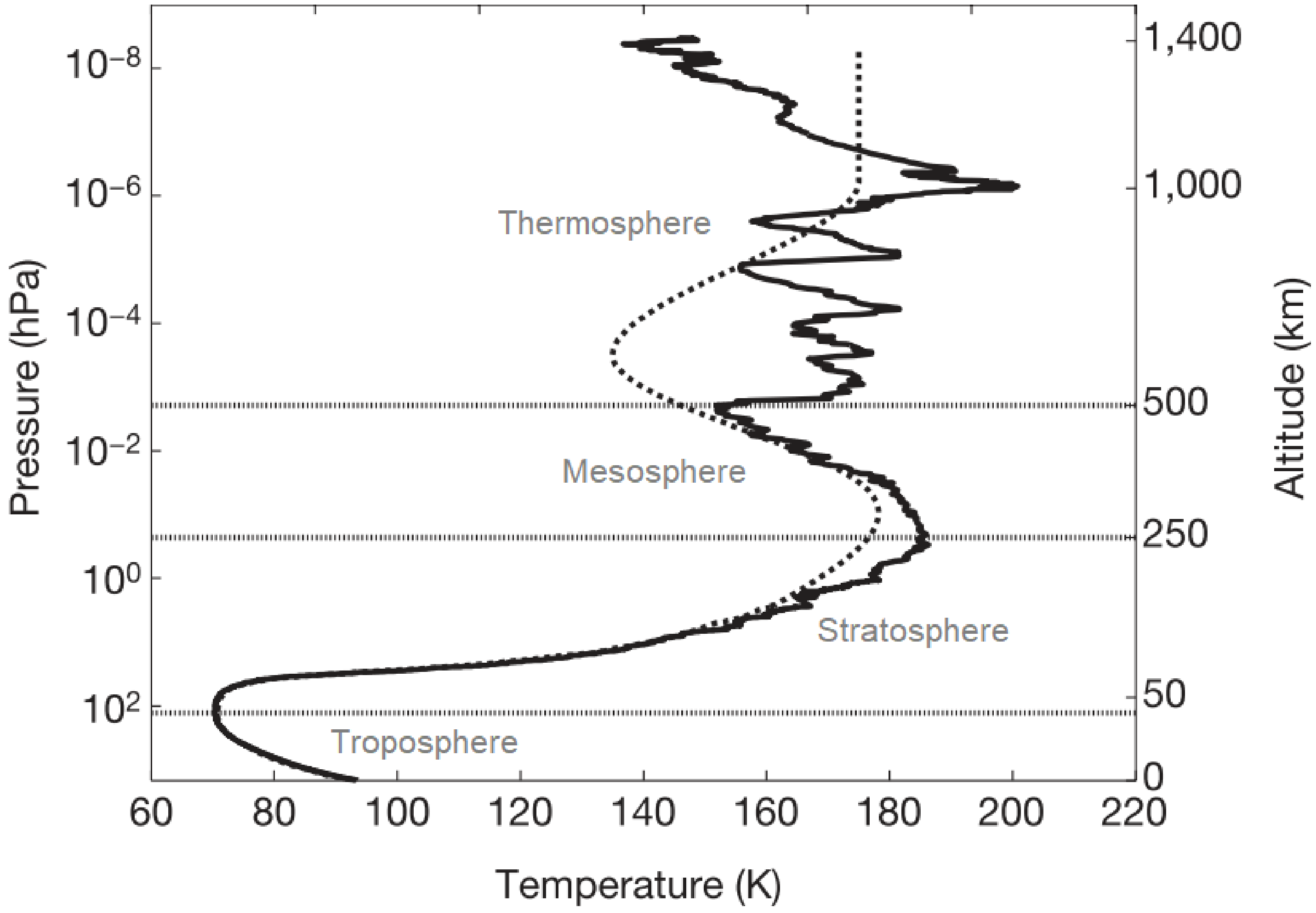
CHEMISTRY IN TITAN

Fulchignoni et al. (2005)



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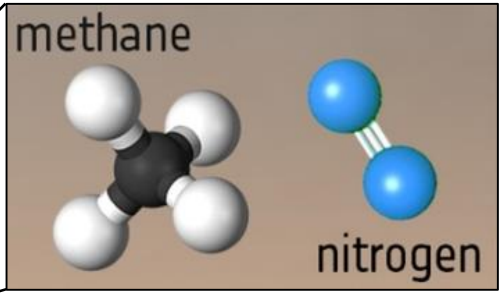

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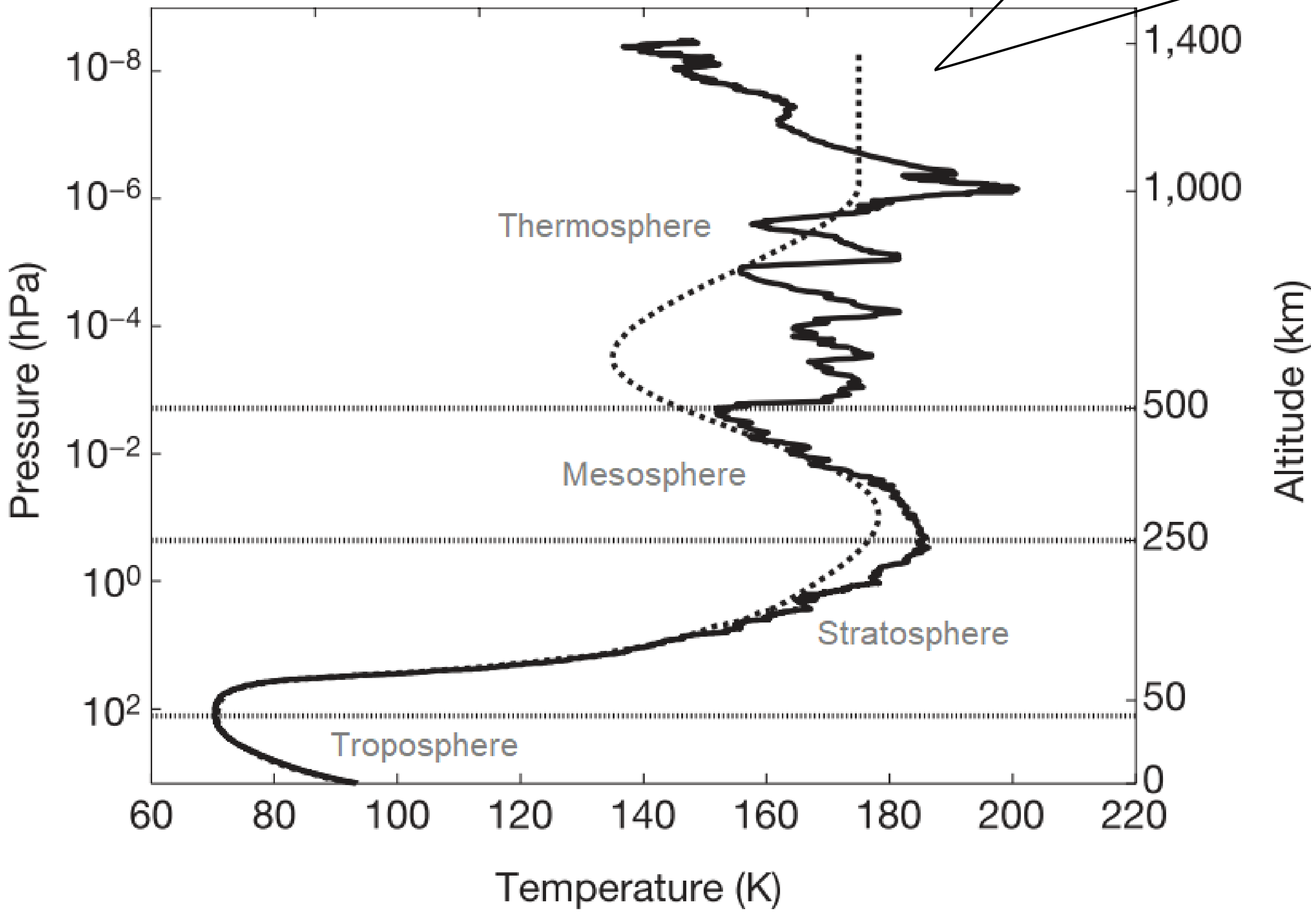

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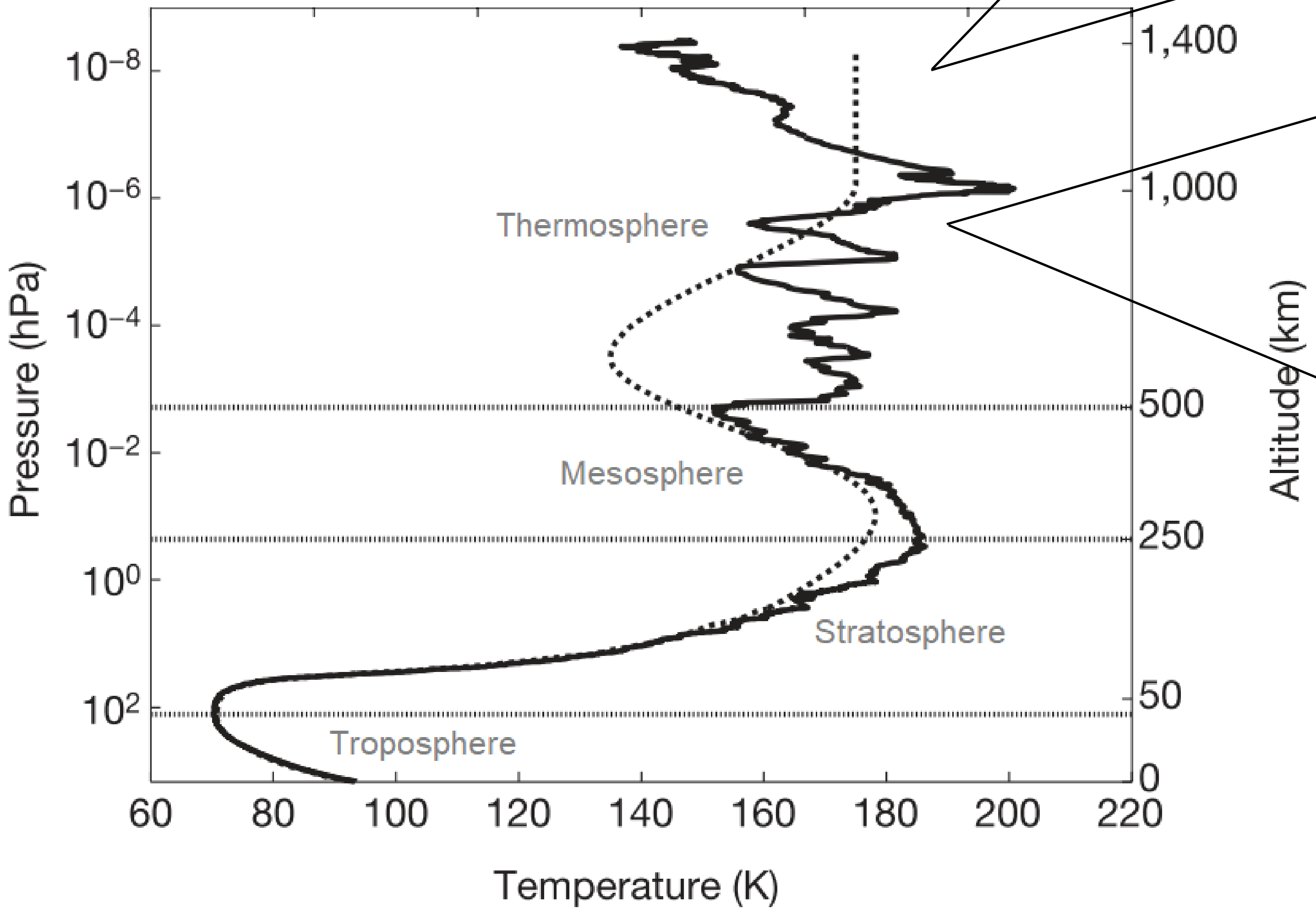
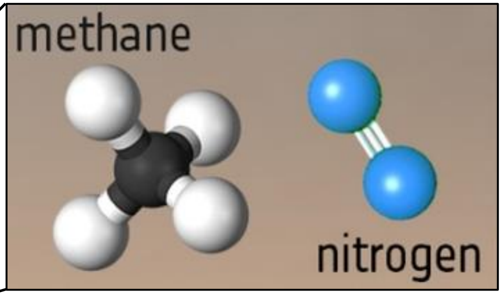
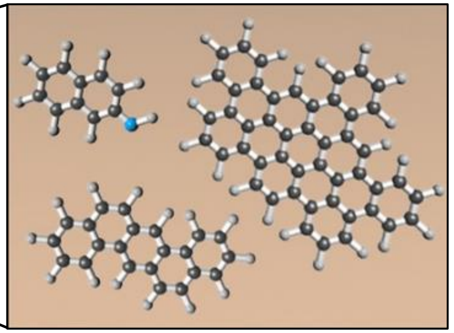




complex organic molecules



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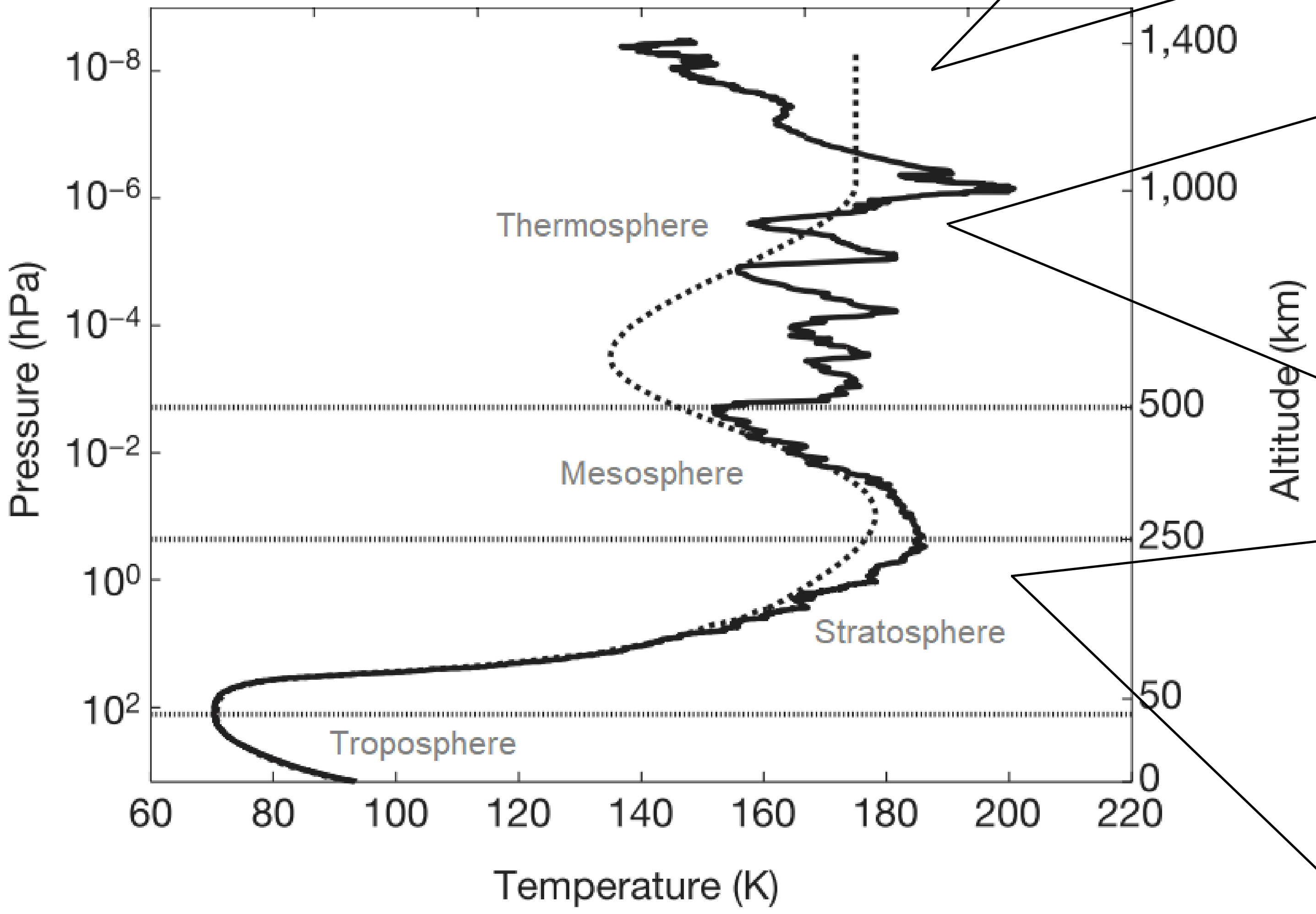

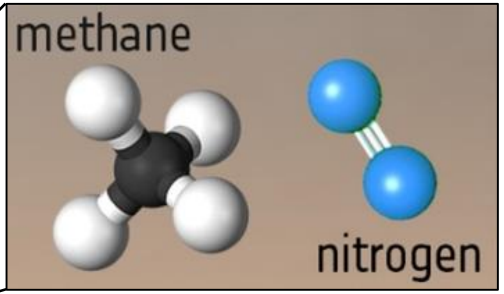

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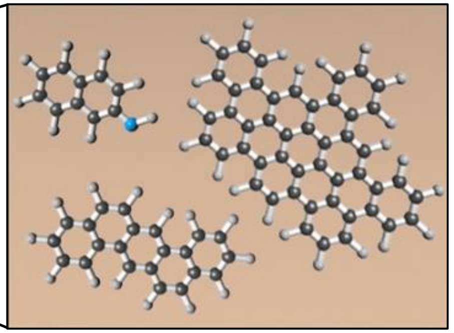
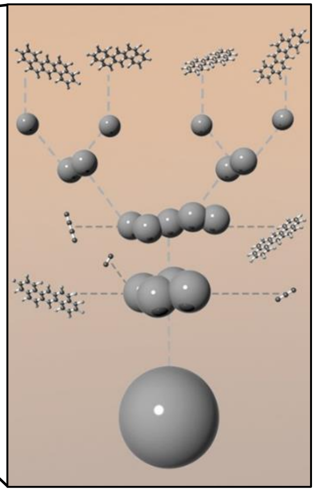


aerosols



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PHOTOCHEMICAL MODEL

- 1D and stationary
- Simulates the formation and destruction of molecules in Titan's upper atmosphere

AstroReactions and ReactionEquations
by Pinotti & Boechat-Roberty (2016)

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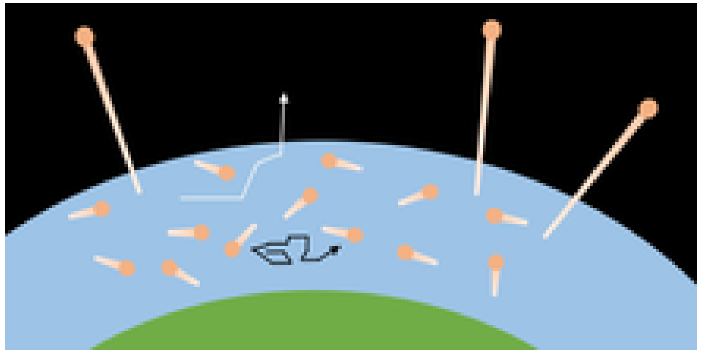
PHOTOCHEMICAL MODEL

- 1D and stationary
- Simulates the formation and destruction of molecules in Titan's upper atmosphere

AstroReactions and ReactionEquations
by Pinotti & Boechat-Roberty (2016)

- Upper atmosphere only ⟶ above the exobase (1450 km)



atmospheric escape

FORMATION AND DESTRUCTION OF ORGANIC MOLECULES IN THE ATMOSPHERE OF TITAN

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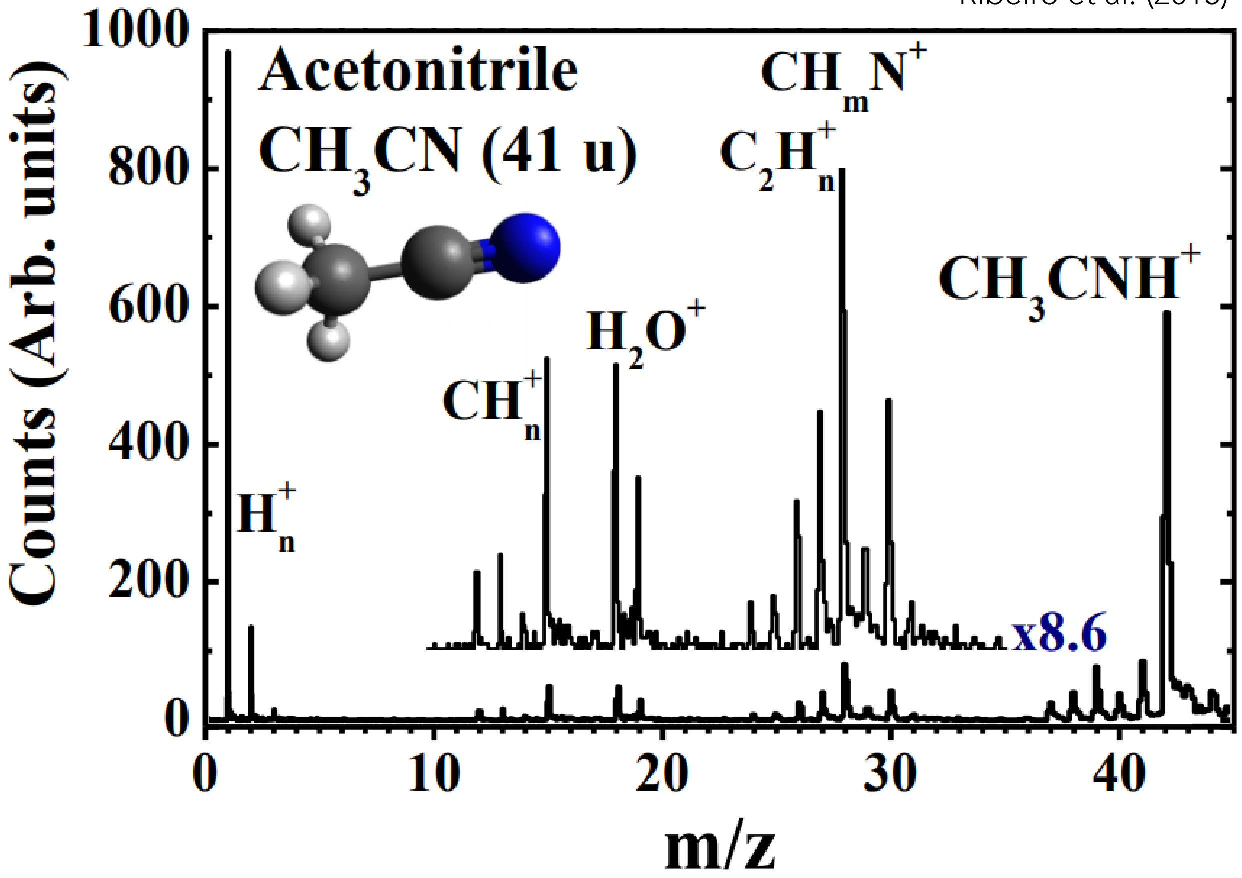
PHOTOCHEMICAL MODEL

selection of species

- literature
- group works (e.g. Ribeiro et al. 2015)

Ribeiro et al. (2015)



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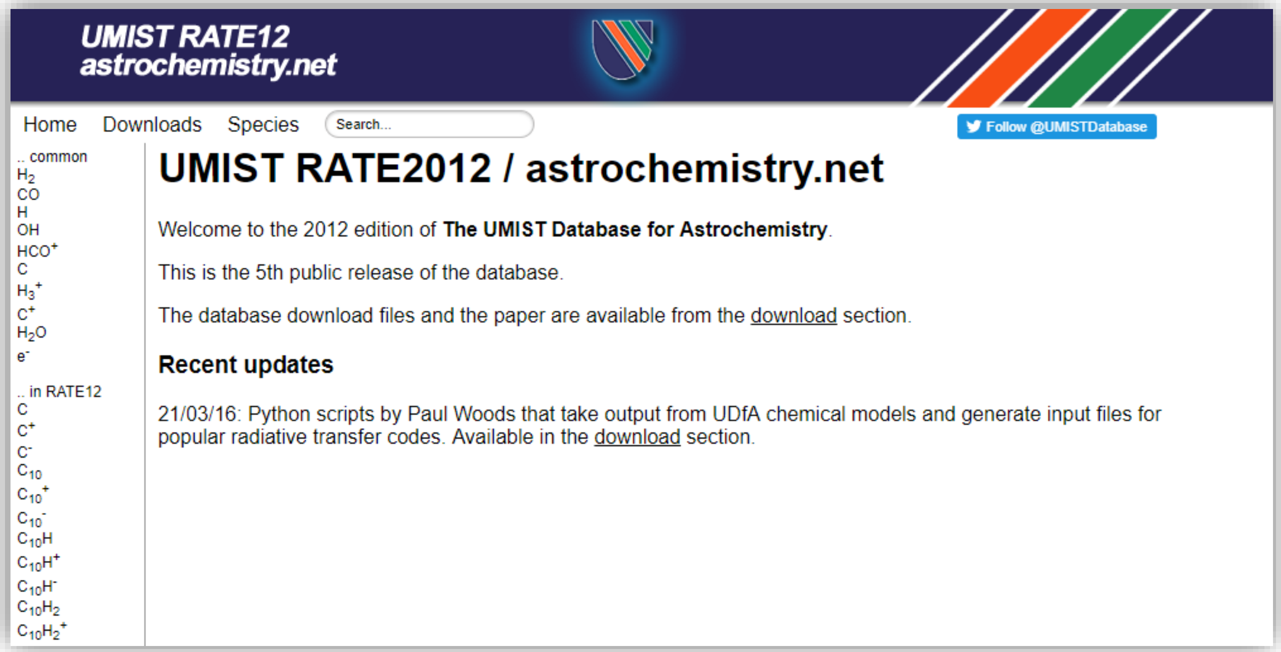
PHOTOCHEMICAL MODEL

selection of species

- literature
- group works (e.g. Ribeiro et al. 2015)
- UMIST database (McElroy et al. 2013)



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PHOTOCHEMICAL MODEL

selection of species

- literature
- group works (e.g. Ribeiro et al. 2015)
- UMIST database (McElroy et al. 2013)
- C,H,O,N molecules only

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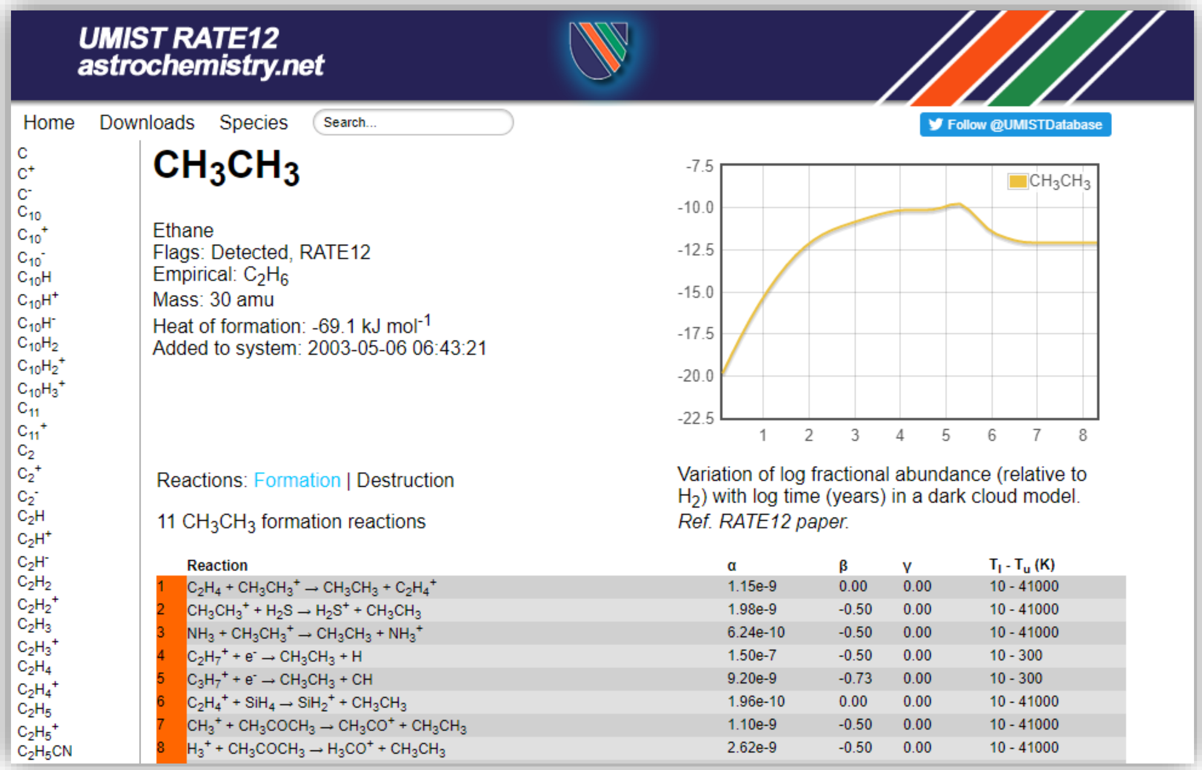
PHOTOCHEMICAL MODEL

selection of species → reactions list for each specie

- UMIST database (McElroy et al. 2013)



	Reaction	α	β	γ	T_l - T_u (K)
1	$C_2H_4 + CH_3CH_3^+ \rightarrow CH_3CH_3 + C_2H_4^+$	1.15e-9	0.00	0.00	10 - 41000
2	$CH_3CH_3^+ + H_2S \rightarrow H_2S^+ + CH_3CH_3$	1.98e-9	-0.50	0.00	10 - 41000
3	$NH_3 + CH_3CH_3^+ \rightarrow CH_3CH_3 + NH_3^+$	6.24e-10	-0.50	0.00	10 - 41000
4	$C_2H_7^+ + e^- \rightarrow CH_3CH_3 + H$	1.50e-7	-0.50	0.00	10 - 300
5	$C_3H_7^+ + e^- \rightarrow CH_3CH_3 + CH$	9.20e-9	-0.73	0.00	10 - 300
6	$C_2H_4^+ + SiH_4 \rightarrow SiH_2^+ + CH_3CH_3$	1.96e-10	0.00	0.00	10 - 41000
7	$CH_3^+ + CH_3COCH_3 \rightarrow CH_3CO^+ + CH_3CH_3$	1.10e-9	-0.50	0.00	10 - 41000
8	$H_3^+ + CH_3COCH_3 \rightarrow H_3CO^+ + CH_3CH_3$	2.62e-9	-0.50	0.00	10 - 41000

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PHOTOCHEMICAL MODEL

selection of species → reactions list for each specie → solving continuity equations

- Continuity equation for a chemical specie i:

$$0 = -\underbrace{\frac{d\Phi_i}{dz}}_{\frac{d(x_i n_{N_2} v_i)}{dz}} + \overbrace{P_i}^{\text{reactions production rate}} - \underbrace{L_i}_{\text{reactions loss rate}}$$

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PHOTOCHEMICAL MODEL

selection of species → reactions list for each specie → solving continuity equations

- Continuity equation for a chemical specie i:

P (solar flux)
p (magnetospheric flux)

$$0 = -\underbrace{\frac{d\Phi_i}{dz}}_{\frac{d(x_i n_{N_2} v_i)}{dz}} + P_i - L_i$$

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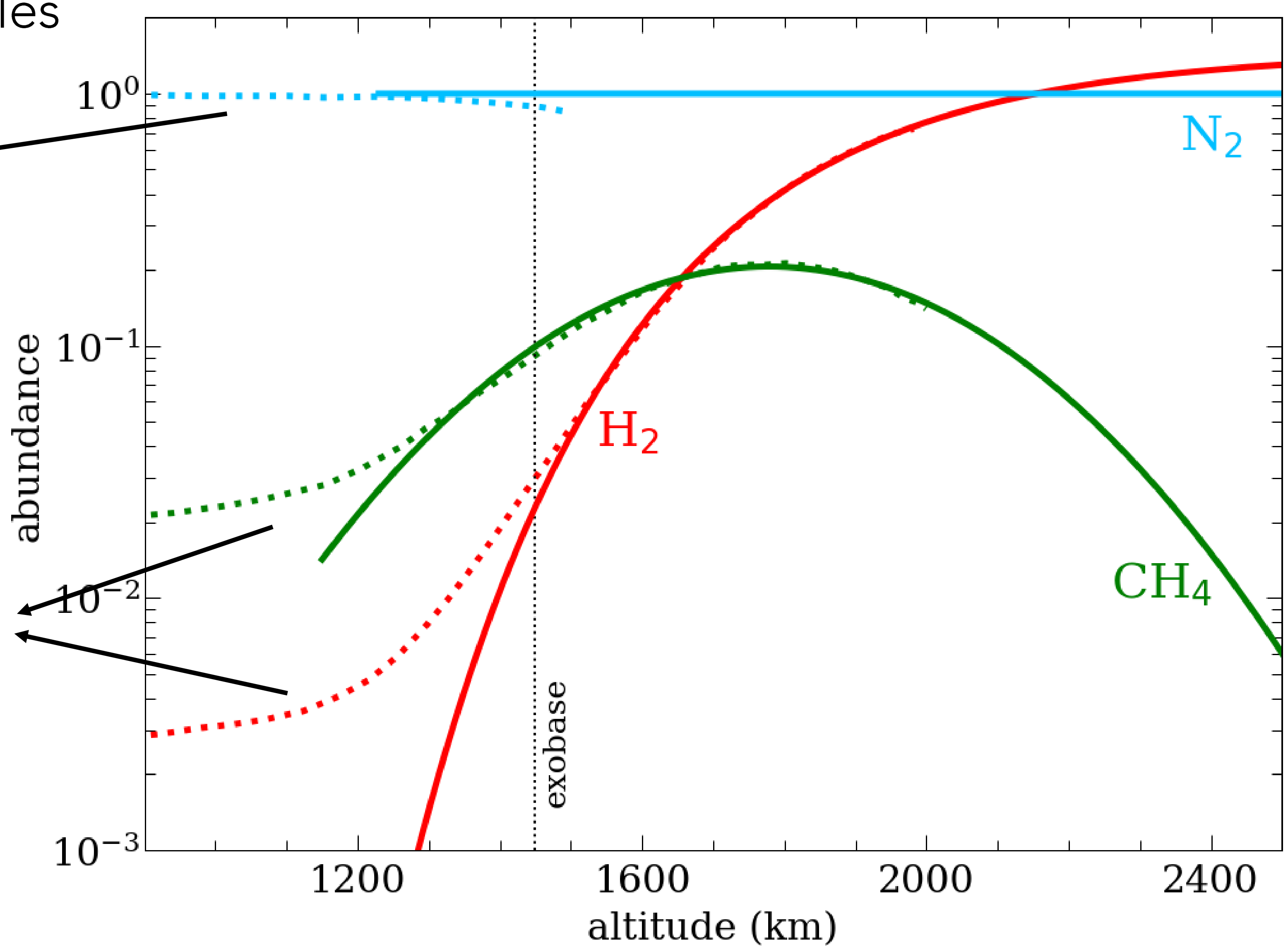
PHOTOCHEMICAL MODEL

Inicial profiles

$N_2 = 1$

De La Haye et al. (2008)



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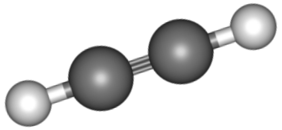
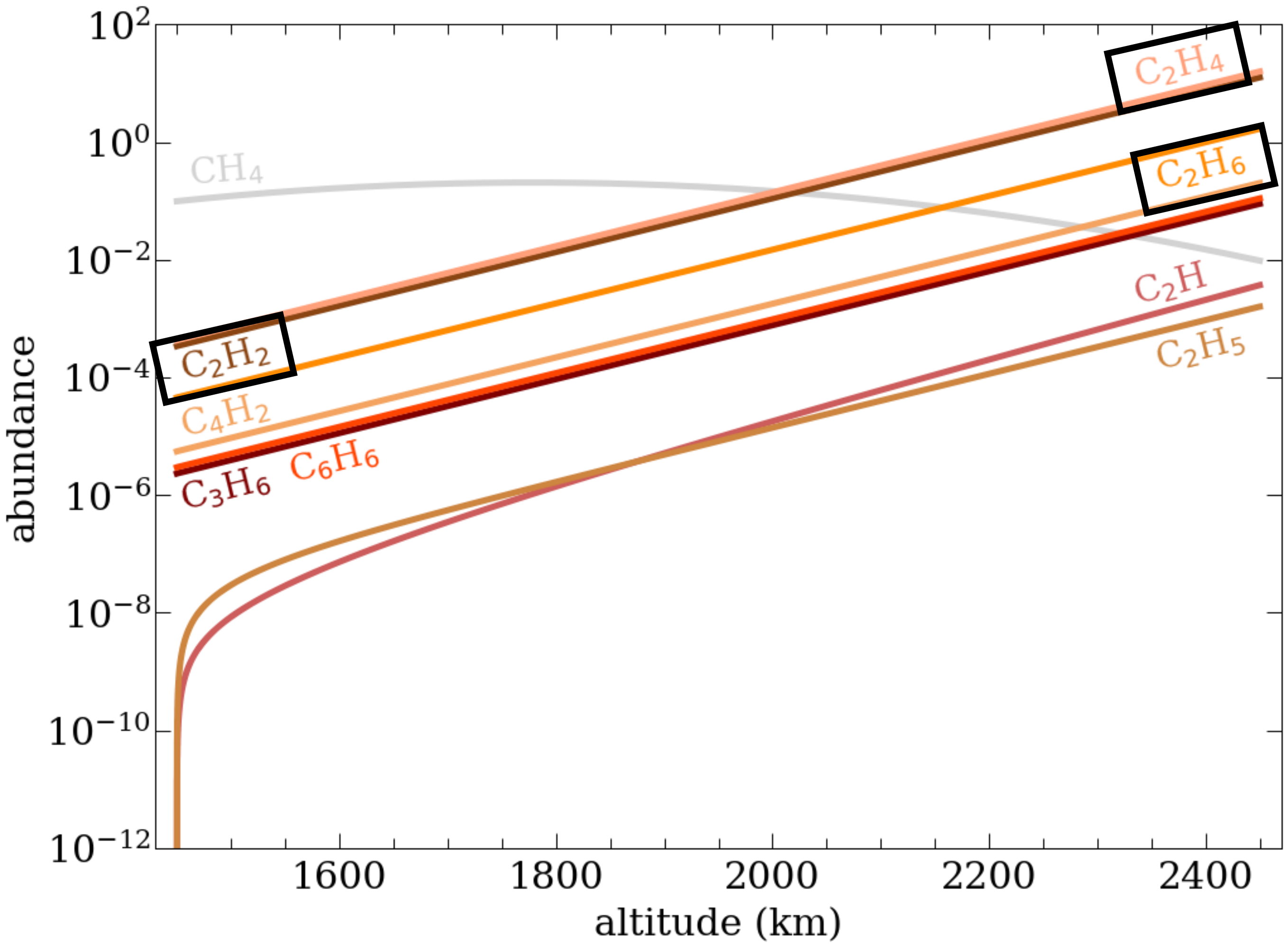
SIMULATING MOLECULE ABUNDANCES

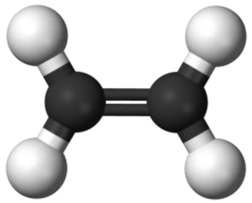
Hydrocarbons

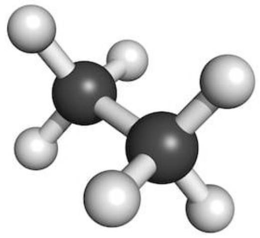
acetylene





etylene





ethane

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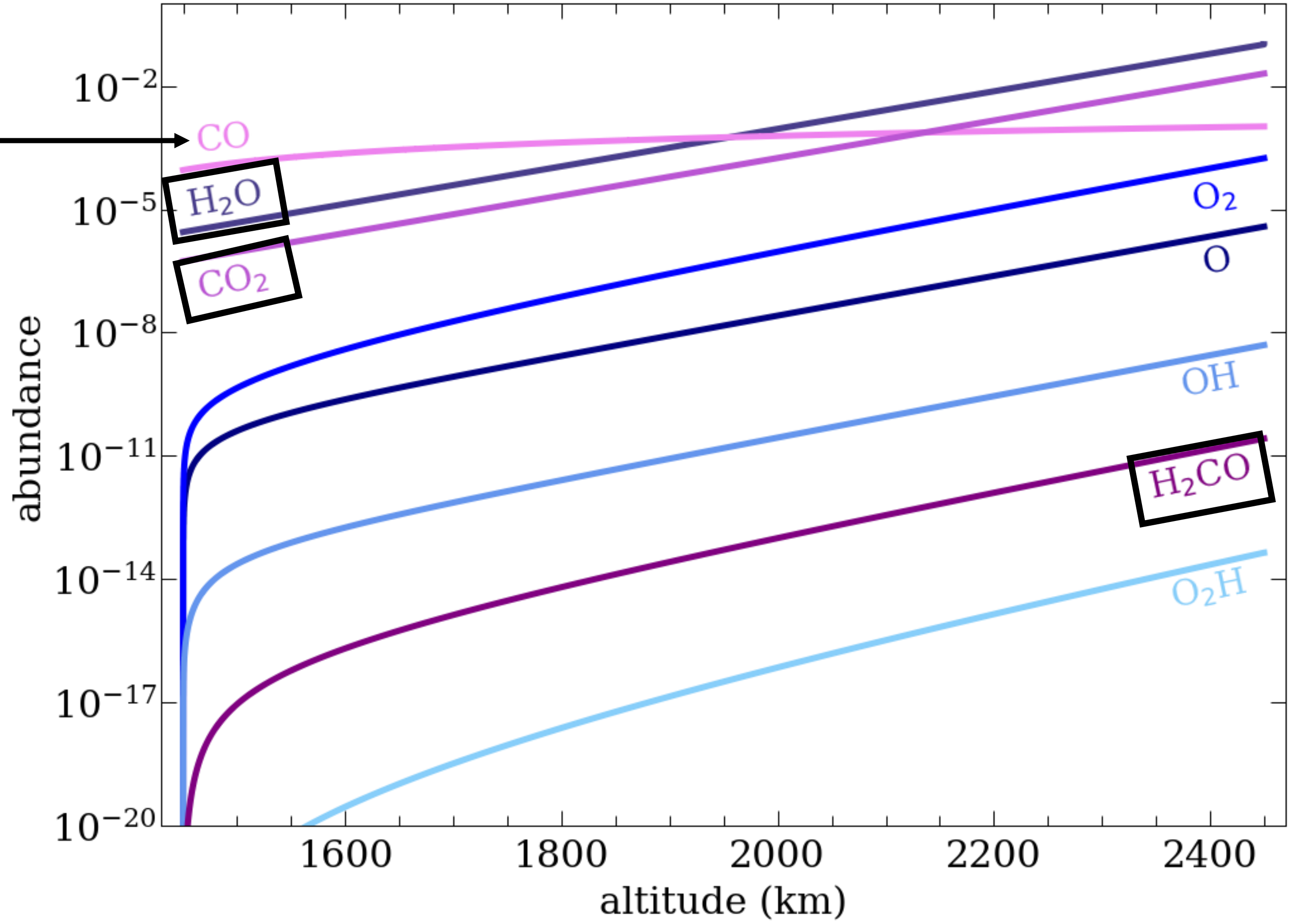
SIMULATING MOLECULE ABUNDANCES

Oxygen-bearing molecules

stable



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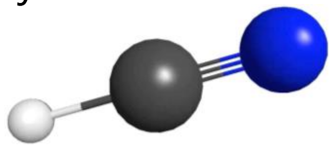
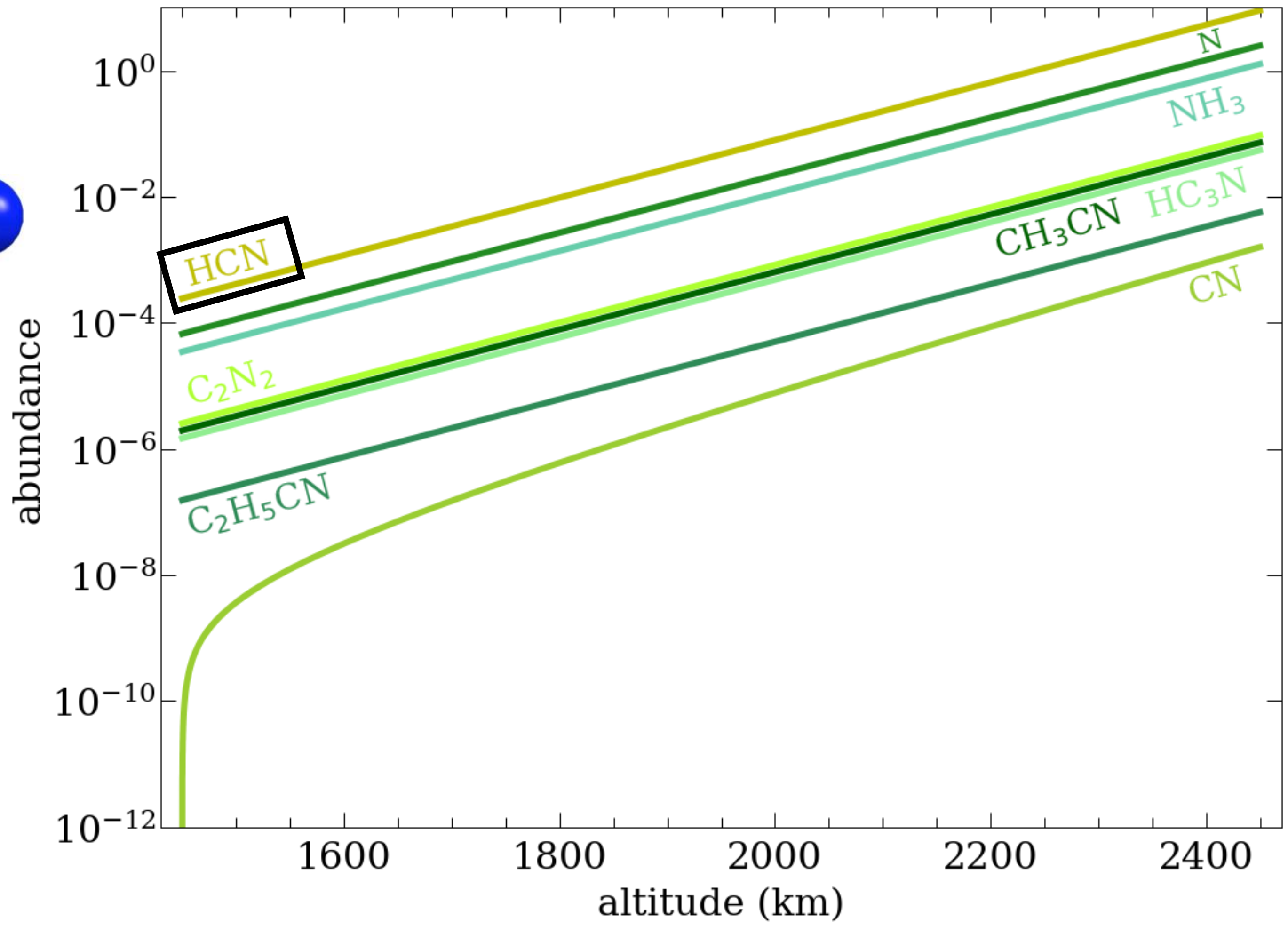
Nitrogen-bearing molecules

hydrogen cyanide





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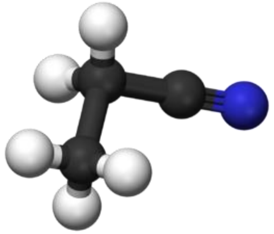
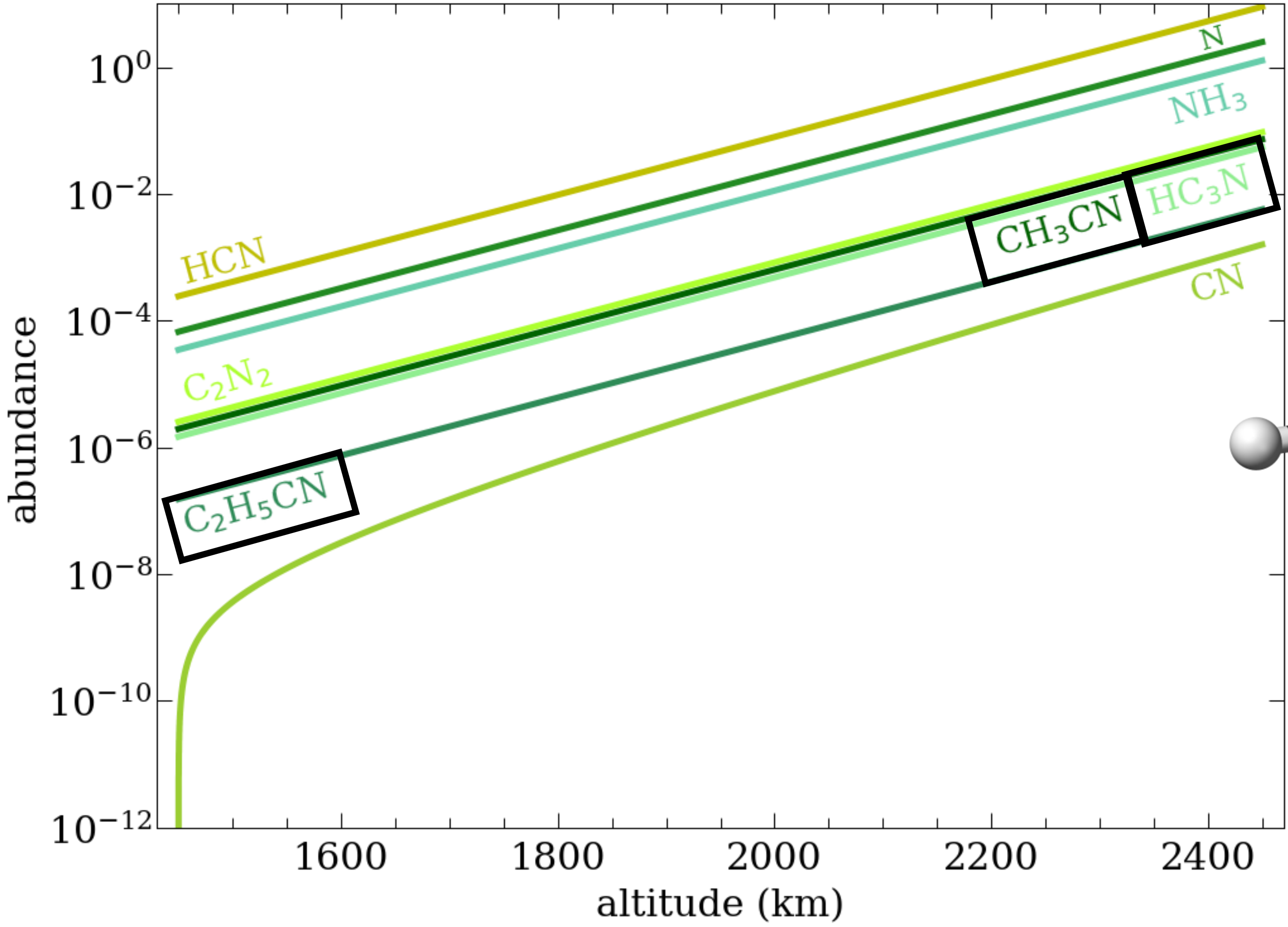
SIMULATING MOLECULE ABUNDANCES

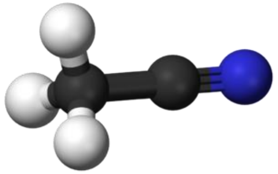
Nitrogen-bearing molecules

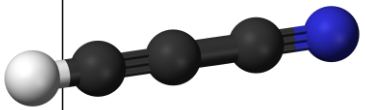
propionitrile





acetonitrile





cyano-acetylene

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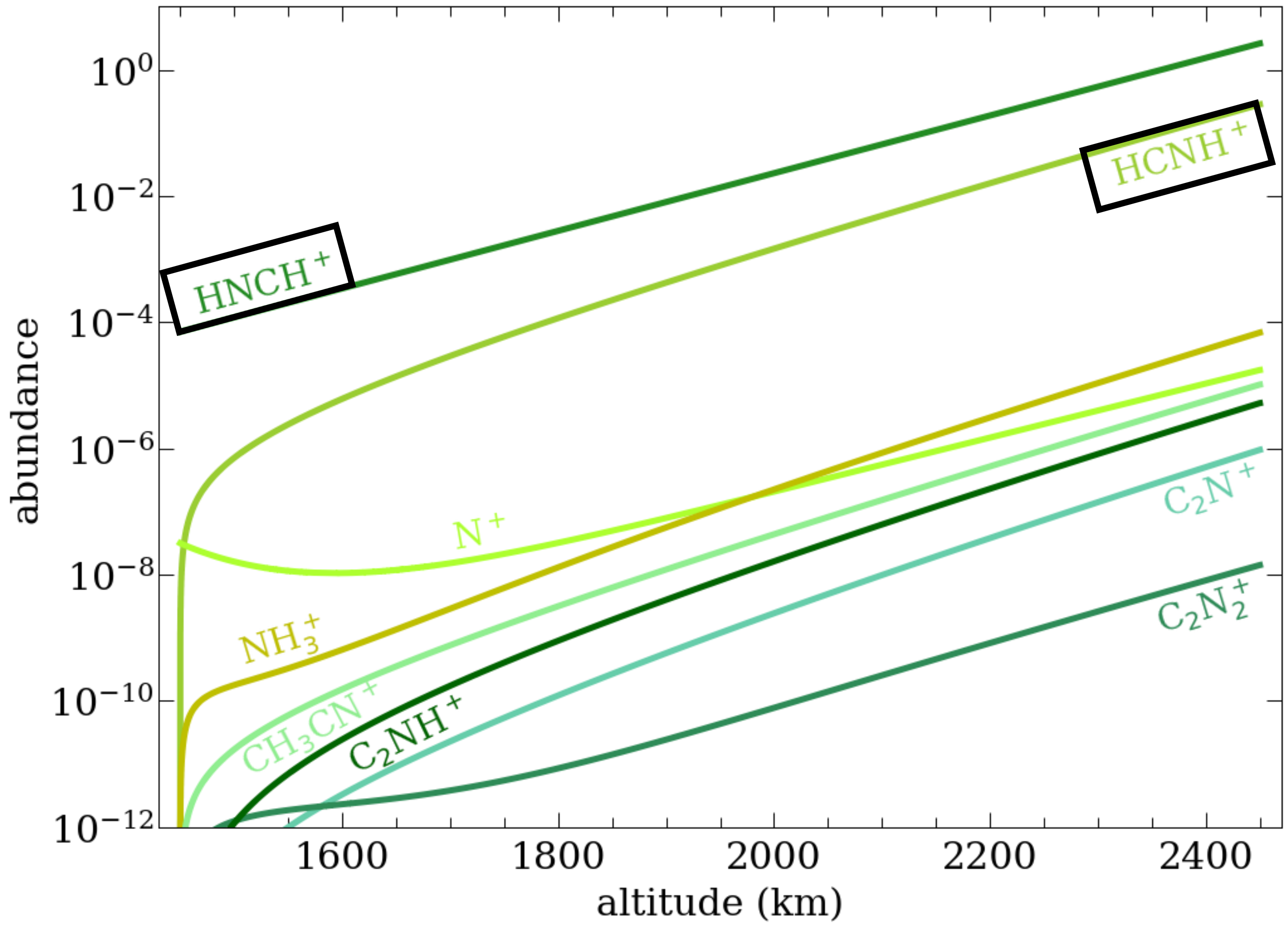
SIMULATING MOLECULE ABUNDANCES

Nitrogen-bearing molecules



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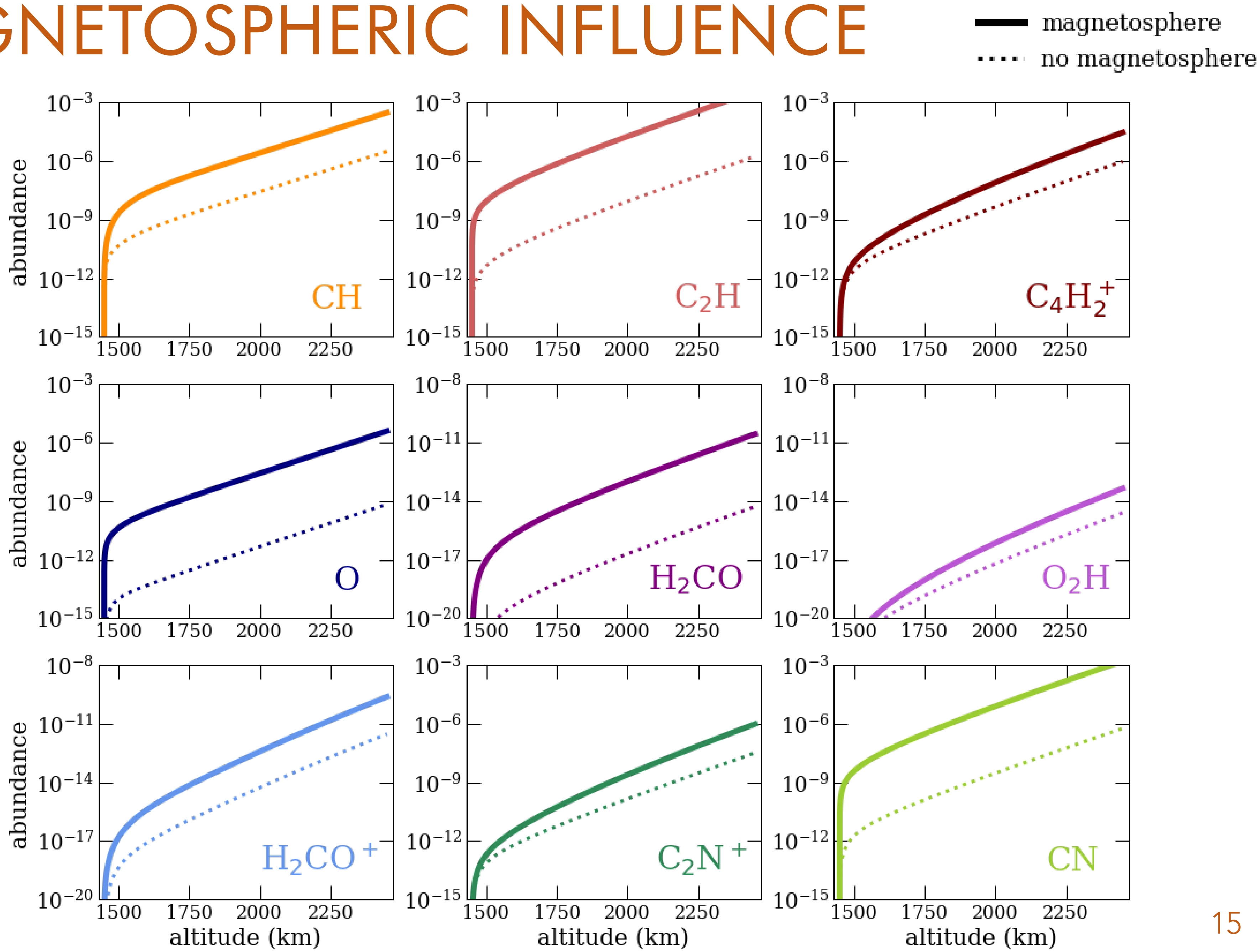
MAGNETOSPHERIC INFLUENCE



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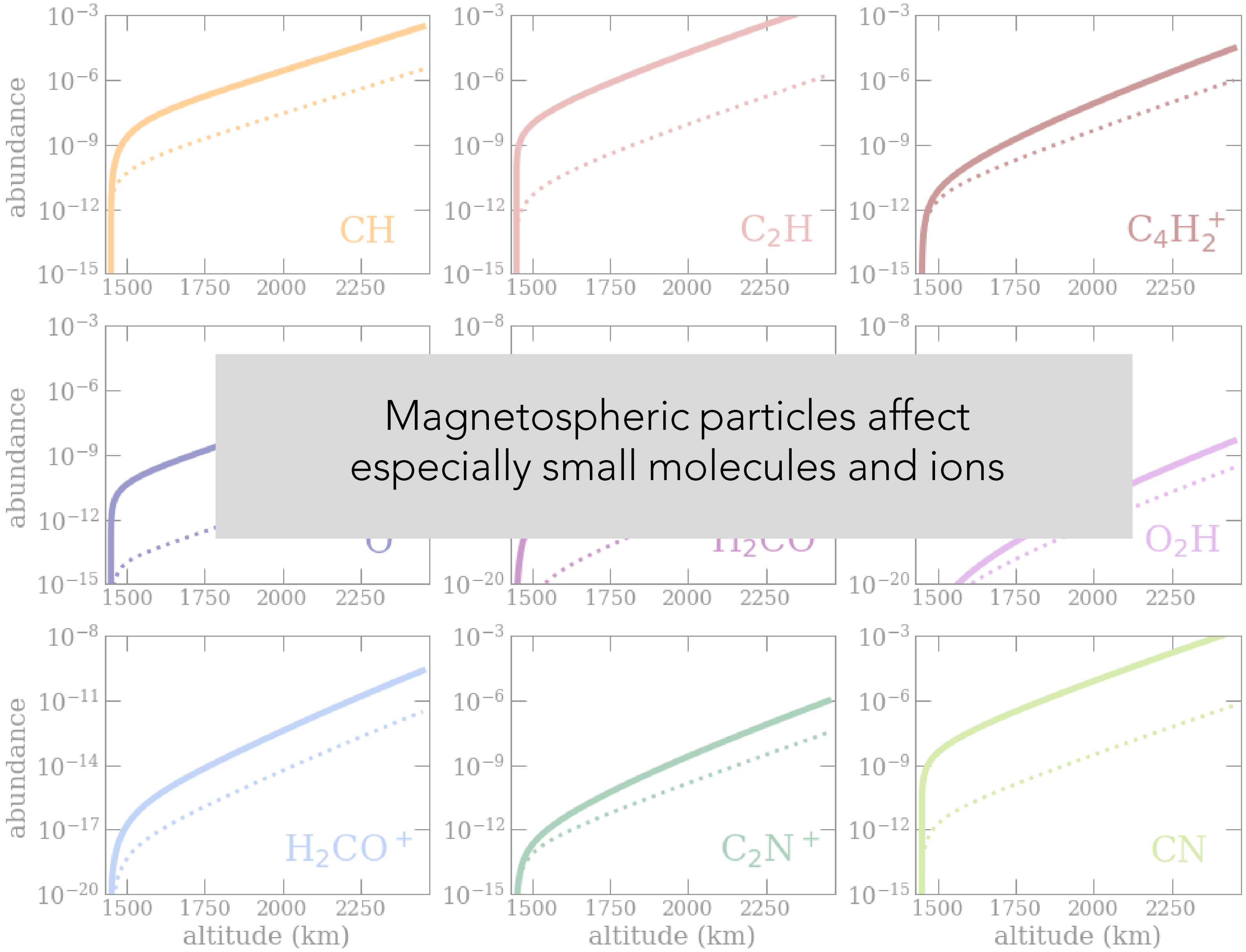
MAGNETOSPHERIC INFLUENCE

magnetosphere
no magnetosphere



Magnetospheric particles affect especially small molecules and ions

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CONCLUSIONS

- Molecule abundances in agreement with literature considering **atmospheric escape** processes

- 3 most abundant hydrocarbons: C_2H_2, C_2H_4, C_2H_6
  - not influenced by O-bearing and N-bearing species

- Evidence of **nitriles**
  - precursors of prebiotic molecules

- Evidence of **magnetospheric influence** in the formation of compounds

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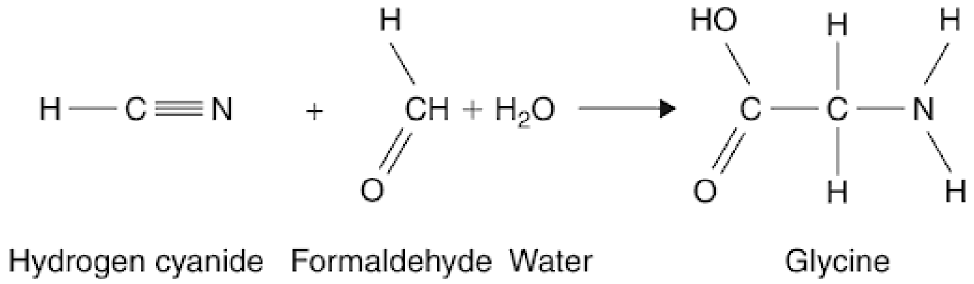
DISCUSSIONS

- Formation of **glycine**: $C_2H_5NO_2$
  - from CH_2OH or CH_3COOH (e.g. Pilling et al. 2011)
  - from HCN + HCOH + H_2O (e.g. Wayne, 2018)



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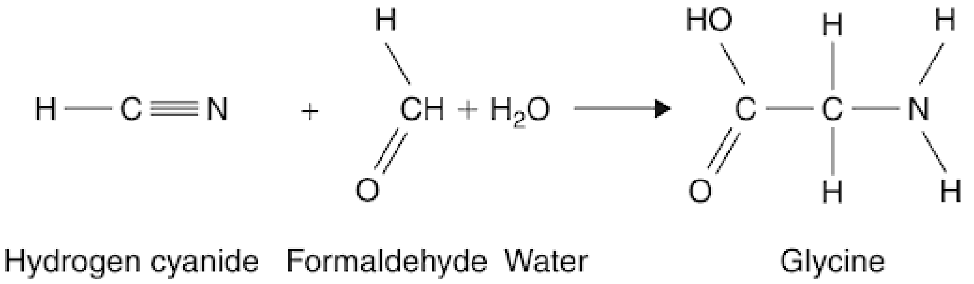
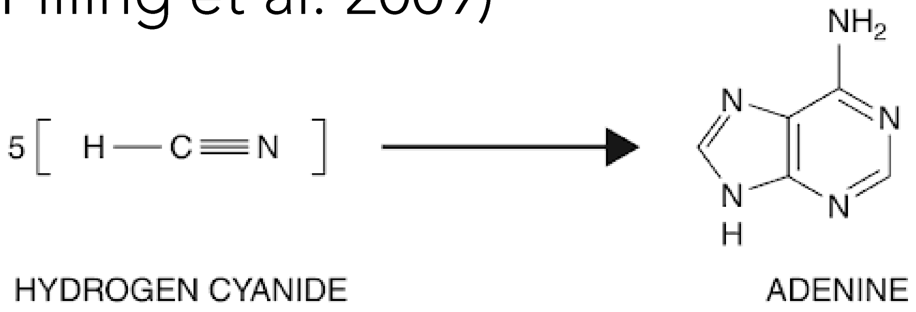


- Formation of **adenine**: $C_5H_5N_5$
  - experimental (e.g. Pilling et al. 2009)
  - from HCN



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PERSPECTIVES

- Upgrade the model
  - Titan's induced magnetic field?
  - complete atmosphere description

- Inclusion of new compounds
  - e.g. PAHs from C_6H_6
  - S and P molecules

- New database (e.g. KIDA)

- Laboratory experiments
  - verify the stability of COMs, especially the ones with astrobiological interest

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APPENDICE:

Constantes de reação:

- entre dois corpos: $k = \alpha \left(\frac{T}{300}\right)^{\beta} exp\left(-\frac{\gamma}{T}\right)$
- com prótons de raios cósmicos: $k_{CRP} = \alpha$
- com fótons de raios cósmicos: $k_{CRPHOT} = \alpha \left(\frac{T}{300}\right)^{\beta} \frac{\gamma}{1-\omega}$
- com fótons do meio interestelar: $k_{PHOTON} = \alpha\, exp(-\gamma A_V)$

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Fator de correção para o fluxo de radiação solar:

- entre dois corpos: $k = \alpha \left(\frac{T}{300}\right)^{\beta} exp\left(-\frac{\gamma}{T}\right)$
- com prótons de raios cósmicos: $k_{CRP} = \alpha$
- com fótons de raios cósmicos: $k_{CRPHOT} = \alpha \left(\frac{T}{300}\right)^{\beta} \frac{\gamma}{1-\omega}$
- com fótons do meio interestelar: $k_{PHOTON} = \alpha\, exp(-\gamma A_V)\, \boldsymbol{P}$

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APPENDICE:

Fator de correção para o fluxo de plasma da magnetosfera de Saturno:

- entre dois corpos: $k = \alpha \left(\frac{T}{300}\right)^{\beta} exp\left(-\frac{\gamma}{T}\right)$
- com prótons de raios cósmicos: $k_{CRP} = \alpha\, \boldsymbol{p}$
- com fótons de raios cósmicos: $k_{CRPHOT} = \alpha \left(\frac{T}{300}\right)^{\beta} \frac{\gamma}{1-\omega}\, \boldsymbol{p}$
- com fótons do meio interestelar: $k_{PHOTON} = \alpha\, exp(-\gamma A_V)\, P$