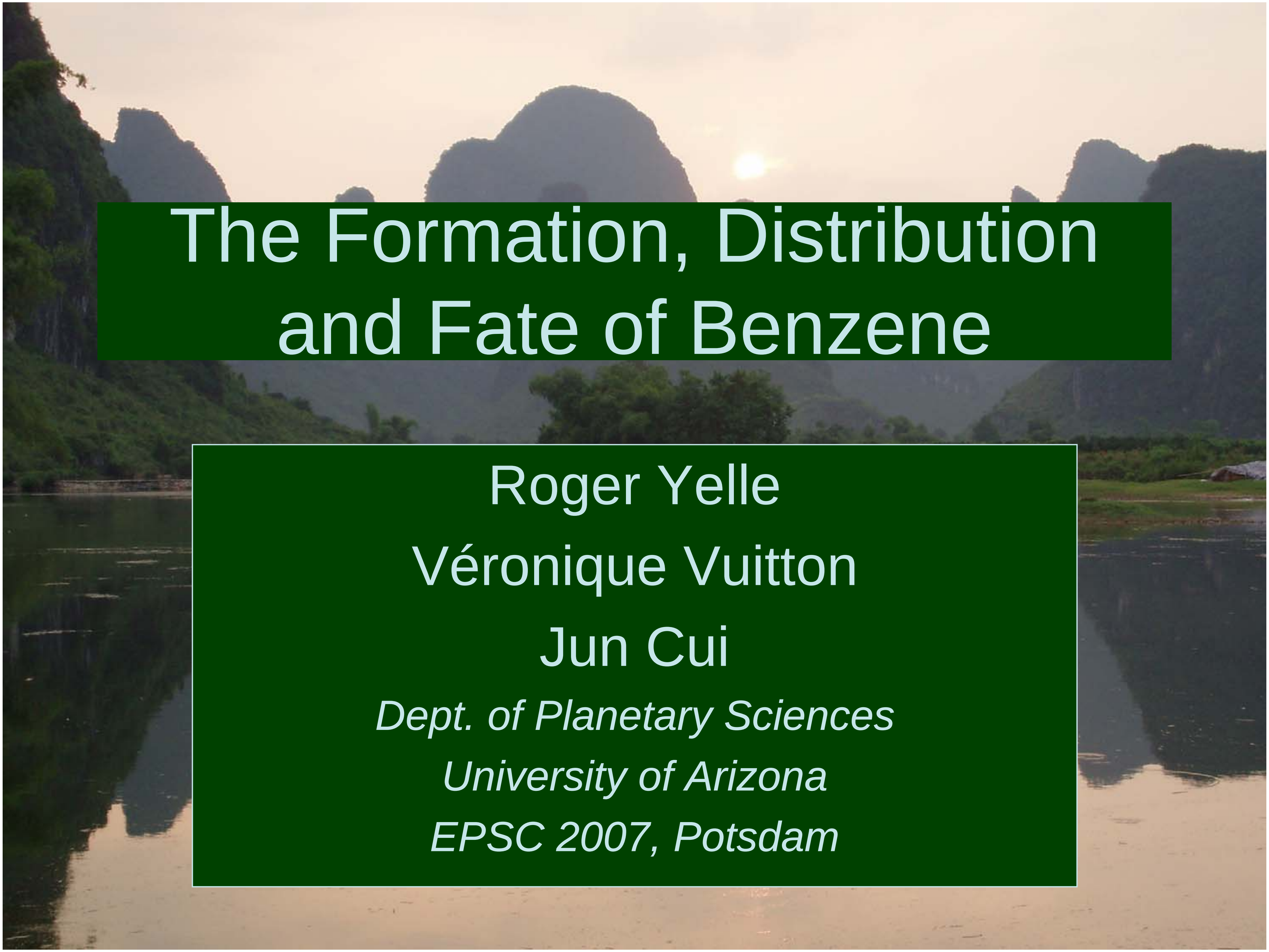

The Formation, Distribution and Fate of Benzene

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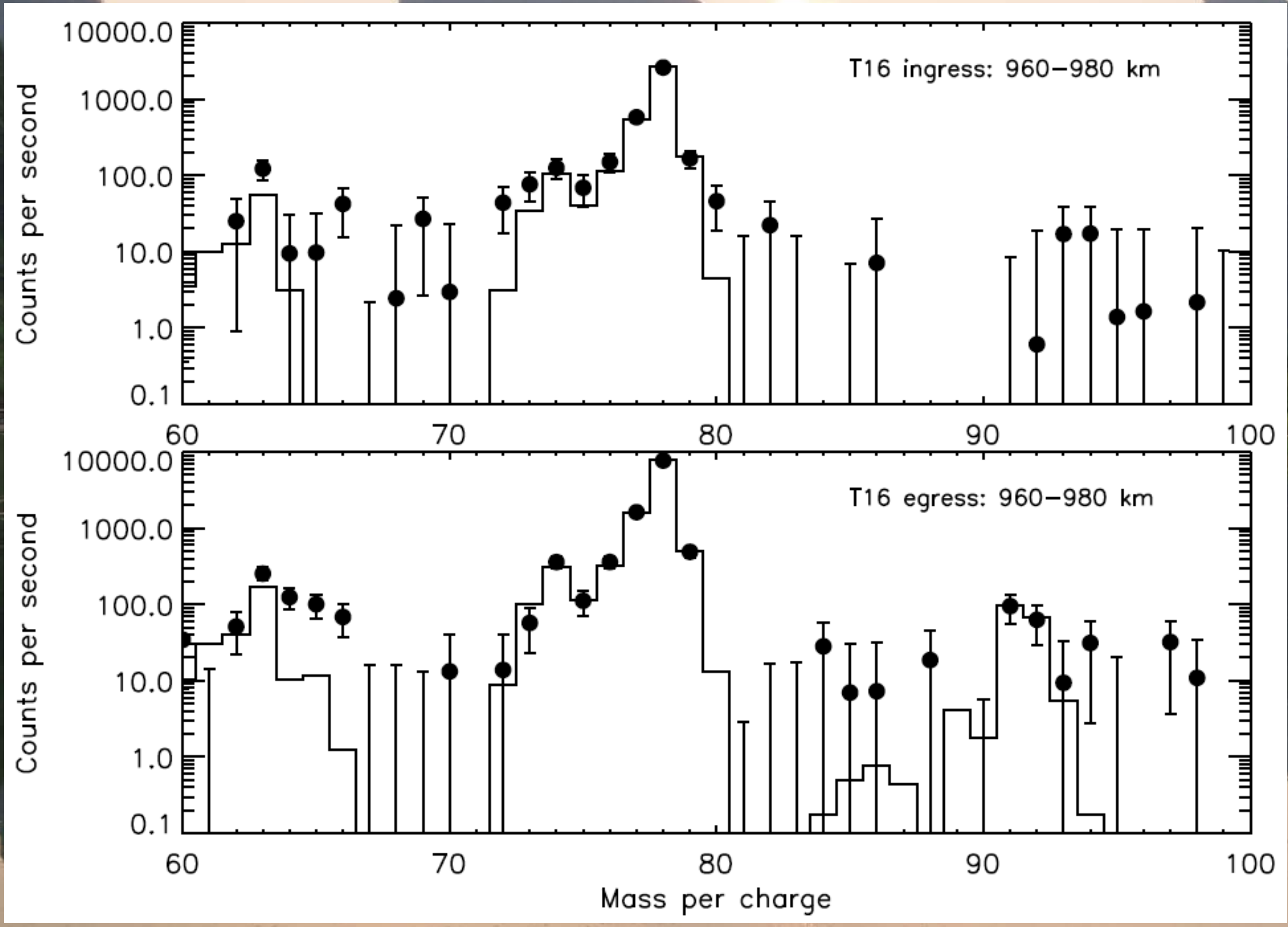
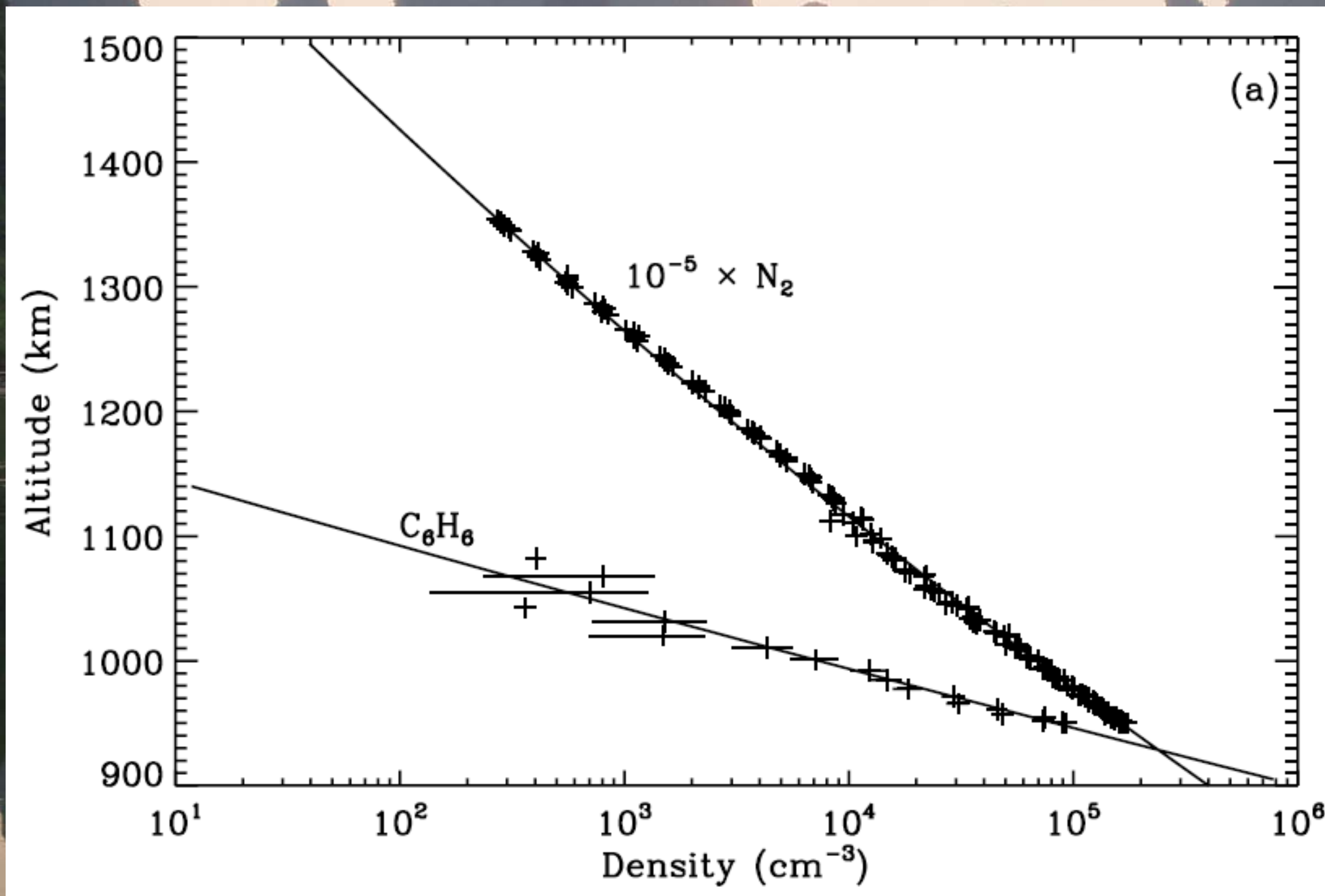
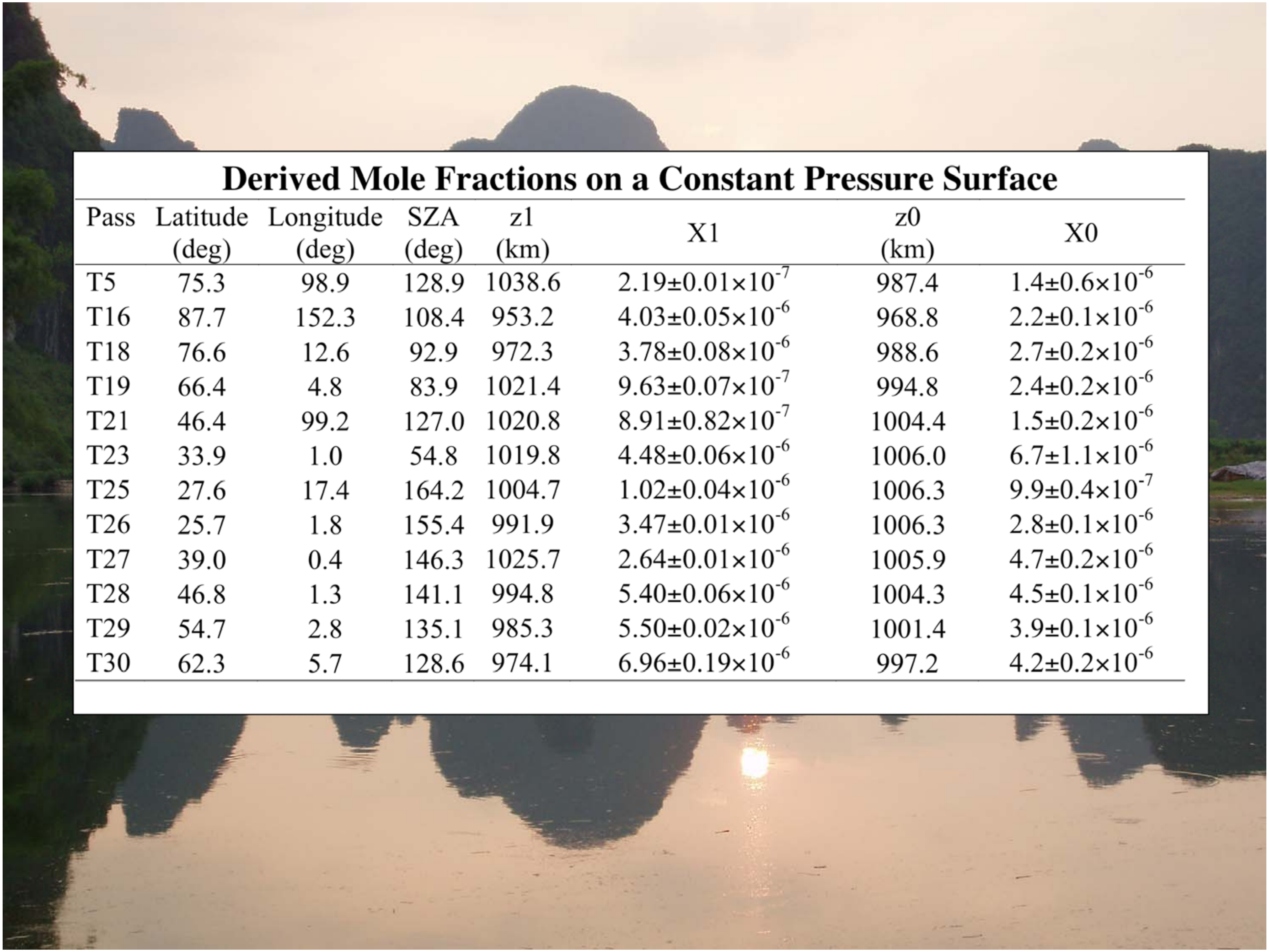
EPSC 2007, Potsdam

INMS Spectra of Benzene and Toluene



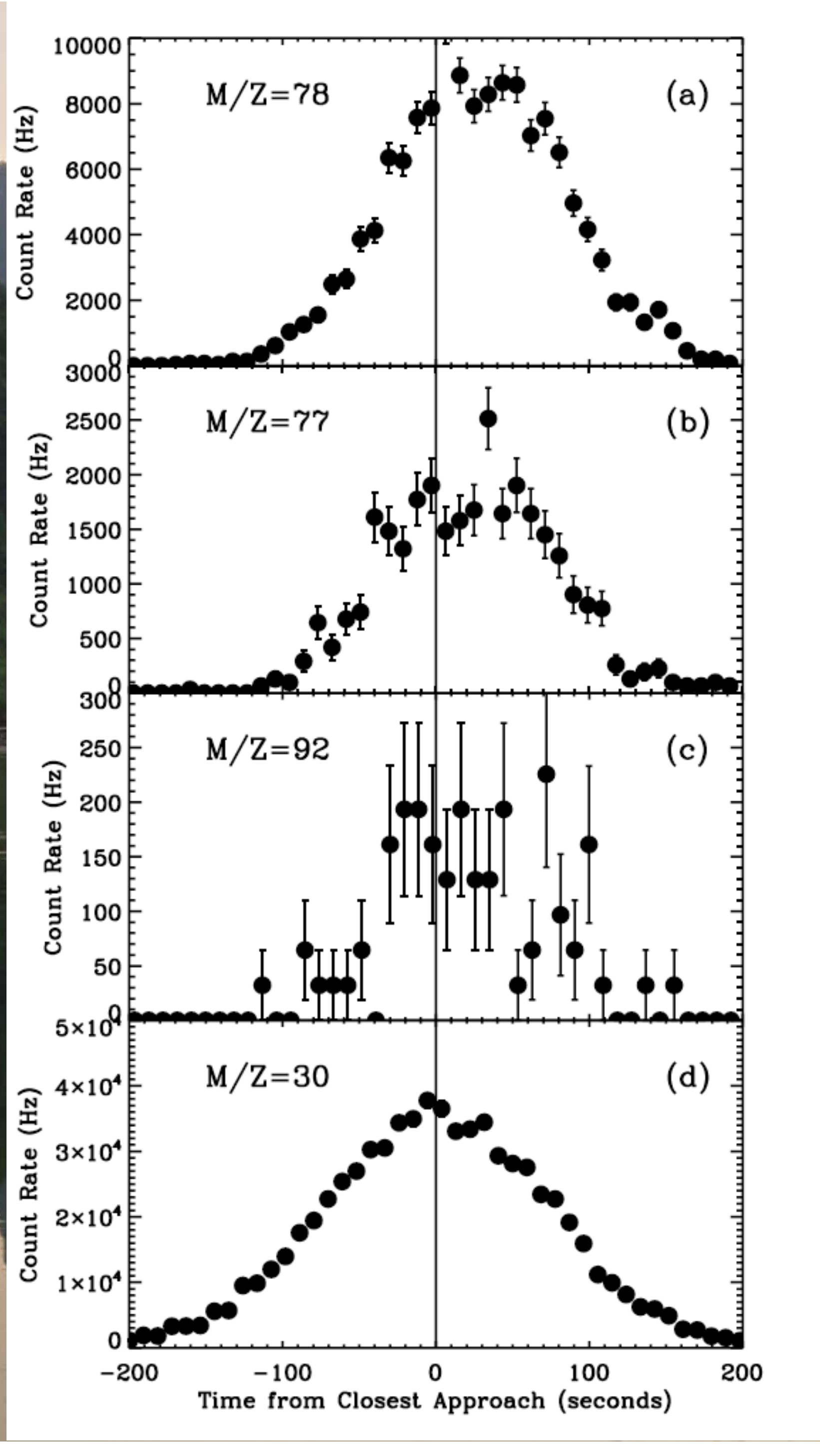
Benzene is Distributed in Diffusive Equilibrium



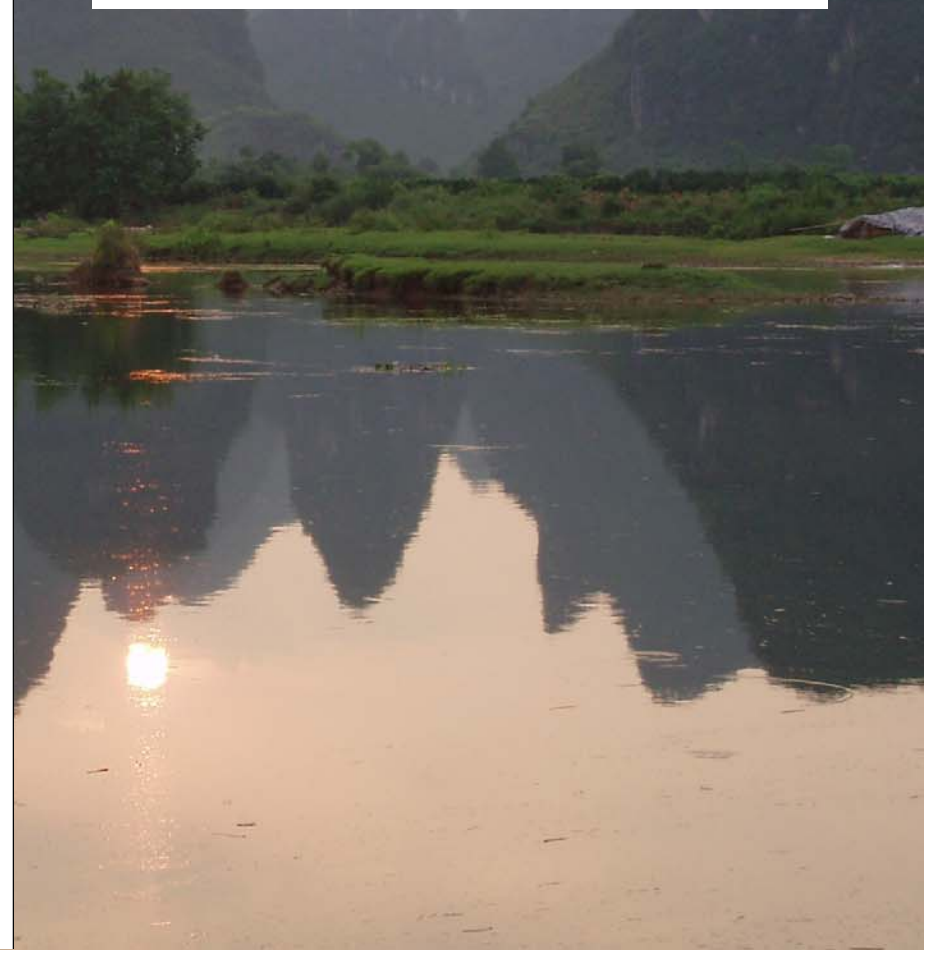


Derived Mole Fractions on a Constant Pressure Surface

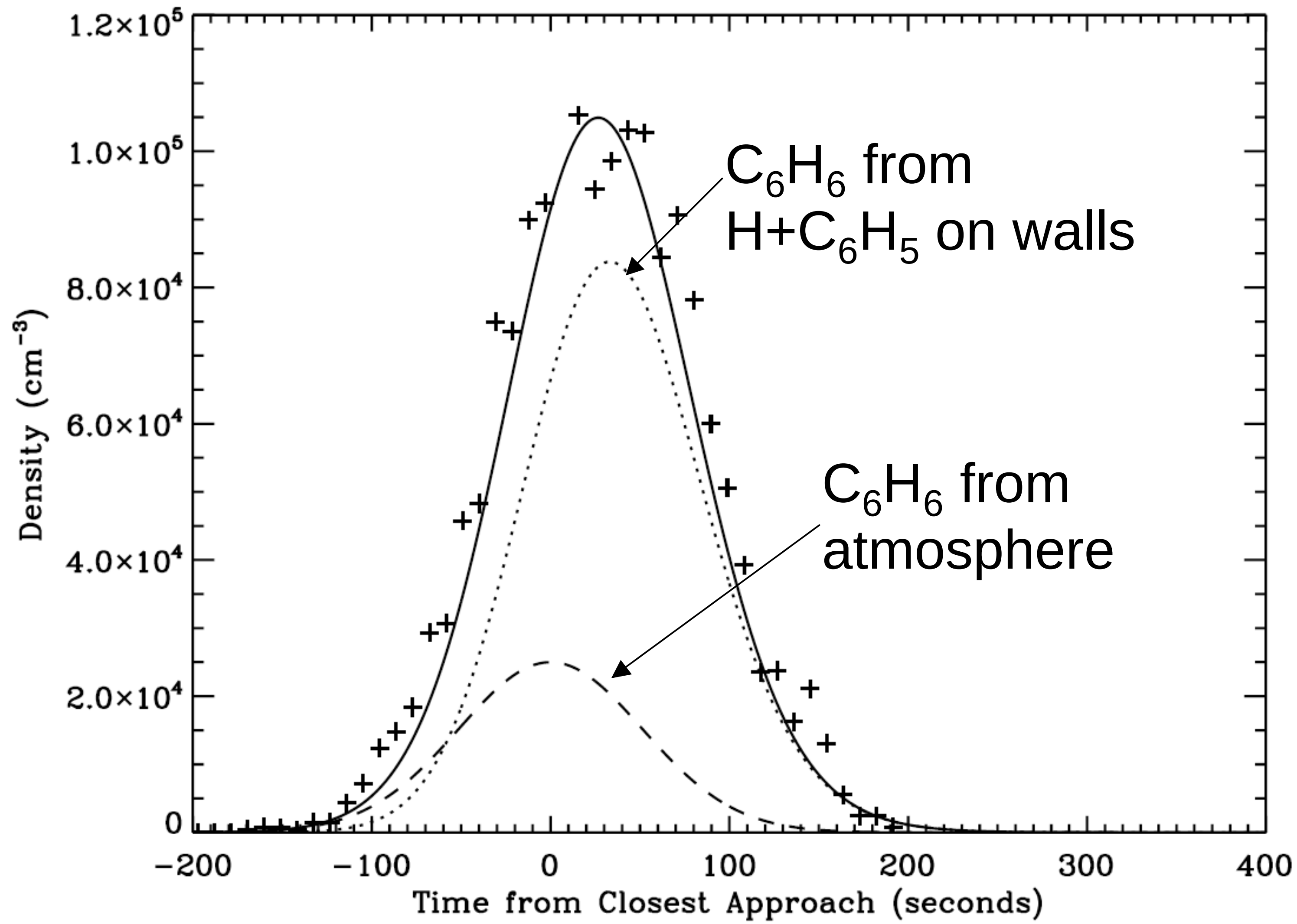
Pass	Latitude (deg)	Longitude (deg)	SZA (deg)	z1 (km)	X1	z0 (km)	X0
T5	75.3	98.9	128.9	1038.6	$2.19\pm0.01\times10^{-7}$	987.4	$1.4\pm0.6\times10^{-6}$
T16	87.7	152.3	108.4	953.2	$4.03\pm0.05\times10^{-6}$	968.8	$2.2\pm0.1\times10^{-6}$
T18	76.6	12.6	92.9	972.3	$3.78\pm0.08\times10^{-6}$	988.6	$2.7\pm0.2\times10^{-6}$
T19	66.4	4.8	83.9	1021.4	$9.63\pm0.07\times10^{-7}$	994.8	$2.4\pm0.2\times10^{-6}$
T21	46.4	99.2	127.0	1020.8	$8.91\pm0.82\times10^{-7}$	1004.4	$1.5\pm0.2\times10^{-6}$
T23	33.9	1.0	54.8	1019.8	$4.48\pm0.06\times10^{-6}$	1006.0	$6.7\pm1.1\times10^{-6}$
T25	27.6	17.4	164.2	1004.7	$1.02\pm0.04\times10^{-6}$	1006.3	$9.9\pm0.4\times10^{-7}$
T26	25.7	1.8	155.4	991.9	$3.47\pm0.01\times10^{-6}$	1006.3	$2.8\pm0.1\times10^{-6}$
T27	39.0	0.4	146.3	1025.7	$2.64\pm0.01\times10^{-6}$	1005.9	$4.7\pm0.2\times10^{-6}$
T28	46.8	1.3	141.1	994.8	$5.40\pm0.06\times10^{-6}$	1004.3	$4.5\pm0.1\times10^{-6}$
T29	54.7	2.8	135.1	985.3	$5.50\pm0.02\times10^{-6}$	1001.4	$3.9\pm0.1\times10^{-6}$
T30	62.3	5.7	128.6	974.1	$6.96\pm0.19\times10^{-6}$	997.2	$4.2\pm0.2\times10^{-6}$



The benzene signal is shifted by ~20 sec. relative to closest approach. Why would this be?

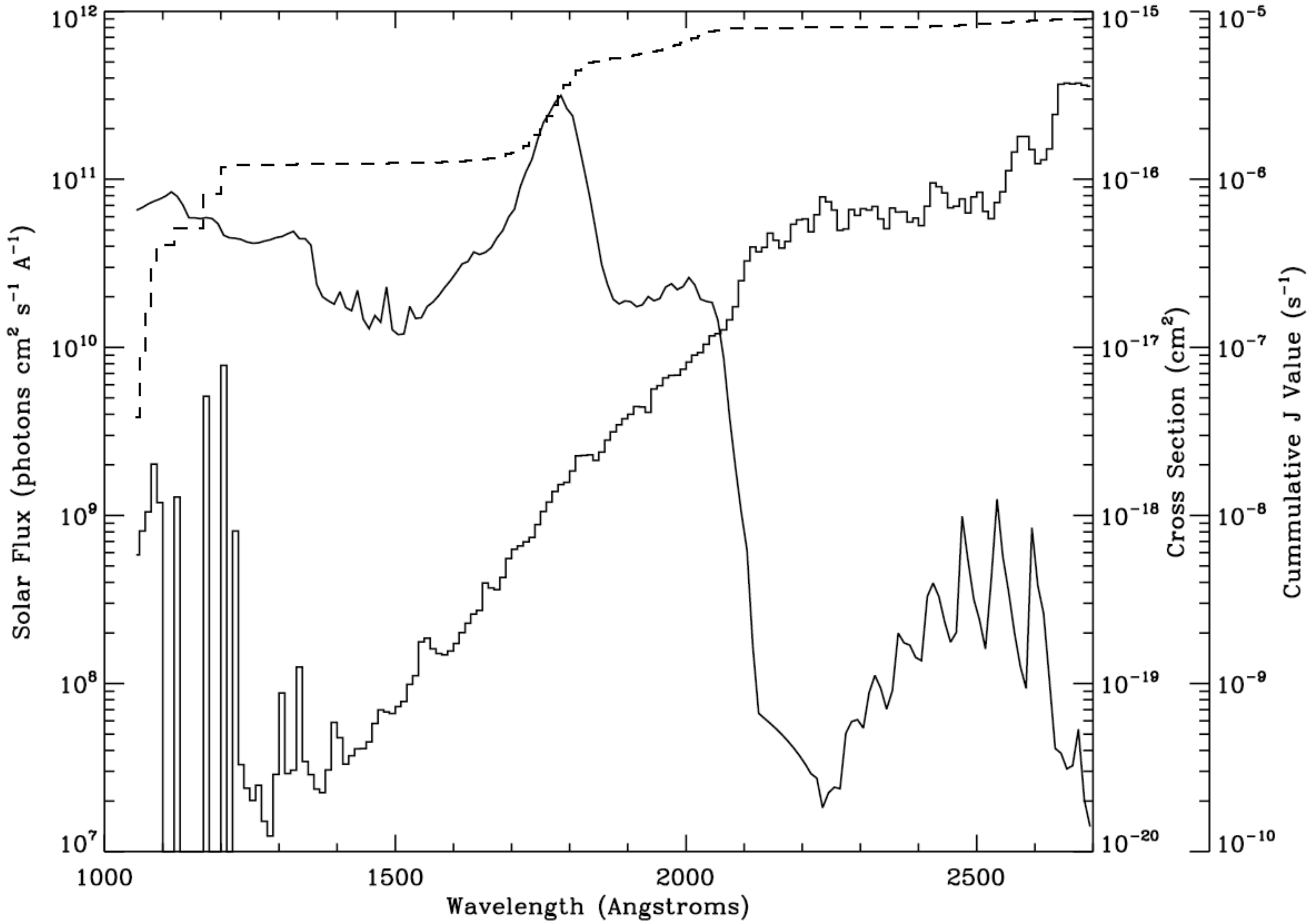


Benzene is formed by recombination of H and C_6H_5 on the walls of the instrument



Benzene has an extremely large photolysis rate.

$$h\nu + C_6H_6 \rightarrow C_6H_5 + H$$



To create benzne at high altitudes requires that molecules react before they diffuse away.

Diffusion time, $t_D \sim H^2/D \sim 1400$ sec.

Benzene must be built up from reactions among simpler species. Assume 5 sequential reaction with CH4, require reaction rate is

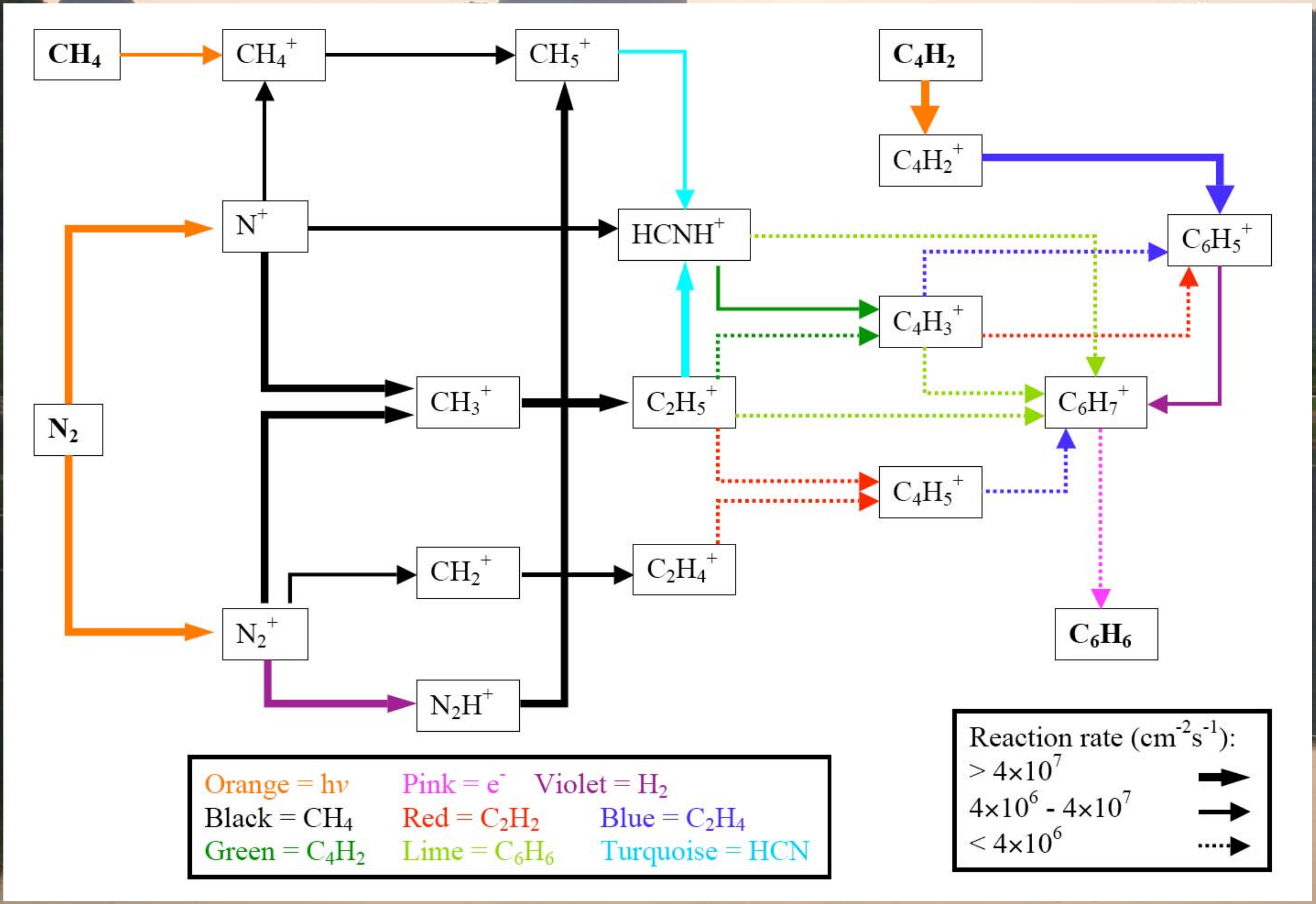
$$k \sim 5/N(CH_4)t_D \sim 5\times10^{-10}\ cm^3s^{-1}$$

Assume 3 sequential reactions with C_2H_x species, required reaction rate is

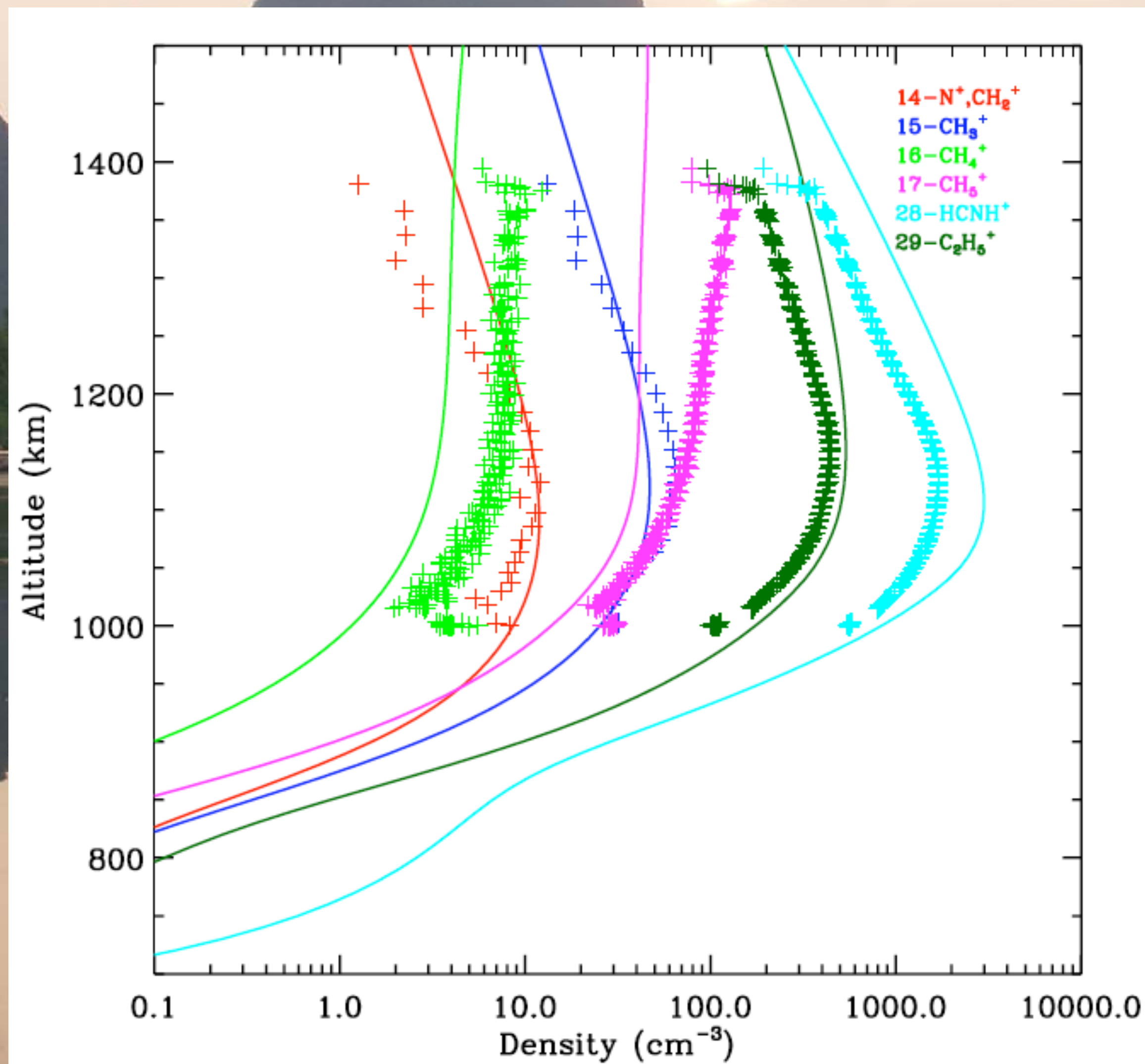
$$k \sim 3/N(C_2H_x)t_D \sim 2\times10^{-9}\ cm^3s^{-1}$$

These values are typical of ion reactions, much faster than typical neutral reaction rates.

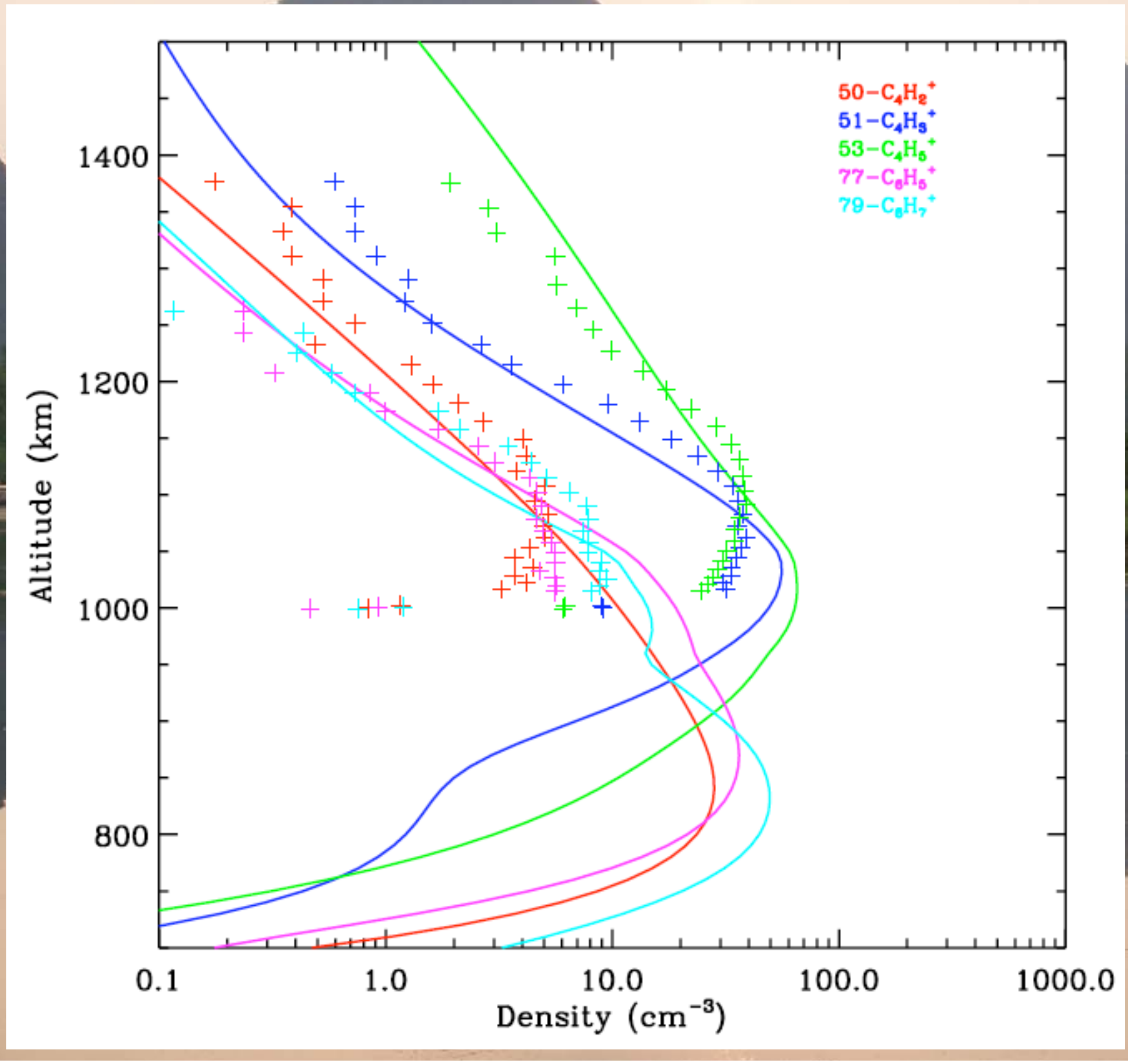
Benzene is synthesized by chemistry in the ionosphere



Results from a 1D Photochemical equilibrium model for Titan’s ionosphere, A.

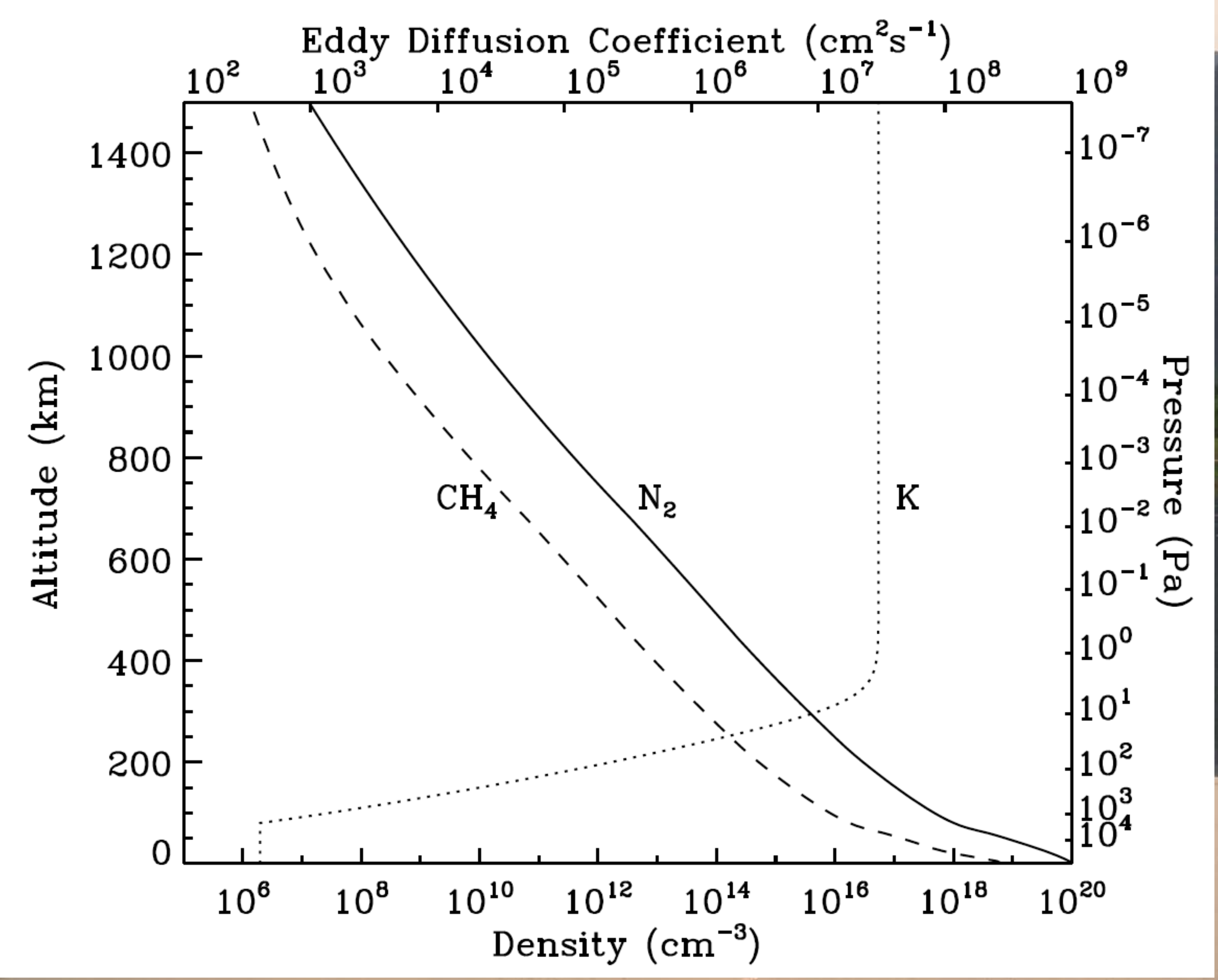


Results from a 1D Photochemical equilibrium model for Titan's ionosphere, B.

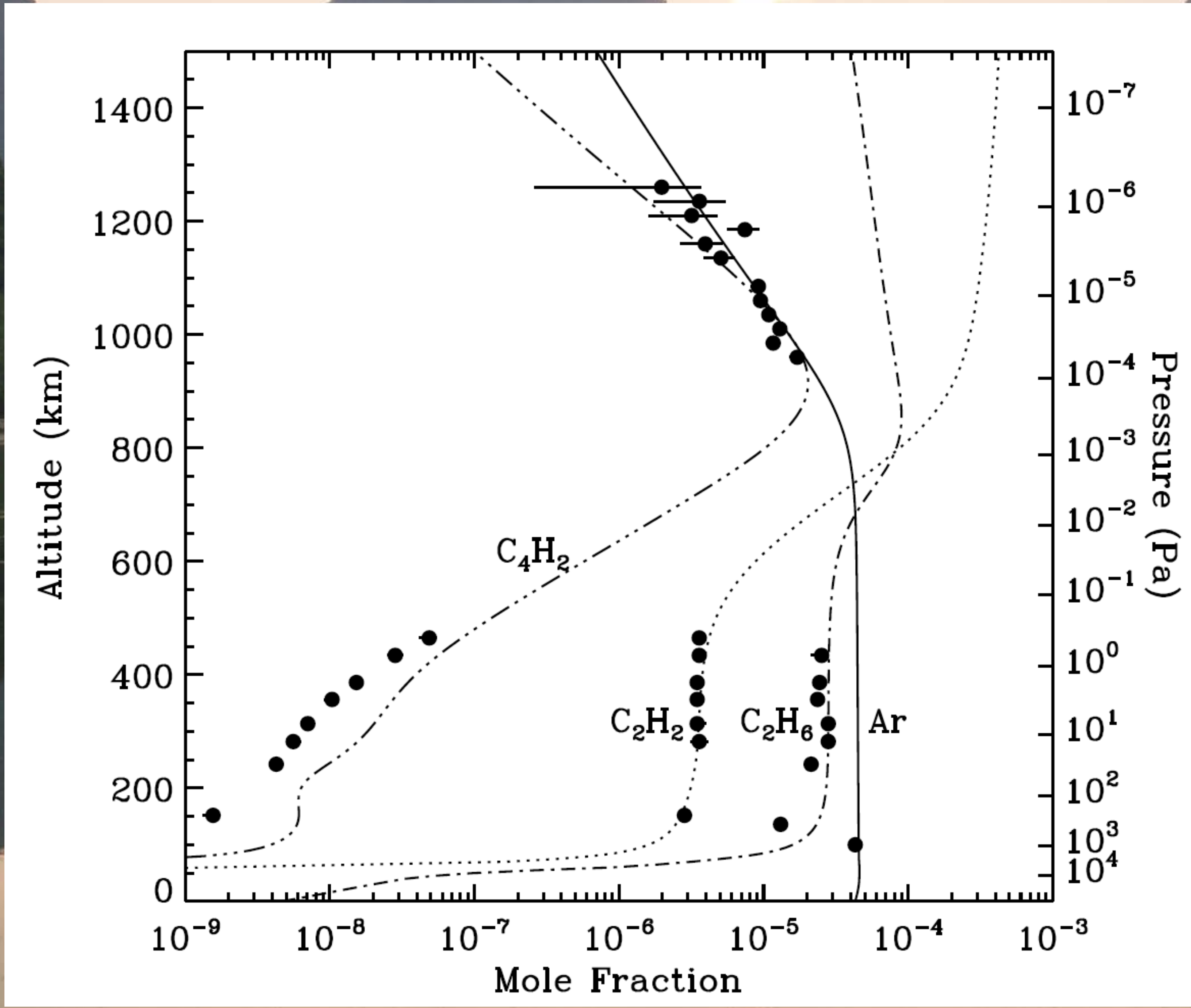


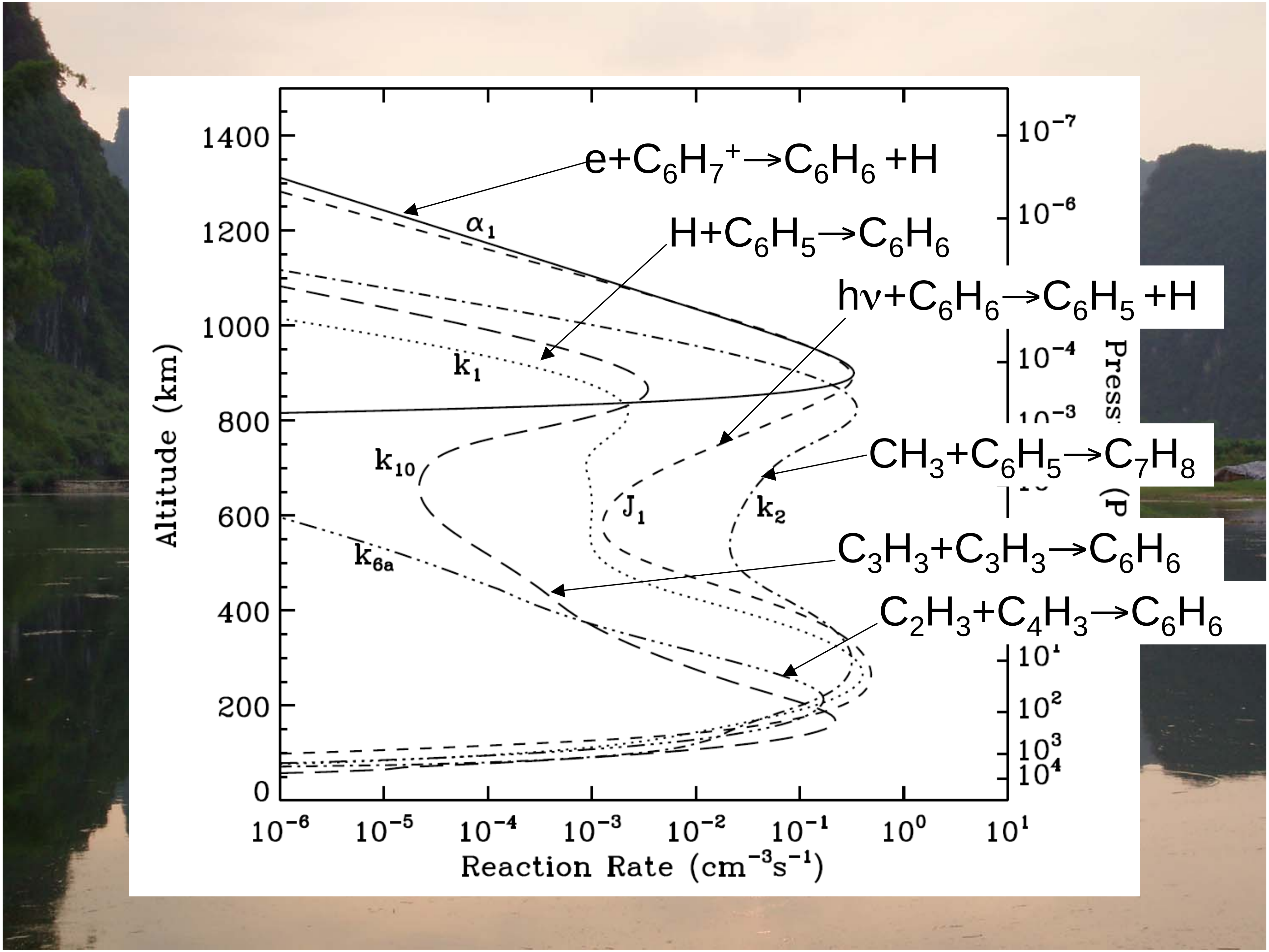
Implied column production rate of C_6H_6, $F=1.4\times10^7\ cm^{-2}s^{-1}$

Model for the background atmosphere



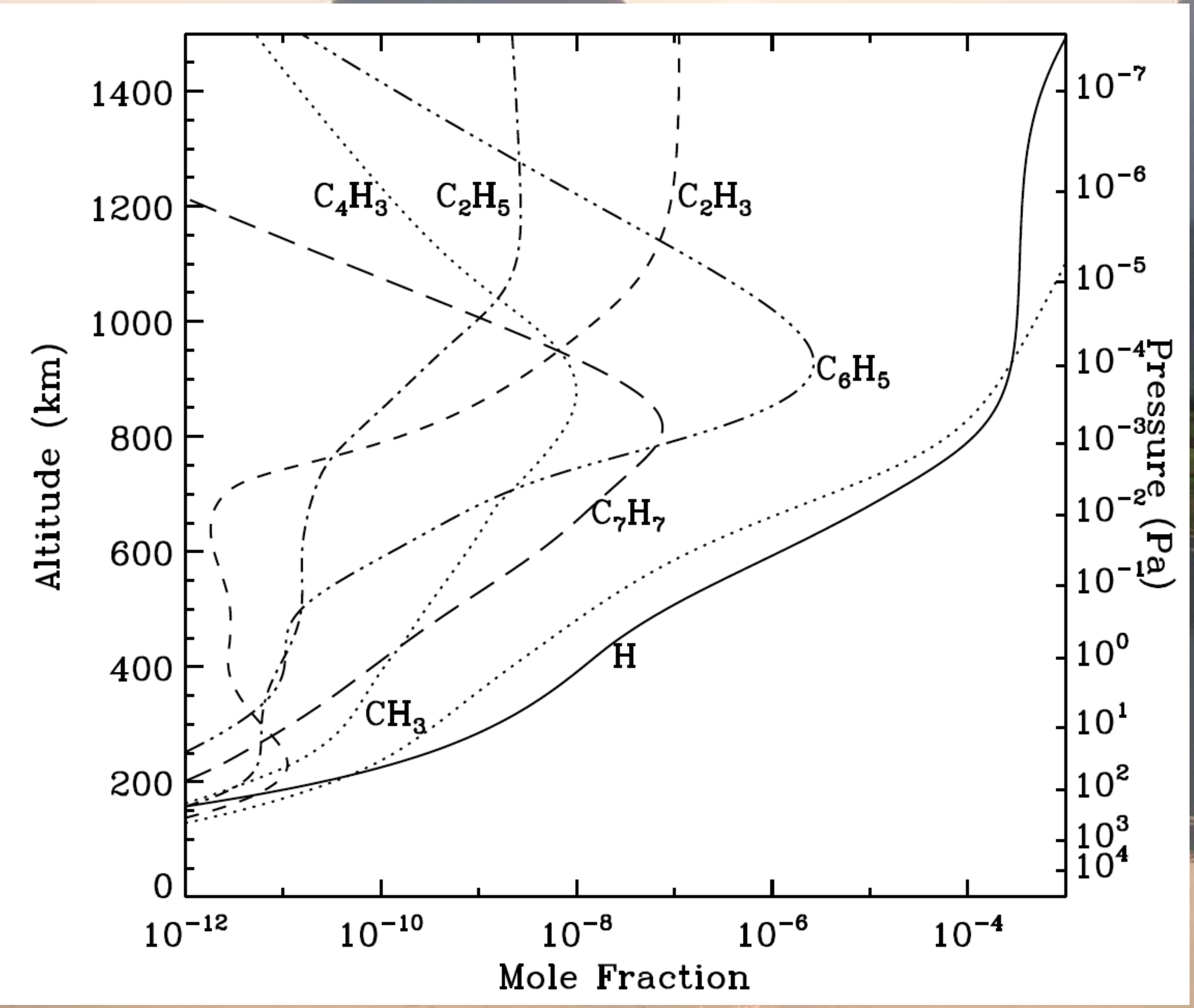
Hydrocarbon chemistry and diffusion rates are constrained by Cassini observations



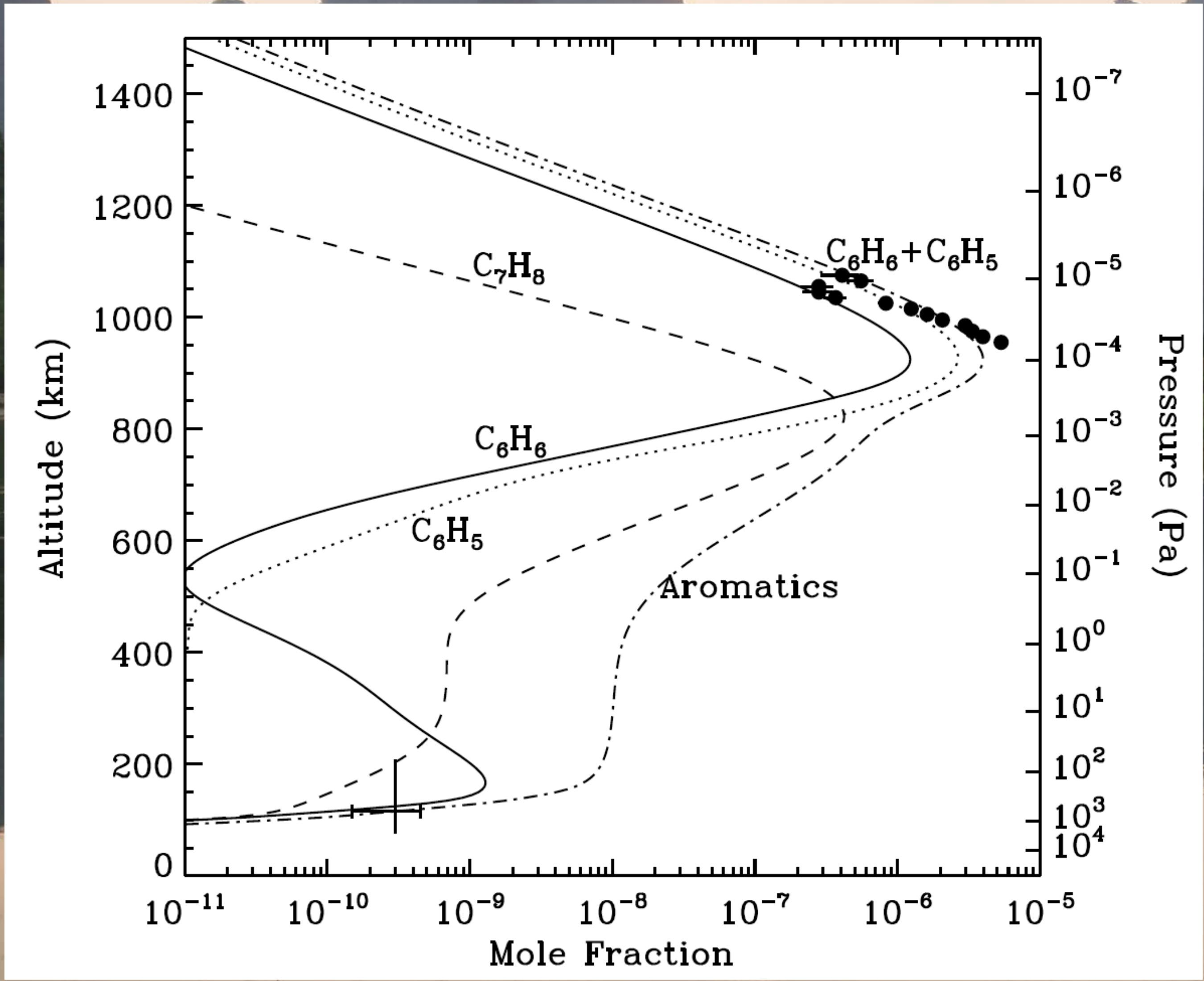


e+C6H7+→C6H6 +H
H+C6H5→C6H6
hν+C6H6→C6H5 +H
CH3+C6H5→C7H8
C3H3+C3H3→C6H6
C2H3+C4H3→C6H6
α1
k1
k10
J1
k2
k6a
Altitude (km)
Reaction Rate (cm−3s−1)
1400
1200
1000
800
600
400
200
0
10−6
10−5
10−4
10−3
10−2
10−1
10^0
10^1
10−7
10−6
10−4
10−3
10^1
10^2
10^3
10^4

Distribution of Radicals in Titan's Atmosphere



Ionospheric and neutral photochemistry produces the required amounts of C_6H_6 and C_6H_5

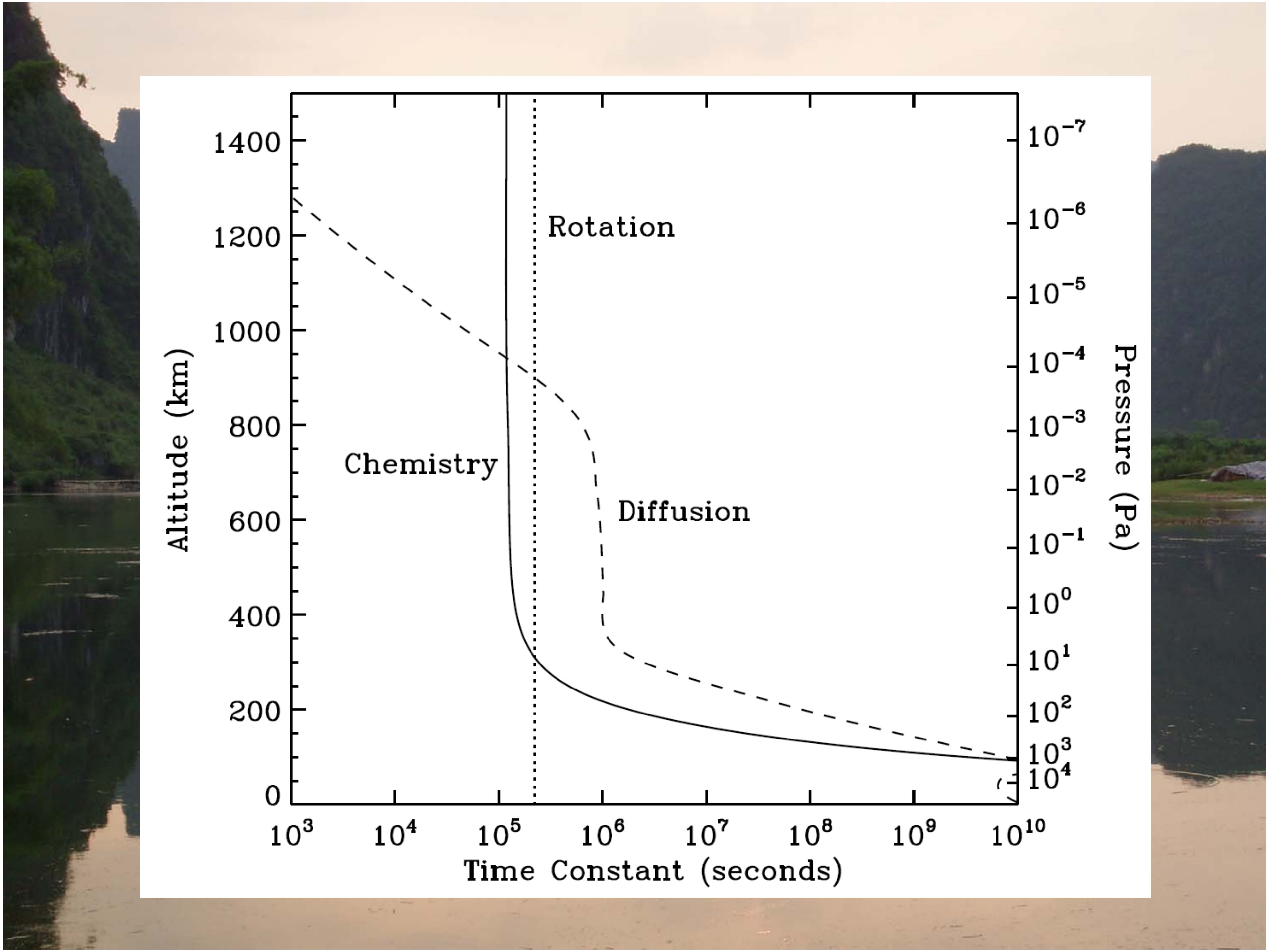


Summary & Conclusions

- The spectra and altitude dependence of the INMS signal indicate atmospheric benzene.
- The time behavior suggests surface chemistry on chamber walls.
- The large C_6H_6 photolysis rate implies that $[C_6H_5]/[C_6H_6]$ ~4, consistent with wall chemistry hypothesis.
- The observed C_6H_6 can be explained as a result of ionospheric chemistry.
- C_6H_6 is destroyed by reaction with radicals, creating heavier aromatics, that, eventually condense and fall to surface.

Many Thanks to

- INMS Colleagues (Waite, Kasprzak, Gell, Fletcher, Müller-Wodarg, Niemann)
- Cassini Operations Team
- Chemistry Colleagues(Imanaka, Smith, Somogyi, Lunine, Hörst, Duituit, Thissen, Pernot, Currasco,…)


Rotation
Chemistry
Diffusion
Altitude (km)
Pressure (Pa)
Time Constant (seconds)
0
200
400
600
800
1000
1200
1400
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}
10^{9}
10^{10}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}