Can AGB stellar winds unveil the origin of the unidentified IR emission bands?

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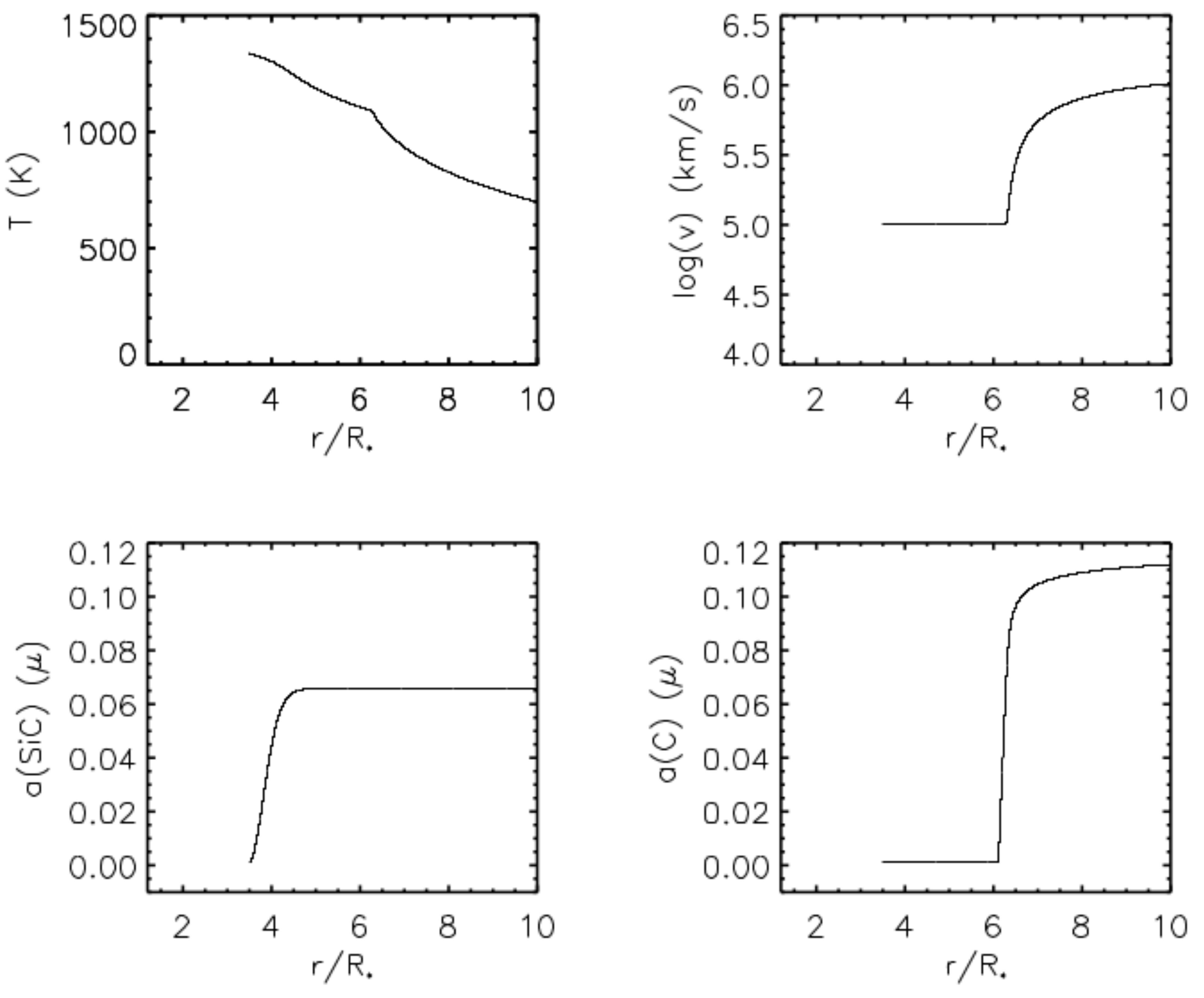
Abstract

The aim of this project is to study PAH (Polycyclic aromatic hydrocarbon)formation in the winds of carbon stars, using a detailed chemical kinetic scheme, to be implemented into the code used to describe the winds of evolved stars. The combination with results from evolutionary models of carbon stars will lead to the determination of the PAH yields expected. This will allow to analyze the production rate of PAHs as function of the mass and metallicity of the stars.



Radial profiles of Temperature (top left panel), velocity (top right panel), grain size of SiC (bottom left panel) and C (bottom right panel) in the wind expanding from the surface of a $M_{\odot}$ model

Goal obtained

Implementation of the current code that describes the dynamics and dust formation in the winds of AGB stars, with the network to describe the formation of PAH, composed by 65 species and 245 reactions

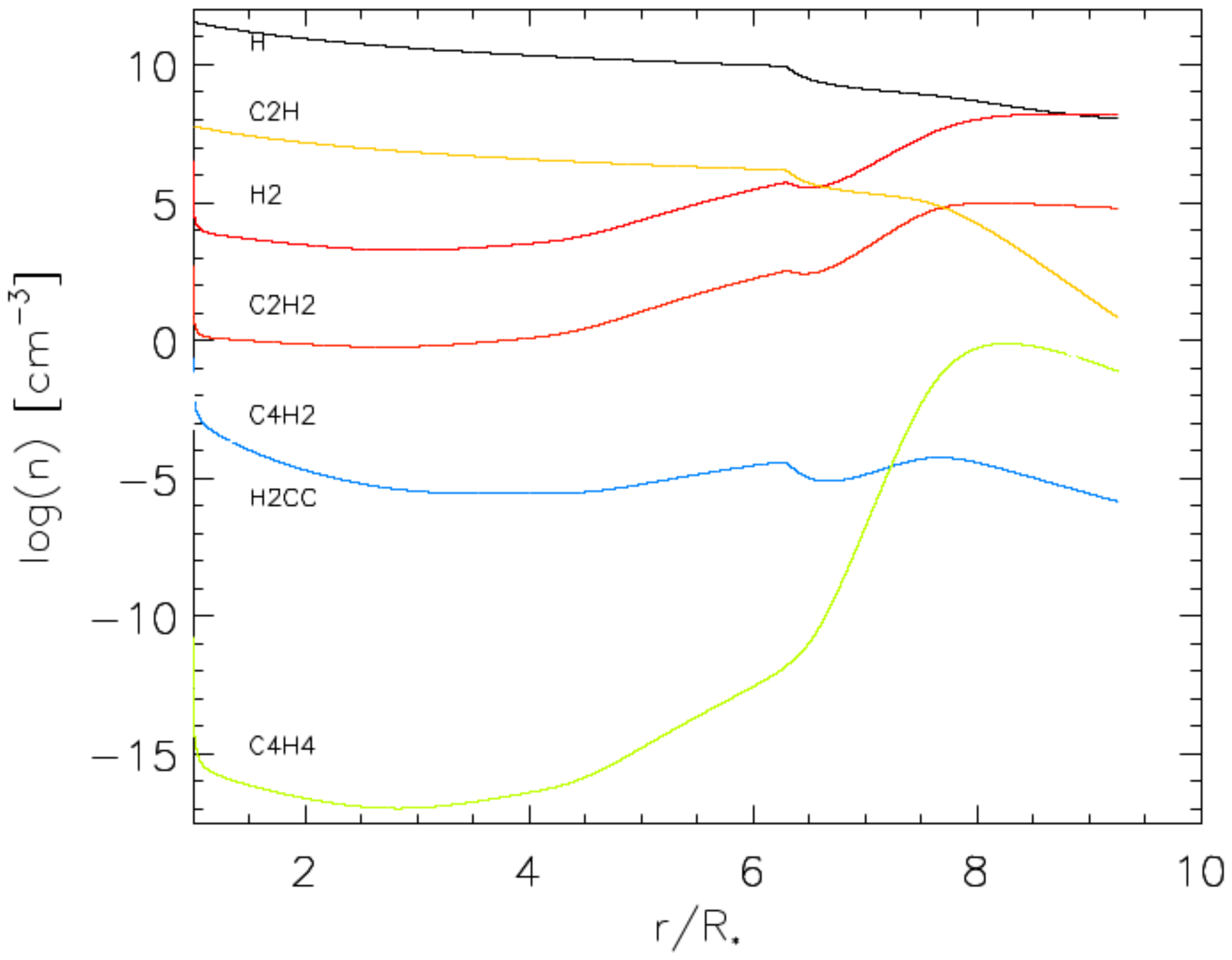
REACTION MECHANISM

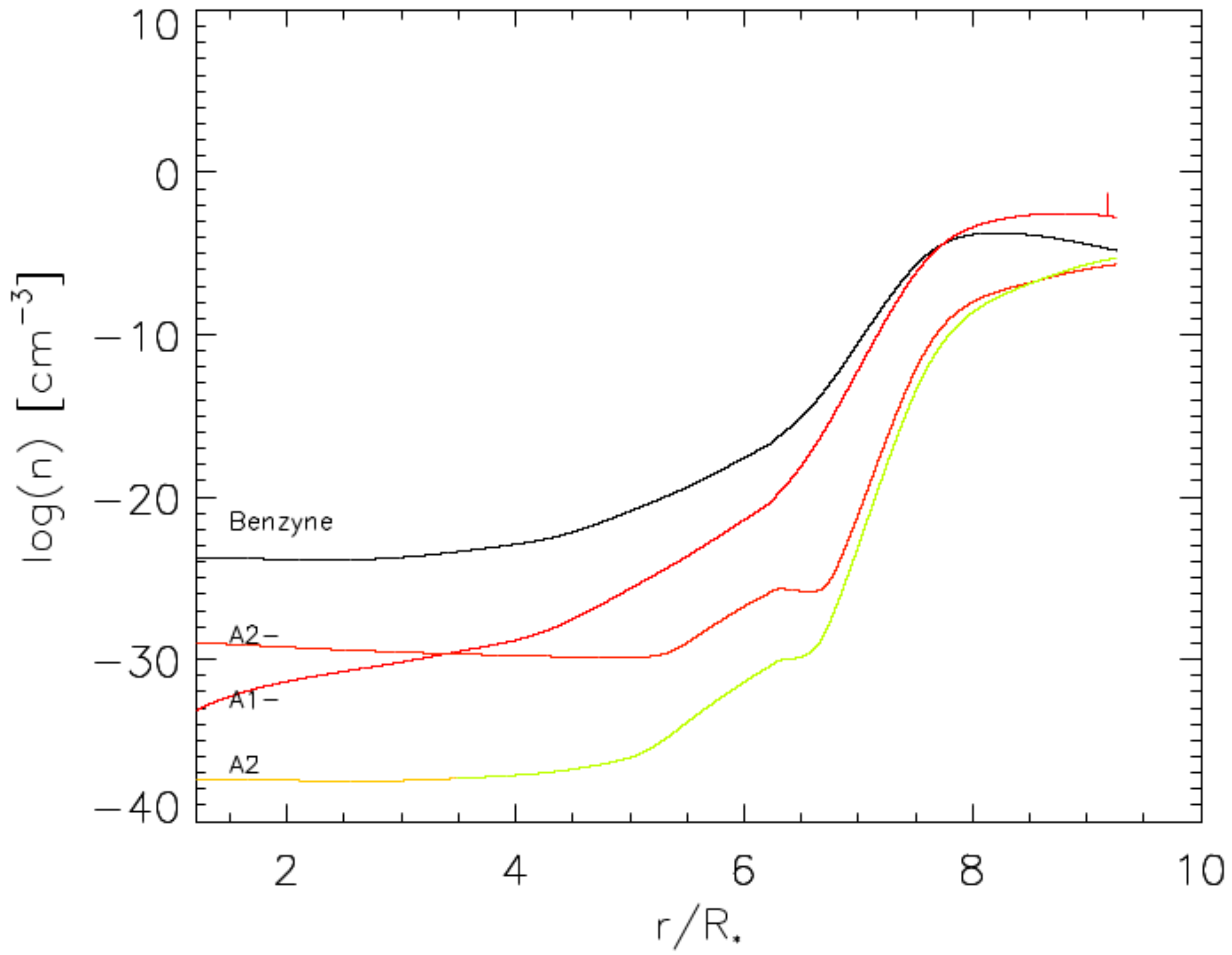
No.[a]	Reaction[b,c]	Forward Rate Coefficient[d] A	n	E	References/ Comments
1	$H + H + H_2 = H_2 + H_2$	9.7(+16)	−0.60		Warnatz 1984
2	$C_2H_2 + M = C_2H + H + M$	4.2(+16)		448	Tanzawa and Gardiner 1980
3	$C_2H_2 + M = H_2CC + M$	3.2(+16)		159	k_3=1.2(+15); Durán, Amorebieta and Colussi 1988
4	$H_2CC + C_2H_2 \rightarrow C_4H_4$	3.2(+12)		8.4	Durán, Amorebieta and Colussi 1988
5	$C_4H_4 + M \rightarrow C_2H_2 + C_2H_2 + M$	2.7(+17)		266	Kiefer *et al.* 1988
6	$C_4H_4 + M = C_4H_2 + H_2 + M$	2.7(+16)		266	$k_6 = 0.1\ k_5$; Kiefer *et al.* 1988
7f	$H_2CC + H_2 \rightarrow C_2H_3 + H$	2.0(+13)		80	estimated, see text
7r	$C_2H_3 + H \rightarrow H_2CC + H_2$	1.5(+13)			$k_{7r} = 0.5\ k_{10}$
8	$C_2H + C_2H_3 = C_2H_2 + C_2H_2$	1.0(+13)			Frenklach *et al.* 1986a
9	$C_2H_3 + M = C_2H_2 + H + M$	1.2(+39)	−7.17	212	Kiefer *et al.* 1985b
10	$C_2H_3 + H = C_2H_2 + H_2$	3.0(+13)			Heinemann,Hofmann–Sievert and Hoyermann 1988
11	$C_2H_3 + C_2H_3 = C_2H_4 + C_2H_2$	1.0(+12)			estimated
12	$C_2H_4 + M = C_2H_3 + H + M$	4.0(+17)		411	Just, Roth and Damm 1976
13	$C_2H_4 + M = C_2H_2 + H_2 + M$	2.5(+17)		332	Just, Roth and Damm 1976
14	$C_2H_4 + H = C_2H_3 + H_2$	1.5(+14)		42.7	Warnatz 1984
15	$C_2H_4 + C_2H = C_2H_3 + C_2H_2$	2.0(+13)			Frenklach, Yuan and Ramachandra 1988
16	$C_2H + H_2 = C_2H_2 + H$	1.1(+13)		12.0	Gardiner *et al.* 1985
17	$C_2H + C_2H_2 = C_4H_2 + H$	4.0(+13)			Tanzawa and Gardiner 1980
18	$C_4H_2 + M = C_4H + H + M$	3.5(+17)		335	Tanzawa and Gardiner 1980
19	$C_4H + H_2 = C_4H_2 + H$	1.1(+13)		12.0	$k_{19} = k_{16}$
20	$C_4H_2 + C_2H = C_4H + C_2H_2$	2.0(+13)			Frenklach *et al.* 1985, 1986b
21	$C_4H_4 + H = C_4H_3S + H_2$	1.5(+14)		42.7	$k_{21} = k_{14}$
22	$C_4H_4 + H = C_4H_3U + H_2$	1.5(+14)		42.7	$k_{22} = k_{14}$
23	$C_4H_4 + C_2H = C_4H_3S + C_2H_2$	4.0(+13)			Tanzawa and Gardiner 1980
24	$C_4H_4 + C_2H = C_4H_3U + C_2H_2$	4.0(+13)			Tanzawa and Gardiner 1980
25	$C_4H_4 + C_4H = C_4H_3S + C_4H_2$	2.0(+13)			Frenklach *et al.* 1985, 1986b
26	$C_4H_4 + C_4H = C_4H_3U + C_4H_2$	2.0(+13)			Frenklach *et al.* 1985, 1986b
27	$C_4H_2 + H + M = C_4H_3S + M$	1.0(+14)			$k_{27} = k_{-9}$
28	$C_4H_2 + H + M = C_4H_3U + M$	1.0(+14)			$k_{28} = k_{-9}$
29	$C_2H_2 + C_2H + M = C_4H_3U + M$				*e*
30	$C_4H_3S + H = C_4H_2 + H_2$	3.0(+13)			$k_{30} = k_{10}$
31	$C_4H_3U + H = C_4H_2 + H_2$	1.5(+13)			$k_{31} = 0.5\ k_{31}$
32	$C_4H_3S + H + M = C_4H_4 + M$	1.0(+15)			Tanzawa and Gardiner 1980
33	$C_4H_3U + H + M = C_4H_4 + M$	1.0(+15)			Tanzawa and Gardiner 1980
34	$C_2H_4 + C_4H = C_2H_3 + C_4H_2$	2.0(+13)			$k_{34} = k_{15}$
35	$C_4H_4 + C_2H = C_4H_2 + C_2H_3$	1.0(+13)			Frenklach, Yuan and Ramachandra 1988
36	$C_2H_4 + C_2H_3 = C_4H_6 + H$	1.0(+11)			estimated
37	$C_4H_6 + H = C_4H_5S + H_2$	1.5(+14)		42.7	$k_{37} = k_{14}$
38	$C_4H_6 + H = C_4H_5U + H_2$	1.5(+14)		42.7	$k_{38} = k_{14}$
39	$C_4H_5S + H = C_4H_4 + H_2$	3.0(+13)			$k_{39} = k_{10}$
40	$C_4H_5U + H = C_4H_4 + H_2$	1.5(+13)			$k_{40} = 0.5\ k_{10}$
41	$C_4H_4 + H + M = C_4H_5S + M$	1.0(+14)			$k_{41} = k_{-9}$
42	$C_4H_4 + H + M = C_4H_5U + M$	1.0(+14)			$k_{42} = k_{-9}$
43	$C_2H + C_4H_2 = C_6H_2 + H$	4.0(+13)			Tanzawa and Gardiner 1980
44	$C_4H + C_2H_2 = C_6H_2 + H$	4.0(+13)			Tanzawa and Gardiner 1980
45	$C_4H + C_4H_2 = C_6H_2 + C_2H$	1.0(+13)			Frenklach *et al.* 1985, 1986b
46	$C_2H + C_4H_4 = C_6H_4 + H$	1.0(+11)			$k_{46} = k_{36}$
47	$C_4H_3U + C_2H_2 = C_6H_4 + H$	1.0(+10)			Westmoreland 1987
48f	$C_4H_3U + C_2H_2 \rightarrow$ benzyne + H	1.5(+10)			Westmoreland 1987
48r	benzyne + H $\rightarrow C_4H_3U + C_2H_2$	3.0(+15)		87.0	Westmoreland 1987
49	benzyne + H = C6H4 + H				*f*
50	benzyne + H = A_1-				*g*
51	$C_4H_3U + C_2H_2 = A_1-$				*h*
52f	$C_2H_3 + C_2H_2 \rightarrow C_4H_5^{\#}$	6.2(+11)		20.3	Durán, Amorebieta and Colussi 1988
52r	$C_4H_5^{\#} \rightarrow C_2H_3 + C_2H_2$	3.3(−06)	5.71		Durán, Amorebieta and Colussi 1988
53	$C_4H_5^{\#} \rightarrow C_4H_4 + H$	2.6(−08)	5.84		Durán, Amorebieta and Colussi 1988
54	$C_4H_5^{\#} + M \rightarrow C_4H_5U + M$	6.8(+12)	0.51		Durán, Amorebieta and Colussi 1988
55	$C_4H_5^{\#} + C_2H_2 \rightarrow C_4H_4 + C_2H_2$	5.8(+14)		6.5	Durán, Amorebieta and Colussi 1988
56	$C_4H_5U + C_2H_2 \rightarrow C_6H_7^{\#}$	6.2(+11)		20.3	Durán, Amorebieta and Colussi 1988
57	$C_6H_7^{\#} \rightarrow A_1 + H$	3.5(+09)	1.49		Durán, Amorebieta and Colussi 1988
58	$C_6H_7^{\#} + M \rightarrow C_6H_7U + M$	1.1(+13)	0.48		Durán, Amorebieta and Colussi 1988
59	$C_6H_7U + H = C_6H_6 + H_2$	1.5(+13)			$k_{59} = 0.5\ k_{10}$

TABLE 1—*Continued*

No.[a]	Reaction[b,c]	Forward Rate Coefficient[d] A	n	E	References/ Comments
60	$C_6H_6 + H = C_6H_5U + H_2$	1.5(+14)		42.7	$k_{60} = k_{15}$
61	$C_6H_5U + H = C_6H_4 + H_2$	1.5(+13)			$k_{61} = 0.5\ k_{10}$
62	$C_4H_5U + M \rightarrow C_2H_3 + C_2H_2 + M$				$k_{62} = k_{29}\ K_{62}$
63	$C_6H_4 + H + M = C_6H_5U + M$	1.0(+14)			$k_{63} = k_{-9}$
64	$C_6H_5U + H + M = C_6H_6 + M$	2.5(+15)		39.7	$k_{64} = k_{-12}$
65	$C_6H_4 + H = C_6H_3U + H_2$	1.5(+14)		42.7	$k_{65} = k_{15}$
66	$C_6H_3U + H + M = C_6H_4 + M$	2.5(+15)		39.7	$k_{66} = k_{-12}$
67	$C_6H_2 + H + M = C_6H_3U + M$	1.0(+14)			$k_{67} = k_{-9}$
68	$C_4H_2 + C_2H + M = C_6H_3U + M$				*e*
69	$C_6H_3U + C_2H_2 = A_1C_2H^{*}$	1.5(+10)			see text
70	$C_4H_3U + C_4H_2 = A_1C_2H-$	1.5(+10)			see text
71	$A_1- + H + M = A_1 + M$	2.5(+15)		39.7	$k_{71} = k_{-12}$
72	$A_1 + H = A_1- + H_2$	2.5(+14)		66.9	T≥1000 K; Kiefer *et al.* 1985a
		3.0(+12)		33.9	T<1000 K; Nicovich and Ravishankara 1984
73	$A_1 + C_2H = A_1- + C_2H_2$	2.0(+13)			Frenklach, Yuan and Ramachandra 1988
74	$A_1 + C_4H = A_1- + C_4H_2$	2.0(+13)			$k_{74} = k_{73}$
75f	$A_1- + C_2H_2 \rightarrow A_1C_2H_2^{\#}$	1.0(+13)			see text
75r	$A_1C_2H_2^{\#} \rightarrow A_1- + C_2H_2$	3.3(−06)	5.71		$k_{75r} = k_{52r}$
76	$A_1C_2H_2^{\#} \rightarrow A_1C_2H + H$	2.6(−08)	5.84		$k_{76} = k_{53}$
77	$A_1C_2H_2^{\#} + M \rightarrow A_1C_2H_2U + M$	6.8(+12)	0.51		$k_{77} = k_{54}$
78	$A_1- + C_2H_2 + M = A_1C_2H_2U + M$				*e*
79	$A_1C_2H + H + M = A_1C_2H_2U + M$	1.0(+14)			$k_{79} = k_{-9}$
80	$A_1C_2H_2U + H = A_1C_2H + H_2$	1.5(+13)			$k_{80} = 0.5\ k_{10}$
81	$A_1C_2H + H = A_1C_2H- + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{81} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{81} = k_{72}$
82	$A_1C_2H + C_2H = A_1C_2H- + C_2H_2$	2.0(+13)			$k_{82} = k_{73}$
83	$A_1C_2H- + H + M = A_1C_2H + M$	2.5(+15)		39.7	$k_{83} = k_{71}$
84	$A_1C_2H + H = A_1C_2H^{*} + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{84} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{84} = k_{72}$
85	$A_1C_2H + C_2H = A_1C_2H^{*} + C_2H_2$	2.0(+13)			$k_{85} = k_{73}$
86	$A_1C_2H^{*} + H + M = A_1C_2H + M$	2.5(+15)		39.7	$k_{86} = k_{71}$
87	$A_1C_2H^{*} + C_2H_2 = A_2{-}X$	5.0(+10)			see text
88	$A_1C_2H_2U + C_2H_2 \rightarrow A_1C_4H_4U^{\#}$	1.0(+13)			see text
89	$A_1C_4H_4U^{\#} \rightarrow A_2 + H$	3.5(+09)	1.49		$k_{89} = k_{57}$
90	$A_1C_4H_4U^{\#} + M \rightarrow A_1C_2H_2U + C_2H_2 + M$	1.1(+13)	0.48		$k_{90} = k_{58}$
91	$A_1- + C_2H_3 + M = A_1C_2H_3 + M$	1.5(−11)		431	*i*
92	$A_1- + C_2H_4 = A_1C_2H_3 + H$	8.6(+11)		16.5	Fahr, Mallard and Stein 1988
93	$A_1 + C_2H_3 = A_1C_2H_3 + H$	1.0(+11)			estimated
94	$A_1C_2H_3 + H = A_1C_2H_2U + H_2$	1.5(+14)		42.7	$k_{94} = k_{15}$
95	$A_1C_2H_3 + H = A_1C_2H_3^{*} + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{95} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{95} = k_{72}$
96	$A_1C_2H_3^{*} + C_2H_2 = A_2 + H$	5.0(+10)			$k_{96} = k_{87}$
97	$A_2{-}X + H + M = A_2 + M$	2.5(+15)		39.7	$k_{97} = k_{71}$
98	$A_2 + H = A_2{-}X + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{98} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{98} = k_{72}$
99	$A_2 + C_2H = A_1{-}X + C_2H_2$	2.0(+13)			$k_{99} = k_{73}$
100	$A_2{-}X + C_2H_2 \rightarrow A_i + H$	1.0(+12)			see text
101	$A_i + H = A_i- + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{101} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{101} = k_{72}$
102f	$A_i- + C_2H_2 \rightarrow A_iC_2H_2^{\#}$	1.0(+13)			$k_{102f} = k_{75f}$
102r	$A_iC_2H_2^{\#} \rightarrow A_i- + C_2H_2$	3.3(−06)	5.71		$k_{102r} = k_{52r}$
103	$A_iC_2H_2^{\#} \rightarrow A_iC_2H + H$	2.6(−08)	5.84		$k_{103} = k_{53}$
104	$A_iC_2H_2^{\#} + M \rightarrow A_iC_2H_2U + M$	6.8(+12)	0.51		$k_{104} = k_{54}$
105	$A_iC_2H_2U + H = A_iC_2H + H_2$	1.5(+13)			$k_{105} = 0.5\ k_{10}$
106	$A_iC_2H + H = A_iC_2H^{*} + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{106} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{106} = k_{72}$
107	$A_iC_2H^{*} + C_2H_2 = A_{i+1}-$	5.0(+10)			$k_{107} = k_{87}$
108	$A_iC_2H_2U + C_2H_2 \rightarrow A_iC_4H_4U^{\#}$	1.0(+13)			$k_{108} = k_{88}$
109	$A_iC_4H_4U^{\#} \rightarrow A_{i+1} + H$	3.5(+09)	1.49		$k_{109} = k_{57}$
110	$A_iC_4H_4U^{\#} + M \rightarrow A_iC_2H_2U + C_2H_2 + M$	1.1(+13)	0.48		$k_{110} = k_{58}$
111	$A_{i+1} + H = A_{i+1}- + H_2$	2.5(+14)		66.9	T≥1000 K; $k_{111} = k_{72}$
		3.0(+12)		33.9	T<1000 K; $k_{111} = k_{72}$
112	$A_{i+1}- + C_2H_2 \rightarrow A_i + H$	1.0(+12)			$k_{112} = k_{100}$

Ongoing: Analysis of the PAH yields produced during the AGB star evolution of a model of initial mass 1.0 $M_{\odot}$ and metallicity Z= 0.004





Concentration profiles of main hydrocarbon (top panel) and small PAH molecules (bottom panel

Next Steps

- Evaluate the PAH formation rate of carbon stars of various mass and chemical composition, during the AGB lifetime
- Calculate synthetic spectra for some selected points along the evolutionary tracks that we compare with the observational data
- Improve the model of stellar wind, taking into account the effect of periodic shocks which are known to be present in the inner wind of AGB stars
- The PAH formation and more generally of the main evolutionary properties of the carbon stars will be reconsidered, based on the updated determination of the mass loss rate and thermodynamic structure of the wind

Critical issues

- Computing Time
- Difficulty to find out the real and complex refractive index for each molecule and compound

Expenses

- Hardware ~3000 euros
- Participation to STARS meeting ~500 euros