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C_1-C_4 在 Pt 催化剂上的多相反应机理

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Heterogeneous Mechanism of C_1-C_4 on a Platinum Catalyst

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表 S1　C_1-C_4 在 Pt 催化剂上的详细壁面反应机理

Table S1　Heterogeneous Reaction Mechanism for C_1-C_4 on Platinum

R1	H +Pt(S) =>H(S)	S_0=1.000	0.0	[12-14]
R2	R2 H_2 +Pt(S) +Pt(S) =>H(S) +H(S)	S_0=0.046	0.0	[12-14]
R3	H_2 +C(S) =>CH_2(S)	S_0=0.040	29.7+4.6θ_c	[12-14]
R4	O +Pt(S) =>O(S)	S_0=1.000	0.0	[12-14]
R5	O_2 +Pt(S)+Pt(S)=>O(S)+O(S)	S_0=0.07(300/T)	0.0	[12-14]
R6	OH +Pt(S) =>OH(S)	S_0=1.000	0.0	[12-14]
R7	H_2O +Pt(S) =>H_2O(S)	S_0=0.750	0.0	[12-14]
R8	CO +Pt(S) =>CO(S)	S_0=0.840	0.0	[12-14]
R9	CO_2 +Pt(S) =>CO_2(S)	S_0=0.005	0.0	[12-14]
R10	CH_3 +Pt(S) =>CH_3(S)	S_0=1.000	0.0	[12-14]
R11	CH_4 +C(S) =>C_2H_4(2S)	S_0=7.000×10^{-9}	23.0+47.5θ_c	[12-14]
R12	CH_4 +Pt(S) +Pt(S) =>CH_3(S)+H(S)	S_0=9.000×10^{-4}	72.0	[12-14]
R13	CH_4 +O(S) +Pt(S) =>CH_3(S) +OH(S)	1.36×10^{10}×$T^{0.7}$	42.0+8θ_o	[12-14]
R14	CH_4+OH(S) +Pt(S) =>CH_3(S) +H_2O(S)	S_0=1.000	10.0	[12-14]
R15	C2H_2 +Pt(S) =>C_2H_2(1S)	S_0=0.050	0.0	[13-14]
R16	C_2H_4 +Pt(S) =>C_2H_4(1S)	S_0=0.015	0.0	[13-14]
R17	C2H_5 +Pt(S) =>C_2H_5(S)	S_0=1.000	0.0	[13-14]
R18	C_2H_6 +Pt(S) +Pt(S) =>C_2H_6(2S)	S_0=0.015	0.0	[13-14]
R19	C_3H_6 +Pt(S) +Pt(S) =>C_3H_6(1S)	S_0=0.980	0.0	[13-14]
R20	C_3H_6 +O(S)+Pt(S) =>C_3H_5(2S)+OH(S)	S_0=0.050	0.0	[13-14]
R21	nC_3H_7 +Pt(S) =>C_3H_7(1S)	S_0=1.000	0.0	Est. [13-14]
R22	C_3H_8 +Pt(S) =>C_3H_8(S)	S_0=1.000	0.0	Est. [13-14]
R23	C_4H_{10} +Pt(S) +Pt(S) =>C_4H_{10}(1S)	S_0=0.950	45.0	[15-16]
R24	C_4H_{10}+Pt(S) +Pt(S)=>C_4H_9(1S)+H(S)	S_0=0.050	56.0	[17]
R25	pC_4H_9 +Pt(S)=>C_4H_9(1S)	S_0=1.000	0.0	Est. [15-17]
R26	sC_4H_9 +Pt(S) =>C_4H_9(2S)	S_0=1.000	0.0	Est. [15-17]
R27	C_4H_8-1 +Pt(S) =>C_4H_8(5S)	S_0=0.015	0.0	Est. [15-17]
R28	C_4H_8-2 +Pt(S) =>C_4H_8(7S)	S_0=0.015	0.0	Est. [13-17]
R29	$CH_2CHCHCH_2$ +Pt(S) =>C_4H_6(5S)	S_0=0.030	0.0	Est. [13-17]
R30	H(S) =>H +Pt(S)	6.000×10^{13}	255.4-5θ_h	[13-14]
R31	H(S) +H(S) =>Pt(S) +Pt(S)+H_2	3.700×10^{21}	67.4-10θ_h	[13-14]
R32	CH_2(S) =>C(S) +H_2	7.690×10^{13}	25.1+50θ_c	[13-14]
R33	O(S) =>O +Pt(S)	1.000×10^{13}	358.8-94.1θ_o	[13-14]
R34	O(S) +O(S) =>Pt(S)+Pt(S) +O_2	3.700×10^{21}	227.4-188.2θ_o	[13-14]
R35	OH(S) =>OH +Pt(S)	5.000×10^{13}	251.1-167.3θ_o	[13-14]
R36	H_2O(S) =>H_2O +Pt(S)	4.500×10^{12}	41.8	[13-14]
R37	CO(S) =>CO +Pt(S)	2.500×10^{16}	146.0-33θ_{co}	[13-14]
R38	CO_2(S) =>CO_2 +Pt(S)	1.000×10^{13}	27.1	[13-14]
R39	CH_3(S) =>Pt(S) +CH_3	1.000×10^{13}	163	[13-14]
R40	CH_3(S) +H(S) =>CH_4 +Pt(S) +Pt(S)	1.500×10^{20}	50.0-2.8θ_h	[13-14]
R41	CH3(S)+H2O(S)=>CH4+OH(S)+Pt(S)	2.500×10^{20}	23.0	[13-14]
R42	CH_3(S) +OH(S) =>CH_4 +O(S) +Pt(S)	3.700×10^{21}	85.9	[13-14]

R43	$C_2H_2(1S)$ =>Pt(S) +C_2H_2	1.000×10^{12}	58.6	[13-14]
R44	$C_2H_4(1S)$ =>Pt(S) +C_2H_4	1.000×10^{13}	50.2	[13-14]
R45	$C_2H_4(2S)$ =>C(S) +CH_4	1.000×10^{10}	$25.5+47.5\theta_c$	[13-14]
R46	$C_2H_5(S)$ =>Pt(S) +C_2H_5	1.000×10^{13}	172.9	[13-14]
R47	$C_2H_6(2S)$ =>Pt(S) +Pt(S) +C_2H_6	1.000×10^{13}	20.9	[13-14]
R48	$C_3H_6(1S)$ =>C_3H_6 +Pt(S) +Pt(S)	1.000×10^{13}	72.7	[13-14]
R49	$C_3H_5(2S)$+OH(S) =>C_3H_6 +O(S) +Pt(S)	3.700×10^{21}	31.0	[13-14]
R50	$C_3H_7(1S)$ =>nC_3H_7 +Pt(S)	1.000×10^{13}	172.9	Est. [13-14]
R51	$C_3H_8(S)$ =>C_3H_8 +Pt(S)	1.000×10^{13}	20.9	Est. [13-14]
R52	$C_4H_6(5S)$ =>$CH_2CHCHCH_2$ +Pt(S)	2.000×10^{13}	100.4	Est. [15-17]
R53	$C_4H_8(5S)$ =>C_4H_8-1 +Pt(S)	1.000×10^{13}	50.2	Est. [15-17]
R54	$C_4H_8(7S)$ =>C_4H_8-2 +Pt(S)	1.000×10^{13}	50.2	Est. [15-17]
R55	$C_4H_9(1S)$ =>pC_4H_9 +Pt(S)	1.000×10^{13}	163	Est. [15-17]
R56	$C_4H_9(2S)$ =>sC_4H_9 +Pt(S)	1.000×10^{13}	163	Est. [15-17]
R57	$C_4H_{10}(1S)$ =>C_4H_{10} +Pt(S)+Pt(S)	1.000×10^{13}	45.0	[15-17]
R58	H(S) +O(S) =>OH(S) +Pt(S)	1.280×10^{21}	112.0	[13-14]
R59	OH(S) +Pt(S) =>H(S) +O(S)	7.390×10^{19}	$77.3-73.2\theta_o$	[13-14]
R60	H(S) +OH(S) =>$H_2O(S)$ +Pt(S)	2.040×10^{21}	66.2	[13-14]
R61	$H_2O(S)$ +Pt(S) =>H(S) +OH(S)	1.150×10^{19}	$101.4+167.3\theta_o$	[13-14]
R62	OH(S) +OH(S) =>H2O(S) +O(S)	7.400×10^{20}	74.0	[13-14]
R63	$H_2O(S)$ +O(S) =>OH(S) +OH(S)	1.000×10^{20}	$43.1+240.5\theta_o$	[13-14]
R64	C(S) +O(S) =>CO(S) +Pt(S)	3.700×10^{19}	0.0	[13-14]
R65	CO(S) +Pt(S) =>C(S) +O(S)	3.700×10^{19}	$236.5-33\theta_{co}$	[13-14]
R66	CO(S) +O(S) =>$CO_2(S)$ +Pt(S)	3.700×10^{19}	$117.6-33\theta_{co}$	[13-14]
R67	$CO_2(S)$ +Pt(S) =>CO(S) +O(S)	3.700×10^{19}	$173.3+94.1\theta_o$	[13-14]
R68	CO(S) +OH(S) =>$CO_2(S)$ +H(S)	2.000×10^{19}	$38.7-30\theta_{co}$	[13-14]
R69	$CO_2(S)$ +H(S) =>CO(S) +OH(S)	2.000×10^{19}	28.3	[13-14]
R70	$CH_3(S)$ +Pt(S) =>$CH_2(S)$ +H(S)	1.262×10^{22}	70.3	[13-14]
R71	$CH_2(S)$ +H(S) =>$CH_3(S)$ +Pt(S)	3.090×10^{22}	$0.0-2.8\theta_h$	[13-14]
R72	$CH_2(S)$ +Pt(S) =>CH(S) +H(S)	7.314×10^{22}	$58.9+50\theta_c$	[13-14]
R73	CH(S) +H(S) =>$CH_2(S)$ +Pt(S)	3.090×10^{22}	$0.0-2.8\theta_h$	[13-14]
R74	CH(S) +Pt(S) =>C(S) +H(S)	3.090×10^{22}	$0.0-2.8\theta_h$	[13-14]
R75	C(S) +H(S) =>CH(S) +Pt(S)	1.248×10^{22}	138.0	[13-14]
R76	$C_4H_{10}(1S)+O(S)=>C_4H_9(1S)+OH(S)+Pt(S)$	3.700×10^{21}	25.1	Est. [14-17]
R77	$C_4H_9(1S)+OH(S)+Pt(S)=>C_4H_{10}(1S)+O(S)$	1.350×10^{30}	77.4	Est. [14-17]
R78	$C_4H_{10}(1S)+O(S)=>C_4H_9(2S)+OH(S)+Pt(S)$	3.700×10^{21}	25.1	Est. [14-17]
R79	$C_4H_9(2S)+OH(S)+Pt(S)=>C_4H_{10}(1S)+O(S)$	1.350×10^{30}	77.4	Est. [14-17]
R80	$C_2H_4(1S)$ =>$C_2H_4(2S)$	1.000×10^{13}	83.3	[13-14]
R81	$C_2H_4(2S)$ =>$C_2H_4(1S)$	1.000×10^{13}	75.3	[13-14]
R82	$C_2H_5(S)$ +H(S) =>$C_2H_6(2S)$	3.700×10^{21}	41.8	[13-14]
R83	$C_2H_6(2S)$ =>$C_2H_5(S)$ +H(S)	7.000×10^{12}	57.7	[13-14]
R84	$CH_3(S)$ +$CH_3(S)$ =>$C_2H_6(2S)$	1.000×10^{21}	14.5	[13-14]
R85	$C_2H_6(2S)$ =>$CH_3(S)$ +$CH_3(S)$	1.000×10^{13}	89.0	[13-14]
R86	$C_2H_5(S)$ +Pt(S) =>$C_2H_4(2S)$+H(S)	1.000×10^{22}	54.4	[13-14]
R87	$C_2H_4(2S)$+H(S) =>$C_2H_5(S)$ +Pt(S)	1.000×10^{21}	29.3	[13-14]

R88	$C_2H_4(2S)+Pt(S) \Rightarrow C_2H_3(1S)+H(S)$	2.000×10^{22}	99.1	[13-14]
R89	$C_2H_3(1S)+H(S) \Rightarrow C_2H_4(2S)+Pt(S)$	3.700×10^{21}	75.3	[13-14]
R90	$C_2H_4(2S)+Pt(S) \Rightarrow C_2H_3(2S)+H(S)$	3.700×10^{21}	128.5	[13-14]
R91	$C_2H_3(2S)+H(S) \Rightarrow C_2H_4(2S)+Pt(S)$	3.700×10^{21}	57.3	[13-14]
R92	$C_2H_4(1S)+Pt(S) \Rightarrow C_2H_3(2S)+H(S)$	3.700×10^{21}	112.7	[13-14]
R93	$C_2H_3(2S)+H(S) \Rightarrow C_2H_4(1S)+Pt(S)$	3.700×10^{21}	33.5	[13-14]
R94	$C_2H_3(2S)+Pt(S) \Rightarrow C_2H_2(3S)+H(S)$	3.700×10^{21}	121.3	[13-14]
R95	$C_2H_2(3S)+H(S) \Rightarrow C_2H_3(2S)+Pt(S)$	3.700×10^{21}	51.7	[13-14]
R96	$C_2H_3(1S)+Pt(S) \Rightarrow CH_3(S)+C(S)$	3.700×10^{21}	$46.9+50\theta_c$	[13-14]
R97	$CH_3(S)+C(S) \Rightarrow C_2H_3(1S)+Pt(S)$	3.700×10^{21}	46.0	[13-14]
R98	$C_2H_2(1S) \Rightarrow C_2H_2(3S)$	1.000×10^{13}	61.5	[13-14]
R99	$C_2H_2(3S) \Rightarrow C_2H_2(1S)$	1.000×10^{13}	4.20	[13-14]
R100	$C_2H_3(1S) \Rightarrow C_2H_3(2S)$	1.000×10^{13}	176.0	[13-14]
R101	$C_2H_3(2S) \Rightarrow C_2H_3(1S)$	1.000×10^{13}	128.6	[13-14]
R102	$C_2H_2(1S)+Pt(S) \Rightarrow C_2H(1S)+H(S)$	3.700×10^{21}	133.5	[13-14]
R103	$C_2H(1S)+H(S) \Rightarrow C_2H_2(1S)+Pt(S)$	3.700×10^{21}	66.9	[13-14]
R104	$C_2H(1S)+Pt(S) \Rightarrow CH(S)+C(S)$	3.700×10^{21}	125.1	[13-14]
R105	$CH(S)+C(S) \Rightarrow C_2H(1S)+Pt(S)$	3.700×10^{21}	121.3	[13-14]
R106	$C_4H_{10}(1S) \Rightarrow C_2H_5(S)+C_2H_5(S)$	1.000×10^{13}	89.0	Est. [13,19]
R107	$C_2H_5(S)+C_2H_5(S) \Rightarrow C_4H_{10}(1S)$	1.000×10^{21}	14.5	Est. [13,19]
R108	$C_4H_{10}(1S) \Rightarrow CH_3(S)+C_3H_7(1S)$	1.000×10^{13}	89.0	Est. [13,19]
R109	$CH_3(S)+C_3H_7(1S) \Rightarrow C_4H_{10}(1S)$	1.000×10^{21}	14.5	Est. [13,19]
R110	$C_4H_{10}(1S) \Rightarrow C_4H_9(1S)+H(S)$	7.000×10^{12}	57.7	[15-17]
R111	$C_4H_9(1S)+H(S) \Rightarrow C_4H_{10}(1S)$	3.700×10^{21}	41.8	[15-17]
R112	$C_4H_{10}(1S) \Rightarrow C_4H_9(2S)+H(S)$	7.000×10^{12}	57.7	[15-17]
R113	$C_4H_9(2S)+H(S) \Rightarrow C_4H_{10}(1S)$	3.700×10^{21}	41.8	[15-17]
R114	$C_3H_7(1S)+Pt(S) \Rightarrow C_3H_6(2S)+H(S)$	1.000×10^{22}	54.4	Est. [13-14]
R115	$C_3H_6(2S)+H(S) \Rightarrow C_3H_7(1S)+Pt(S)$	1.000×10^{21}	29.3	Est. [13-14]
R116	$C_3H_6(1S) \Rightarrow C_3H_6(2S)+Pt(S)$	1.000×10^{13}	83.3	Est. [13-14]
R117	$C_3H_6(2S)+Pt(S) \Rightarrow C_3H_6(1S)$	1.000×10^{13}	753.0	Est. [13-14]
R118	$C_3H_5(2S)+O(S) \Rightarrow C_3H_4(2S)+OH(S)$	3.700×10^{21}	95.0	[13-14]
R119	$C_3H_4(2S)+O(S) \Rightarrow C_3H_3(2S)+OH(S)$	3.700×10^{21}	0.0	[13-14]
R120	$C_3H_3(2S)+O(S) \Rightarrow C2H2(S)+CHO(S)$	1.360×10^{40}	0.0	[13-14]
R121	$CHO(S)+Pt(S) \Rightarrow OH(S)+C(S)$	1.360×10^{40}	0.0	[13-14]
R122	$C_2H_2(2S)+O(S) \Rightarrow CHO(S)+CH(2S)$	1.360×10^{40}	0.0	[13-14]
R123	$CH(2S)+O(S) \Rightarrow OH(S)+C(S)$	3.700×10^{40}	0.0	[13-14]
R124	$C_3H_6(1S) \Rightarrow C_3H_5(1S)+H(S)$	1.000×10^{13}	75.4	[13-14]
R125	$C_3H_5(1S)+H(S) \Rightarrow C_3H_6(1S)$	3.700×10^{21}	48.8	[13-14]
R126	$C_3H_5(1S)+Pt(S) \Rightarrow C_2H_3(1S)+CH_2(S)$	3.700×10^{21}	108.2	[13-14]
R127	$C_2H_3(1S)+CH_2(S) \Rightarrow C_3H_5(1S)+Pt(S)$	3.700×10^{21}	32.0	[13-14]
R128	$CH_3(S)+O(S) \Rightarrow CH_2(S)+OH(S)$	3.700×10^{21}	36.6	[13-14]
R129	$CH_2(S)+OH(S) \Rightarrow CH_3(S)+O(S)$	3.700×10^{21}	251.0	[13-14]
R130	$CH_2(S)+O(S) \Rightarrow CH(S)+OH(S)$	3.700×10^{21}	251.0	[13-14]
R131	$CH(S)+OH(S) \Rightarrow CH_2(S)+O(S)$	3.700×10^{21}	252.0	[13-14]
R132	$CH(S)+O(S) \Rightarrow C(S)+OH(S)$	3.700×10^{21}	251.0	[13-14]

R133	C(S) +OH(S) =>CH(S) +O(S)	3.700×10^{21}	224.8	[13-14]
R134	C_2H_3(1S)+O(S) =>C_2H_3O(S)+Pt(S)	3.700×10^{19}	62.3	[13-14]
R135	C_2H_3O(S)+Pt(S) =>C_2H_3(1S)+O(S)	3.700×10^{21}	$90.0+45\theta_o$	[13-14]
R136	C_3H_6(2S)+Pt(S) =>C_3H_5(3S)+H(S)	2.000×10^{22}	99.1	[13-14]
R137	C_3H_5(3S)+H(S) =>C_3H_6(2S)+Pt(S)	3.700×10^{21}	75.3	[13-14]
R138	C_3H_5(3S)+Pt(S) =>C(S)+C_2H_5(S)	3.700×10^{21}	$46.9+50\theta_c$	[13-14]
R139	C(S)+C_2H_5(S) =>C_3H_5(3S)+Pt(S)	3.700×10^{21}	46.0	[13-14]
R140	C_4H_9(1S)+Pt(S) =>C_4H_8(4S)+H(S)	1.000×10^{22}	54.4	Est. [15-17]
R141	C_4H_8(4S)+H(S) =>C_4H_9(1S)+Pt(S)	1.000×10^{21}	29.3	Est. [15-17]
R142	C_4H_8(4S) =>C_4H_8(5S)	1.000×10^{13}	75.3	Est. [13-17]
R143	C_4H_8(5S) =>C_4H_8(4S)	1.000×10^{13}	83.3	Est. [13-16]
R144	C_4H_8(5S)+Pt(S) =>C_3H_5(2S)+CH_3(S)	1.000×10^{13}	89.0	Est. [13,19]
R145	C_3H_5(2S)+CH_3(S) =>C_4H_8(5S)+Pt(S)	1.000×10^{21}	14.5	Est. [13,19]
R146	C_3H_5(2S)+H(S) =>C_3H_6(1S)	3.700×10^{21}	48.8	[13-14]
R147	C_3H_6(1S) =>C_3H_5(2S)+H(S)	1.000×10^{13}	75.4	[13-14]
R148	C_4H_8(5S)+Pt(S) =>C_4H_7(4S)+H(S)	3.700×10^{21}	48.8	[15-17]
R149	C_4H_7(4S)+H(S) =>C_4H_8(5S)+Pt(S)	1.000×10^{13}	75.4	[15-17]
R150	C_4H_7(4S)+Pt(S) =>C_4H_6(4S)+H(S)	1.000×10^{22}	54.4	Est. [15-17]
R151	C_4H_6(4S)+H(S) =>C_4H_7(4S)+Pt(S)	1.000×10^{21}	29.3	Est. [15-17]
R152	C_4H_6(4S)+Pt(S) =>C_4H_5(2S)+H(S)	2.000×10^{22}	99.1	Est. [15-17]
R153	C_4H_5(2S)+H(S) =>C_4H_6(4S)+Pt(S)	3.700×10^{21}	75.3	Est. [15-17]
R154	C_4H_5(2S)+Pt(S) =>C(S)+C_3H_5(2S)	3.700×10^{21}	$46.9+50\theta_c$	Est. [13,19]
R155	C(S)+C_3H_5(2S) =>C_4H_5(2S)+Pt(S)	3.700×10^{21}	46.0	Est. [13,19]
R156	C_4H_6(4S) =>C_4H_6(5S)	1.000×10^{13}	75.3	Est. [13-14]
R157	C_4H_6(5S) =>C_4H_6(4S)	1.000×10^{13}	83.3	Est. [13-14]
R158	C_4H_8(4S)+Pt(S) =>C_4H_7(5S)+H(S)	2.000×10^{22}	99.1	[15-17]
R159	C_4H_7(5S)+H(S) =>C_4H_8(4S)+Pt(S)	3.700×10^{21}	75.3	[15-17]
R160	C_4H_7(5S)+Pt(S) =>C(S)+C_3H_7(1S)	3.700×10^{21}	$46.9+50\theta_c$	Est. [13,19]
R161	C(S)+C_3H_7(1S) =>C_4H_7(5S)+Pt(S)	3.700×10^{21}	46.0	Est. [13,19]
R162	C_4H_9(2S)+Pt(S) =>C_4H_8(6S)+H(S)	7.000×10^{12}	57.7	[15-17]
R163	C_4H_8(6S)+H(S) =>C_4H_9(2S)+Pt(S)	3.700×10^{21}	41.8	[15-17]
R164	C_4H_8(6S) =>C_4H_8(7S)	1.000×10^{13}	75.3	Est. [13-14]
R165	C_4H_8(7S) =>C_4H_8(6S)	1.000×10^{13}	83.3	Est. [13-14]
R166	C_4H_8(6S) =>C_4H_8(5S)	1.000×10^{13}	75.3	Est. [13-14]
R167	C_4H_8(5S) =>C_4H_8(6S)	1.000×10^{13}	83.3	Est. [13-14]
R168	C_4H_8(6S)+Pt(S) =>CH_3(S)+C_3H_5(3S)	1.000×10^{13}	89.0	Est. [13,19]
R169	CH_3(S)+C_3H_5(3S) =>C_4H_8(6S)+Pt(S)	1.000×10^{21}	14.5	Est. [13,19]
R170	C_4H_8(6S)+Pt(S) =>C_2H_3(1S)+C_2H_5(S)	1.000×10^{13}	89.0	Est. [13,19]
R171	C_2H_3(1S)+C_2H_5(S)=>C_4H_8(6S)+Pt(S)	1.000×10^{21}	14.5	Est. [13,19]

Units: S_0[-], A[s^{-1}, K^{-n}], Ea [kJ/mol]

a) S_0 represent the adsorption coefficient, A represent preexponential factor

b) Ea represent the activation energy

c) θ represent the coverage dependence

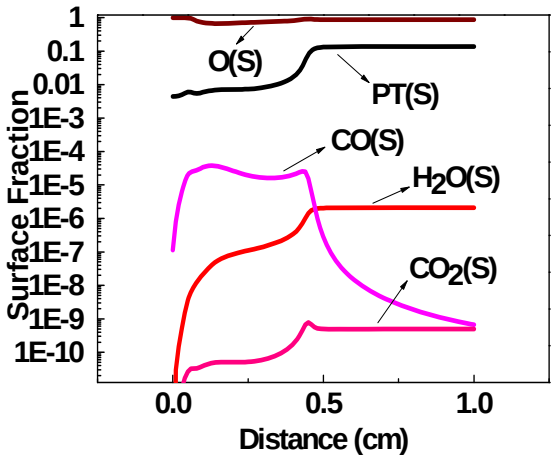

图 S1　CH_4:O_2 摩尔比为 0.05 时壁面组分的分布

Fig.S1　Distribution of surface species at mole ratio CH_4:O_2=0.05

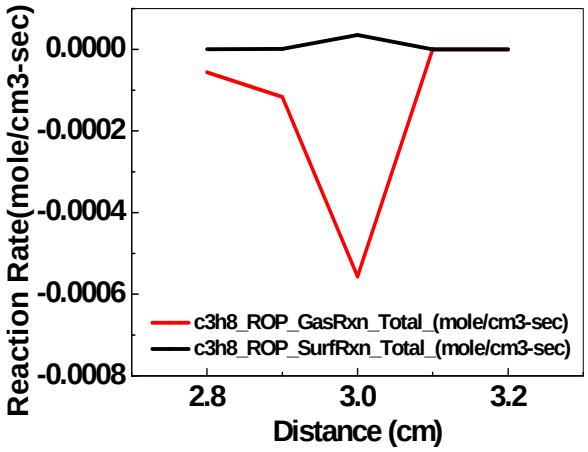

图 S2　丙烷的气相反应与壁面反应速率

Fig.S2　Gas and surface reaction rate of propane