Electronic supplementary information (ESI) for:

Matching precursor kinetics to afford a more robust CVD chemistry: a case study of the C chemistry for silicon carbide using SiF_4 as Si precursor

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Supporting Table 1. Chemical reaction scheme for the kinetic model.

		Forward reaction rate (cm^3, mol, s)			Backward reaction rate (cm^3, mol, s)			Ref.
	Reaction	**A**	**n**	**Ea/R (K)**	**A**	**n**	**Ea/R (K)**	
1	$H_2 + H_2 \rightleftharpoons H + H + H_2$	$9.033 \cdot 10^{14}$	0	48350	by equilibrium			1
2	$CH_3 + H_2 \rightleftharpoons CH_4 + H$	$1.084 \cdot 10^{3}$	2.88	4060	$6.142 \cdot 10^{5}$	2.50	4825	2
3	$CH_3 + CH_3 \rightleftharpoons C_2H_5 + H$	$5.420 \cdot 10^{13}$	0	8080	$3.613 \cdot 10^{13}$	0	0	2
4	$CH_3 + CH_3 + M \rightleftharpoons C_2H_6 + M$	Pressure dependent						2
	k_0	$1.269 \cdot 10^{41}$	-7.00	1390	$1.566 \cdot 10^{49}$	-8.37	47290	
	k_∞	$3.613 \cdot 10^{13}$	0	0	$4.500 \cdot 10^{21}$	-1.37	45900	
	Troe parameters: a ⇌ 0.62, T* = 1180, T*** = 73				a = 0.62, T* = 1180, T*** = 73			
5	$CH_4 + M \rightleftharpoons CH_3 + H + M$	Pressure dependent						1
	k_0	$7.226 \cdot 10^{17}$	0	47000	$6.467 \cdot 10^{23}$	-1.80	0	
	k_∞	$2.400 \cdot 10^{16}$	0	52800	$2.108 \cdot 10^{14}$	0	0	
	Troe parameters: a = 1, T* = 1350, T*** = 1, T** = 7830				a = 0.37, T* = 61, T*** = 3315			
6	$CH_4 + CH_3 \rightleftharpoons C_2H_5 + H_2$	$1.024 \cdot 10^{13}$	0	11500	by equilibrium			3
7	$C_2H_2 + H + M \rightleftharpoons C_2H_3 + M$	Pressure dependent						2
	k_0	$5.802 \cdot 10^{27}$	-3.47	475	$3.975 \cdot 10^{27}$	-3.50	18070	
	k_∞	$5.540 \cdot 10^{8}$	1.64	1055	$3.900 \cdot 10^{8}$	1.62	18650	
	Troe parameters: a = -0.98, T* = 6000, T*** = 10, T** = 0				a=-0.98, T*=6000, T***=10, T**=0			
8	$C_2H_2 + H_2 \rightleftharpoons C_2H_3 + H$	$2.409 \cdot 10^{12}$	0	32714	$1.204 \cdot 10^{13}$	0.00	0	4, 5
9	$C_2H_3 + H_2 \rightleftharpoons C_2H_4 + H$	$3.016 \cdot 10^{4}$	2.63	4306	$2.349 \cdot 10^{2}$	3.62	5670	4, 2
10	$C_2H_3 + CH_3 \rightleftharpoons C_2H_2 + CH_4$	$3.914 \cdot 10^{11}$	0	0	by equilibrium			4
11	$C_2H_3 + CH_3 \rightleftharpoons C_3H_6$	$1.000 \cdot 10^{10}$	1.00	0	$1.099 \cdot 10^{21}$	-1.20	49191	6
12	$C_2H_3 + CH_4 \rightleftharpoons C_2H_4 + CH_3$	$1.451 \cdot 10^{0}$	4.02	2754	$6.022 \cdot 10^{7}$	1.56	8370	4
13	$C_2H_3 + C_2H_3 \rightleftharpoons C_2H_4 + C_2H_2$	$8.431 \cdot 10^{13}$	0	0	$2.409 \cdot 10^{13}$	0	34398	2, 4
14	$C_2H_4 + M \rightleftharpoons C_2H_2 + H_2 + M$	$7.950 \cdot 10^{12}$	0.44	44741	by equilibrium			4
15	$C_2H_4 + M \rightleftharpoons C_2H_3 + H + M$	$2.589 \cdot 10^{17}$	0	48600	by equilibrium			2
16	$C_2H_4 + H + M \rightleftharpoons C_2H_5 + M$	$8.414 \cdot 10^{8}$	1.49	499	$4.900 \cdot 10^{9}$	1.19	18642	4
17	$C_2H_4 + H_2 \rightleftharpoons C_2H_5 + H$	$1.018 \cdot 10^{13}$	0	34278	$4.215 \cdot 10^{13}$	0	0	4, 2
18	$C_2H_4 + CH_3 \rightleftharpoons i\text{-}C_3H_7$	$4.600 \cdot 10^{4}$	1.00	2160	$1.995 \cdot 10^{10}$	0	14855	6, 7
19	$C_2H_4 + CH_3 \rightleftharpoons n\text{-}C_3H_7$	$2.200 \cdot 10^{8}$	1.00	2916	$9.550 \cdot 10^{13}$	0	15610	6, 7
20	$C_2H_4 + C_2H_4 \rightleftharpoons C_2H_5 + C_2H_3$	$4.818 \cdot 10^{14}$	0	35961	$4.818 \cdot 10^{11}$	0	0	20
21	$C_2H_5 + H \rightleftharpoons C_2H_6$	$5.446 \cdot 10^{13}$	0.16	0	$3.076 \cdot 10^{42}$	-7.93	55895	8, 9
22	$C_2H_5 + H_2 \rightleftharpoons C_2H_6 + H$	$3.071 \cdot 10^{0}$	3.60	4250	$1.445 \cdot 10^{9}$	1.50	3730	2, 5
23	$C_2H_5 + CH_3 \rightleftharpoons C_2H_4 + CH_4$	$9.033 \cdot 10^{11}$	0	0	by equilibrium			2
24	$C_2H_5 + CH_4 \rightleftharpoons C_2H_6 + CH_3$	$8.618 \cdot 10^{-2}$	4.14	6322	$1.506 \cdot 10^{-7}$	6.00	3043	4, 5
25	$C_2H_5 + C_2H_3 \rightleftharpoons C_2H_6 + C_2H_2$	$4.818 \cdot 10^{11}$	0	0	by equilibrium			4
26	$C_2H_5 + C_2H_4 \rightleftharpoons C_2H_6 + C_2H_3$	$4.878 \cdot 10^{-7}$	5.82	6000	$6.014 \cdot 10^{2}$	3.30	5280	2, 4
27	$C_2H_5 + C_2H_5 \rightleftharpoons C_2H_6 + C_2H_4$	$1.385 \cdot 10^{12}$	0	0	by equilibrium			2
28	$C_3H_6 + H \rightleftharpoons i\text{-}C_3H_7$	$1.319 \cdot 10^{13}$	0	785	$6.310 \cdot 10^{13}$	0	18581	10, 7
29	$C_3H_6 + H \rightleftharpoons n\text{-}C_3H_7$	$1.319 \cdot 10^{13}$	0	1636	$1.259 \cdot 10^{14}$	0	18632	10, 7
30	$C_3H_6 + C_2H_4 \rightleftharpoons i\text{-}C_3H_7 + C_2H_3$	$7.226 \cdot 10^{15}$	-0.65	37051	by equilibrium			10
31	$C_3H_6 + C_2H_4 \rightleftharpoons n\text{-}C_3H_7 + C_2H_3$	$6.022 \cdot 10^{13}$	0	37966	by equilibrium			10
32	$i\text{-}C_3H_7 + H \rightleftharpoons C_3H_6 + H_2$	$3.613 \cdot 10^{12}$	0	0	by equilibrium			11
33	$n\text{-}C_3H_7 + H \rightleftharpoons C_3H_6 + H_2$	$1.813 \cdot 10^{12}$	0	0	by equilibrium			11
34	$i\text{-}C_3H_7 + CH_3 \rightleftharpoons C_3H_6 + CH_4$	$9.408 \cdot 10^{10}$	0.68	0	by equilibrium			11
35	$n\text{-}C_3H_7 + CH_3 \rightleftharpoons C_3H_6 + CH_4$	$1.145 \cdot 10^{13}$	-0.32	0	by equilibrium			11
36	$i\text{-}C_3H_7 + C_2H_3 \rightleftharpoons C_3H_8 + C_2H_2$	$1.520 \cdot 10^{14}$	-0.70	0	by equilibrium			11
37	$n\text{-}C_3H_7 + C_2H_3 \rightleftharpoons C_3H_8 + C_2H_2$	$1.210 \cdot 10^{12}$	0	0	by equilibrium			11
38	$i\text{-}C_3H_7 + C_2H_4 \rightleftharpoons C_3H_6 + C_2H_5$	$2.650 \cdot 10^{10}$	0	3320	by equilibrium			11
39	$n\text{-}C_3H_7 + C_2H_4 \rightleftharpoons C_3H_6 + C_2H_5$	$2.650 \cdot 10^{9}$	0	3320	by equilibrium			11

40	$i\text{-}C_3H_7 + C_2H_5 \rightleftharpoons C_3H_6 + C_2H_6$	$2.300 \cdot 10^{13}$	-0.35	0	by equilibrium			11
41	$n\text{-}C_3H_7 + C_2H_5 \rightleftharpoons C_3H_6 + C_2H_6$	$1.451 \cdot 10^{12}$	0	0	by equilibrium			11
42	$i\text{-}C_3H_7 + C_2H_5 \rightleftharpoons C_3H_8 + C_2H_4$	$1.844 \cdot 10^{13}$	-0.35	0	by equilibrium			11
43	$n\text{-}C_3H_7 + C_2H_5 \rightleftharpoons C_3H_8 + C_2H_4$	$1.150 \cdot 10^{12}$	0	0	by equilibrium			11
44	$i\text{-}C_3H_7 + i\text{-}C_3H_7 \rightleftharpoons C_3H_8 + C_3H_6$	$2.529 \cdot 10^{12}$	0	0	by equilibrium			2
45	$i\text{-}C_3H_7 + n\text{-}C_3H_7 \rightleftharpoons C_3H_8 + C_3H_6$	$5.143 \cdot 10^{13}$	-0.35	0	by equilibrium			11
46	$n\text{-}C_3H_7 + n\text{-}C_3H_7 \rightleftharpoons C_3H_8 + C_3H_6$	$1.686 \cdot 10^{12}$	0	0	by equilibrium			11
47	$C_3H_8 \rightleftharpoons C_2H_5 + CH_3$	$1.100 \cdot 10^{17}$	0	42456	$3.673 \cdot 10^{13}$	0	0	5, 2
48	$C_3H_8 \rightleftharpoons i\text{-}C_3H_7 + H$	$7.200 \cdot 10^{14}$	-0.03	47958	$2.000 \cdot 10^{13}$	0	0	6
49	$C_3H_8 \rightleftharpoons n\text{-}C_3H_7 + H$	$7.600 \cdot 10^{15}$	-0.34	50356	$2.000 \cdot 10^{13}$	0	0	6
50	$C_3H_8 + H \rightleftharpoons i\text{-}C_3H_7 + H_2$	$8.700 \cdot 10^{6}$	2.00	2518	$7.800 \cdot 10^{12}$	0	7991	6
51	$C_3H_8 + H \rightleftharpoons n\text{-}C_3H_7 + H_2$	$5.600 \cdot 10^{7}$	2.00	3877	$9.100 \cdot 10^{12}$	0	7281	6
52	$C_3H_8 + CH_3 \rightleftharpoons i\text{-}C_3H_7 + CH_4$	$1.097 \cdot 10^{15}$	0	12659	$4.400 \cdot 10^{15}$	1.00	16174	7, 6
53	$C_3H_8 + CH_3 \rightleftharpoons n\text{-}C_3H_7 + CH_4$	$1.097 \cdot 10^{15}$	0	12659	$4.400 \cdot 10^{15}$	1.00	16174	7, 6
54	$C_3H_8 + C_2H_3 \rightleftharpoons i\text{-}C_3H_7 + C_2H_4$	$1.000 \cdot 10^{11}$	0	5237	by equilibrium			7
55	$C_3H_8 + C_2H_3 \rightleftharpoons n\text{-}C_3H_7 + C_2H_4$	$1.000 \cdot 10^{11}$	0	5237	by equilibrium			7
56	$C_3H_8 + C_2H_5 \rightleftharpoons i\text{-}C_3H_7 + C_2H_6$	$1.000 \cdot 10^{11}$	0	5237	by equilibrium			7
57	$C_3H_8 + C_2H_5 \rightleftharpoons n\text{-}C_3H_7 + C_2H_6$	$1.000 \cdot 10^{11}$	0	5237	by equilibrium			7
58	$C_3H_8 + i\text{-}C_3H_7 \rightleftharpoons C_3H_8 + n\text{-}C_3H_7$	$8.430 \cdot 10^{-3}$	4.20	4390	$8.400 \cdot 10^{-4}$	4.00	2381	11
59	$SiF_4 + H \rightleftharpoons SiF_3 + HF$	$1.402 \cdot 10^{10}$	1.54	29012	by equilibrium			calc.
60	$SiF_3 + H \rightleftharpoons SiHF_3$	$1.618 \cdot 10^{7}$	1.48	2.24	by equilibrium			calc.
61	$SiHF_3 \rightleftharpoons SiF_2 + HF$	$6.129 \cdot 10^{12}$	0.54	44230	by equilibrium			calc.
62	$SiHF_3 + HF \rightleftharpoons SiF_4 + H_2$	$3.593 \cdot 10^{3}$	2.51	15393	by equilibrium			calc.
63	$SiHF_3 + H \rightleftharpoons SiF_3 + H_2$	$6.893 \cdot 10^{8}$	1.76	3375	by equilibrium			calc.
64	$SiHF_3 + H \rightleftharpoons SiHF_2 + HF$	$2.189 \cdot 10^{9}$	1.58	28106	by equilibrium			calc.
65	$SiHF_2 \rightleftharpoons SiF + HF$	$1.706 \cdot 10^{12}$	0.51	33602	by equilibrium			calc.
66	$SiHF_2 \rightleftharpoons SiF_2 + H$	$5.758 \cdot 10^{12}$	0.38	18967	by equilibrium			calc.
67	$SiHF_2 + H \rightleftharpoons SiH_2F_2$	$3.207 \cdot 10^{13}$	0.58	45761	by equilibrium			calc.
68	$SiHF_2 + HF \rightleftharpoons SiF_3 + H_2$	$1.938 \cdot 10^{3}$	2.44	13513	by equilibrium			calc.
69	$SiH_2F_2 \rightleftharpoons SiF_2 + H_2$	$1.079 \cdot 10^{12}$	0.58	41421	by equilibrium			calc.
70	$SiH_2F_2 \rightleftharpoons SiHF + HF$	$3.164 \cdot 10^{12}$	0.57	45220	by equilibrium			calc.
71	$SiH_2F_2 + HF \rightleftharpoons SiHF_3 + H_2$	$3.549 \cdot 10^{3}$	2.45	13811	by equilibrium			calc.
72	$SiH_2F_2 + H \rightleftharpoons SiH_2F + HF$	$3.019 \cdot 10^{9}$	1.66	25835	by equilibrium			calc.
73	$SiH_2F_2 + H \rightleftharpoons SiHF_2 + H_2$	$4.712 \cdot 10^{8}$	1.76	2372	by equilibrium			calc.
74	$SiH_2F \rightleftharpoons SiF + H_2$	$3.667 \cdot 10^{11}$	0.62	24003	by equilibrium			calc.
75	$SiH_2F + H \rightleftharpoons SiH_3F$	$1.097 \cdot 10^{7}$	1.42	2.37	by equilibrium			calc.
76	$SiH_2F + HF \rightleftharpoons SiHF_2 + H_2$	$2.253 \cdot 10^{3}$	2.45	13784	by equilibrium			calc.
77	$SiH_3F \rightleftharpoons SiHF + H_2$	$1.729 \cdot 10^{12}$	0.58	32318	by equilibrium			calc.
78	$SiH_3F + H \rightleftharpoons SiH_2F + H_2$	$9.951 \cdot 10^{8}$	1.71	1814	by equilibrium			calc.
79	$SiH_3F + HF \rightleftharpoons SiH_2F_2 + H_2$	$1.029 \cdot 10^{4}$	2.38	13503	by equilibrium			calc.
80	$SiHF + H \rightleftharpoons SiH_2F$	$7.666 \cdot 10^{7}$	1.54	2.11	by equilibrium			calc.
81	$SiHF + HF \rightleftharpoons SiF_2 + H_2$	$3.956 \cdot 10^{3}$	2.37	1094	by equilibrium			calc.
82	$SiF + H \rightleftharpoons SiHF$	$1.236 \cdot 10^{9}$	1.28	1.52	by equilibrium			calc.
83	$Si + HF \rightleftharpoons SiF + H$	$1.963 \cdot 10^{8}$	1.59	9818	by equilibrium			calc.
84	$SiH_2 + HF \rightleftharpoons SiH_3F$	$1.620 \cdot 10^{4}$	2.38	2357	by equilibrium			calc.
85	$SiH_4 + HF \rightleftharpoons SiH_3F + H_2$	$1.097 \cdot 10^{5}$	2.39	16335	by equilibrium			calc.
86	$SiF_2 + H \rightleftharpoons SiF + HF$	$1.129 \cdot 10^{9}$	1.46	21938	by equilibrium			calc.
87	$SiHF + H \rightleftharpoons SiF + H_2$	$4.359 \cdot 10^{9}$	1.59	318	by equilibrium			calc.
88	$SiH_4 \rightleftharpoons SiH_2 + H_2$	$1.585 \cdot 10^{28}$	-4.79	30420	by equilibrium			12
89	$SiH_2 \rightleftharpoons Si + H_2$	$1.202 \cdot 10^{12}$	0.5	0	by equilibrium			12

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