Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information.

Visualization of the geometry optimized molecular structures for the adsorbates at vacancy sites of the H-saturated $(GaN)_{24}$ cluster that are listed in Table 1.

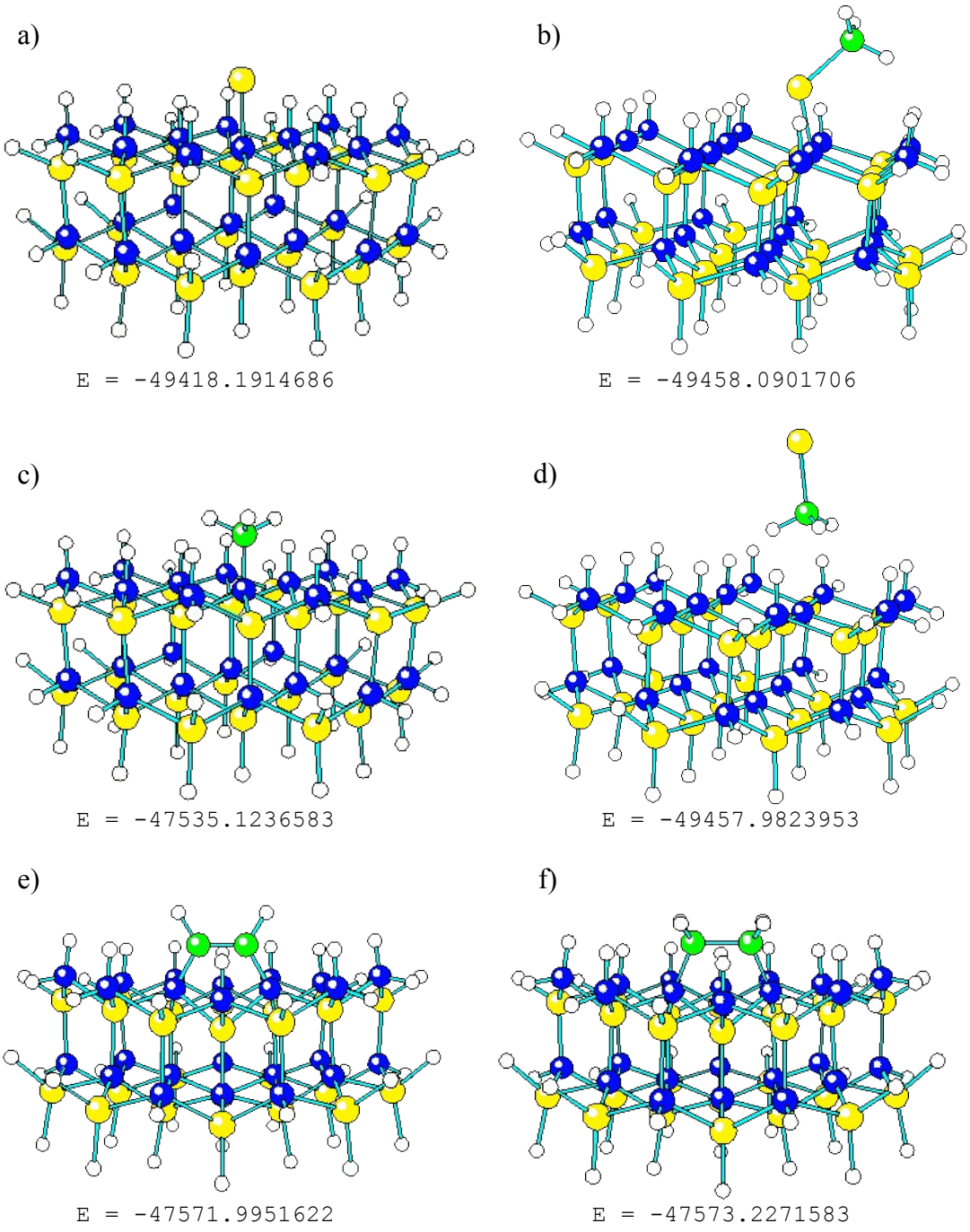

Fig. S1. a) Ga(ads), b) $GaCH_3$(ads), c) CH_3(ads), d) $GaCH_3$(ads), physisorbed at the CH_3 part, e) C_2H_2(ads), f) C_2H_4(ads). The B3LYP/6-31G(d,p) energies (in Hartrees) are given as inserts (the energy of the sole fully H-saturated (GaN)24 cluster is -47495.8123203 Hartree). Yellow: Ga, blue: N, green: C, white: H atoms.

Calculated molefractions of the most abundant species in the gas phase.

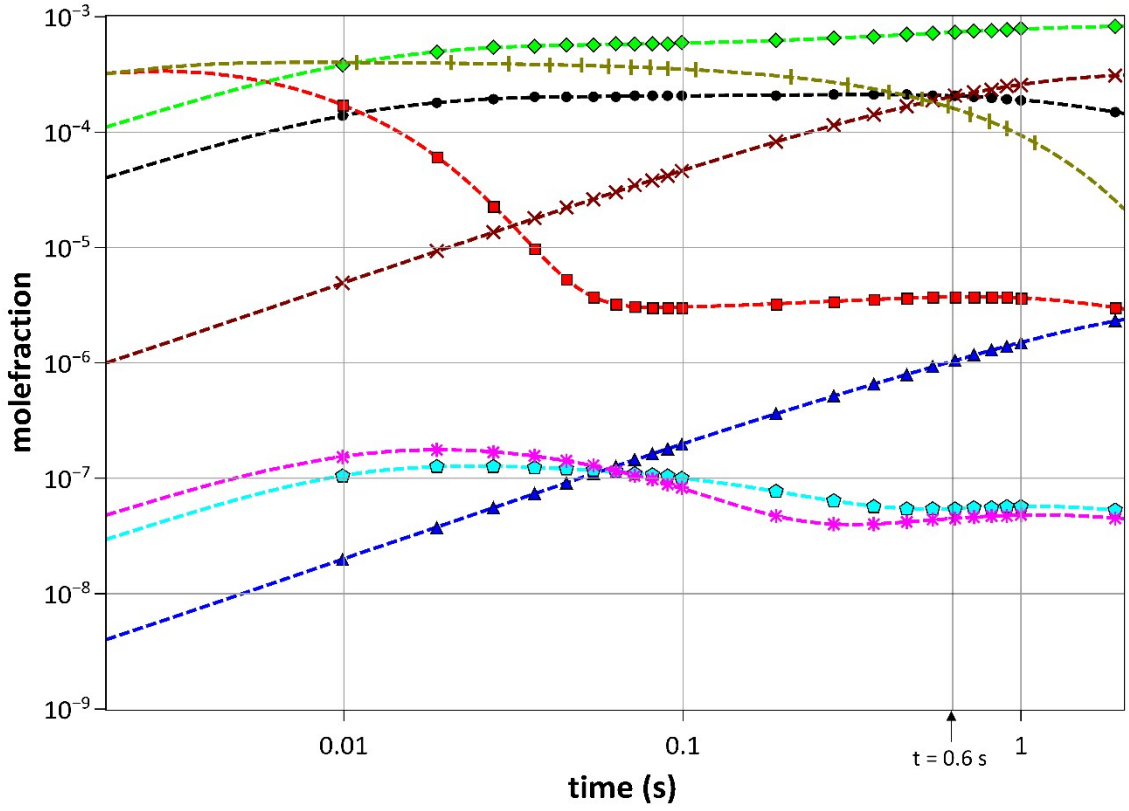

Fig. S2 Calculated molefractions of the most abundant species in the gas phase. (H_2, N_2, and NH_3 are omitted.) Process conditions: T = 1050°C, NH_3/TMGa = 157.
H (●), CH_3 (■), CH_4 (♦), C_2H_2 (▲), C_2H_4 (⌓), C_2H_6 (*), Ga (×), $GaCH_3$ (|).

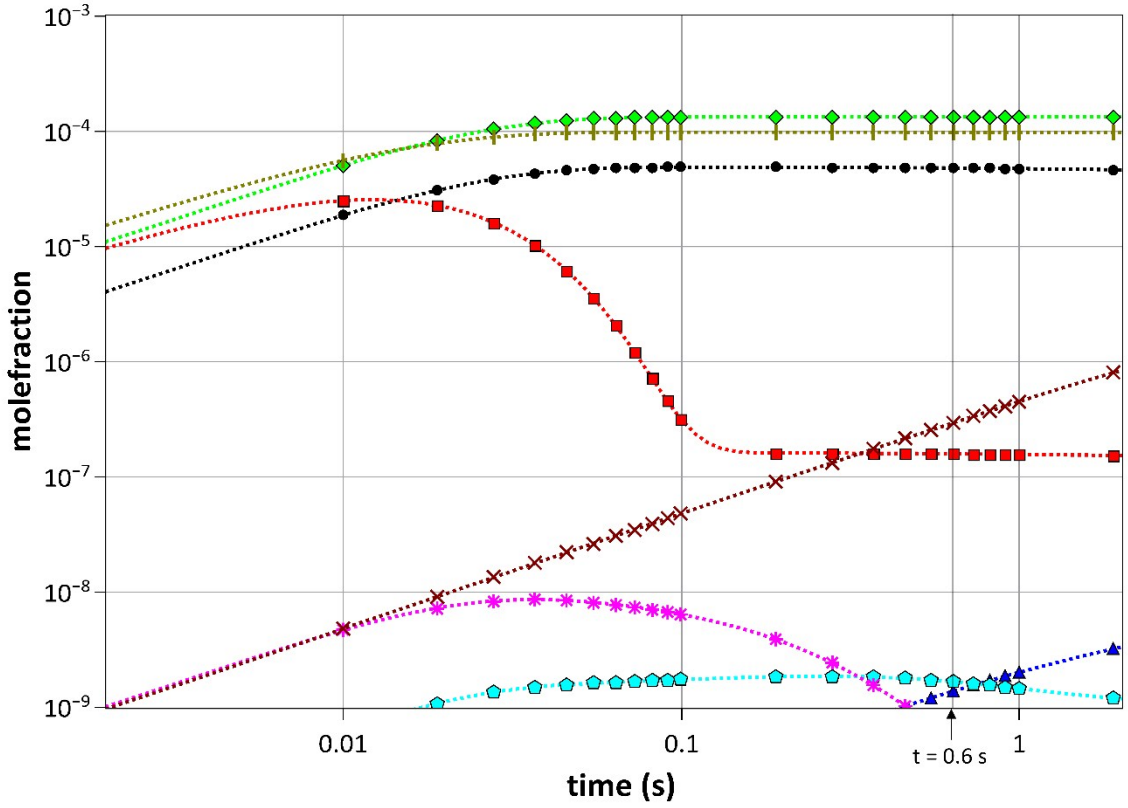

Fig. S3 Calculated molefractions of the most abundant species in the gas phase. (H_2, N_2, and NH_3 are omitted.) Process conditions: T = 800°C, NH_3/TMGa flow = 625.
H (●), CH_3 (■), CH_4 (♦), C_2H_2 (▲), C_2H_4 (⌓), C_2H_6 (*), Ga (×), $GaCH_3$ (|).

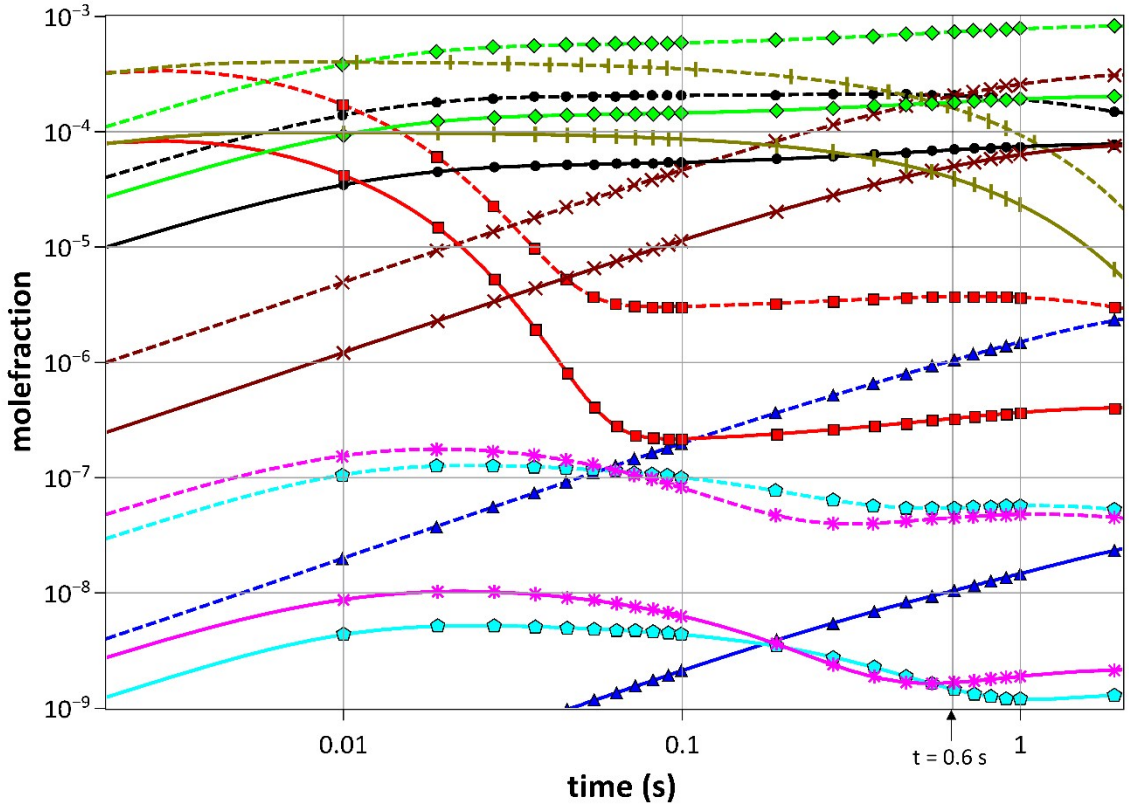

Fig. S4 Calculated molefractions of the most abundant species in the gas phase. (H_2, N_2, and NH_3 are omitted.) Comparing low and high TMGa flow rates at T = 1050°C: NH_3/TMGa = 625 (solid lines), NH_3/TMGa = 157 (dashed lines).
H (●), CH_3 (■), CH_4 (♦), C_2H_2 (▲), C_2H_4 (⌂), C_2H_6 (*), Ga (×), $GaCH_3$ (|).

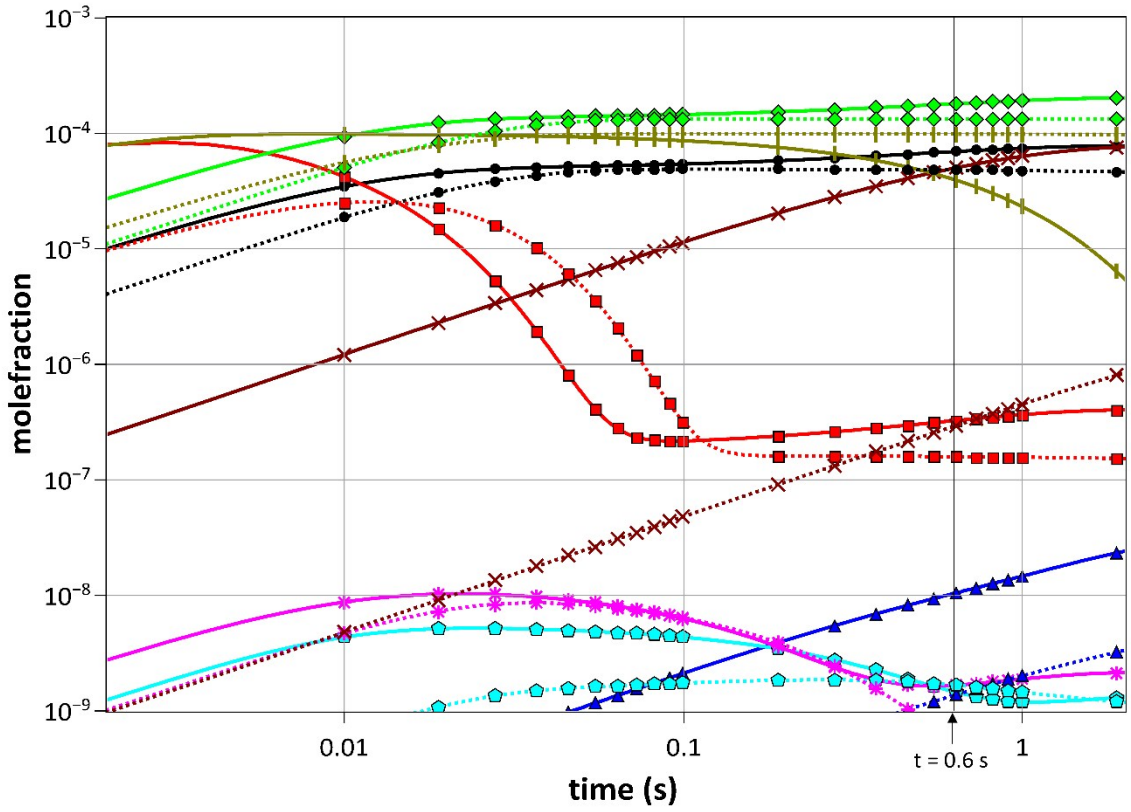

Fig. S5 Calculated molefractions of the most abundant species in the gas phase. (H_2, N_2, and NH_3 are omitted.) Comparing low and high process temperature at NH_3/TMGa = 625: T = 1050°C (solid lines), T = 800°C (dotted lines).
H (●), CH_3 (■), CH_4 (♦), C_2H_2 (▲), C_2H_4 (⌓), C_2H_6 (*), Ga (×), $GaCH_3$ (|).

Gas phase reaction schemes.

Table S1 Hydrocarbon reaction scheme. The rate constants are calculated using the modified Arrhenius expression format $k = AT^n e^{-E_a/RT}$.

	Reaction	A (m^3, mol, s)	n	Ea/R (K)	Ref.
1	$H_2 + CH \leftrightarrow CH_3$	$0.1445 \cdot 10^{12}$	0.00	1800	a
2	$CH + CH \leftrightarrow C_2H + H$	$0.1000 \cdot 10^{12}$	0.00	0	b
3	$CH + CH \leftrightarrow C_2H_2$	$0.1204 \cdot 10^{12}$	0.00	0	c
4	$CH_2^{(1)} \leftrightarrow CH + H$	$0.3771 \cdot 10^{16}$	0.00	45000	d
5	$CH_2^{(3)} \leftrightarrow CH + H$	$0.9394 \cdot 10^{16}$	0.00	45000	e
6	$H + CH_2^{(1)} \leftrightarrow H + CH_2^{(3)}$	$0.1000 \cdot 10^{12}$	0.00	0	f
7	$H_2 + CH_2^{(1)} \leftrightarrow H_2 + CH_2^{(3)}$	$0.6022 \cdot 10^{10}$	0.00	0	e
8	$CH_2^{(1)} + CH_4 \leftrightarrow CH_2^{(3)} + CH_4$	$0.1867 \cdot 10^{10}$	0.00	250	e
9	$C_2H_2 + CH_2^{(1)} \leftrightarrow C_2H_2 + CH_2^{(3)}$	$0.6624 \cdot 10^{13}$	-0.90	0	e
10	$CH_2^{(1)} + C_2H_4 \leftrightarrow CH_2^{(3)} + C_2H_4$	$0.1144 \cdot 10^{11}$	0.00	280	e
11	$CH_2^{(1)} + C_2H_6 \leftrightarrow CH_2^{(3)} + C_2H_6$	$0.2168 \cdot 10^{11}$	0.00	0	e
12	$CH_2^{(1)} + C_3H_6 \leftrightarrow CH_2^{(3)} + C_3H_6$	$0.3011 \cdot 10^{11}$	0.00	0	g
13	$H + CH_2^{(1)} \leftrightarrow H_2 + CH$	$0.3011 \cdot 10^{11}$	0.00	0	h
14	$H + CH_2^{(3)} \leftrightarrow H_2 + CH$	$0.1204 \cdot 10^{12}$	0.00	0	e
15	$H_2 + CH_2^{(1)} \leftrightarrow CH_3 + H$	$0.6022 \cdot 10^{11}$	0.00	0	e
16	$H_2 + CH_2^{(3)} \leftrightarrow CH_3 + H$	$0.5012 \cdot 10^{3}$	2.00	3600	i
17	$CH + CH_2^{(1)} \leftrightarrow H + C_2H_2$	$0.4000 \cdot 10^{11}$	0.00	0	j
18	$CH + CH_2^{(3)} \leftrightarrow H + C_2H_2$	$0.4000 \cdot 10^{11}$	0.00	0	j
19	$CH_2^{(1)} + CH_2^{(1)} \leftrightarrow H_2 + C_2H_2$	$0.3011 \cdot 10^{11}$	0.00	0	h
20	$CH_2^{(1)} + CH_2^{(3)} \leftrightarrow H_2 + C_2H_2$	$0.1807 \cdot 10^{11}$	0.00	0	h
21	$CH_2^{(3)} + CH_2^{(3)} \leftrightarrow H_2 + C_2H_2$	$0.1204 \cdot 10^{12}$	0.00	400	a
22	$CH_3 + M \leftrightarrow H + CH_2^{(1)} + M$	$0.1024 \cdot 10^{14}$	0.00	46000	e
23	$CH_3 + M \leftrightarrow H + CH_2^{(3)} + M$	$0.1024 \cdot 10^{14}$	0.00	46000	e
24	$H_2 + CH_3 \leftrightarrow H + CH_4$	$0.1084 \cdot 10^{1}$	2.88	4100	e
25	$CH + CH_3 \leftrightarrow H + C_2H_3$	$0.3000 \cdot 10^{11}$	0.00	0	j
26	$CH_3 + CH_2^{(1)} \leftrightarrow H + C_2H_4$	$0.1199 \cdot 10^{11}$	0.00	-290	i
27	$CH_3 + CH_2^{(3)} \leftrightarrow H + C_2H_4$	$0.7226 \cdot 10^{11}$	0.00	0	e
28	$CH_3 + CH_3 \leftrightarrow H + C_2H_5$	$0.5420 \cdot 10^{11}$	0.00	8100	e
29	$CH_3 + CH_3 + M \rightarrow C_2H_6 + M$	$0.3613 \cdot 10^{8}$	0.00	0	e
30	$C_2H_6 + M \rightarrow 2.0\ CH_3 + M$	$0.4500 \cdot 10^{19}$	-1.37	46000	e
31	$CH_4 + M \rightarrow CH_3 + H + M$	$0.2400 \cdot 10^{14}$	0.00	53000	k
32	$CH_3 + H + M \rightarrow CH_4 + M$	$0.2108 \cdot 10^{9}$	0.00	0	k
33	$CH + CH_4 \leftrightarrow CH_3 + CH_2^{(1)}$	$0.1325 \cdot 10^{14}$	-0.94	29	e
34	$CH + CH_4 \leftrightarrow CH_3 + CH_2^{(3)}$	$0.1325 \cdot 10^{14}$	-0.94	29	e
35	$CH + CH_4 \leftrightarrow H + C_2H_4$	$0.1325 \cdot 10^{14}$	-0.94	29	e
36	$CH + CH_4 \leftrightarrow C_2H_5$	$0.1626 \cdot 10^{12}$	0.00	0	l
37	$CH_2^{(1)} + CH_4 \leftrightarrow 2.0\ CH_3$	$0.9334 \cdot 10^{10}$	0.00	250	e
38	$CH_2^{(3)} + CH_4 \leftrightarrow 2.0\ CH_3$	$0.2455 \cdot 10^{4}$	2.00	4200	i
39	$CH_2^{(1)} + CH_4 \leftrightarrow H + C_2H_5$	$0.7467 \cdot 10^{10}$	0.00	250	e

40	$CH_2^{(3)} + CH_4 \leftrightarrow H + C_2H_5$	$0.1964 \cdot 10^4$	2.00	4200	est.
41	$CH_2^{(1)} + CH_4 \leftrightarrow C_2H_6$	$0.5687 \cdot 10^{10}$	0.00	0	est.
42	$CH_2^{(3)} + CH_4 \leftrightarrow C_2H_6$	$0.4550 \cdot 10^{10}$	0.00	0	est.
43	$CH_3 + CH_4 \leftrightarrow H_2 + C_2H_5$	$0.1024 \cdot 10^{11}$	0.00	12000	m
44	$H_2 + C_2H \leftrightarrow H + C_2H_2$	$0.2108 \cdot 10^4$	2.32	440	e
45	$C_2H + CH_2^{(1)} \leftrightarrow CH + C_2H_2$	$0.1807 \cdot 10^{11}$	0.00	0	h
46	$C_2H + CH_2^{(3)} \leftrightarrow CH + C_2H_2$	$0.1807 \cdot 10^{11}$	0.00	0	h
47	$CH_3 + C_2H \leftrightarrow H + C_3H_3$	$0.2409 \cdot 10^{11}$	0.00	0	h
48	$C_2H + CH_4 \leftrightarrow CH_3 + C_2H_2$	$0.2168 \cdot 10^8$	0.94	330	e
49	$C_2H_2 + M \leftrightarrow C_2H + H + M$	$0.2630 \cdot 10^{13}$	0.00	62000	h
50	$H + C_2H_2 + M \rightarrow C_2H_3 + M$	$0.5540 \cdot 10^3$	1.64	1100	e
51	$C_2H_3 + M \rightarrow H + C_2H_2 + M$	$0.3900 \cdot 10^6$	1.62	19000	e
52	$H_2 + C_2H_2 \leftrightarrow H + C_2H_3$	$0.2409 \cdot 10^{10}$	0.00	33000	h
53	$CH + C_2H_2 \leftrightarrow H + C_3H_2$	$0.1000 \cdot 10^{12}$	0.00	0	j
54	$C_2H_2 + CH_2^{(1)} \leftrightarrow H + C_3H_3$	$0.2698 \cdot 10^{14}$	-0.90	0	e
55	$C_2H_2 + CH_2^{(3)} \leftrightarrow H + C_3H_3$	$0.1204 \cdot 10^{11}$	0.00	3300	e
56	$C_2H_2 + CH_2^{(1)} + M \leftrightarrow C_3H_4A + M$	$0.2698 \cdot 10^{11}$	-0.90	0	e
57	$C_2H_2 + CH_2^{(1)} + M \leftrightarrow C_3H_4P + M$	$0.6745 \cdot 10^{10}$	-0.90	0	e
58	$C_2H_2 + CH_2^{(3)} + M \leftrightarrow C_3H_4A + M$	$0.1204 \cdot 10^8$	0.00	3300	e
59	$C_2H_2 + CH_2^{(3)} + M \leftrightarrow C_3H_4P + M$	$0.3312 \cdot 10^{10}$	0.00	4600	e
60	$CH_3 + C_2H_2 \leftrightarrow H + C_3H_4A$	$0.5160 \cdot 10^7$	0.86	11000	n
61	$CH_3 + C_2H_2 \leftrightarrow H + C_3H_4P$	$0.2561 \cdot 10^7$	1.10	6900	n
62	$CH_3 + C_2H_2 \leftrightarrow CH_2CHCH_2$	$0.1396 \cdot 10^2$	2.21	8300	o
63	$C_2H_2 + C_2H_2 \leftrightarrow C_2H + C_2H_3$	$0.9635 \cdot 10^{10}$	0.00	42000	h
64	$H_2 + C_2H_3 \leftrightarrow H + C_2H_4$	$0.3016 \cdot 10^2$	2.63	4300	h
65	$CH + C_2H_3 \leftrightarrow C_2H_2 + CH_2^{(1)}$	$0.5000 \cdot 10^{11}$	0.00	0	est.
66	$CH + C_2H_3 \leftrightarrow C_2H_2 + CH_2^{(3)}$	$0.5000 \cdot 10^{11}$	0.00	0	j
67	$CH_2^{(1)} + C_2H_3 \leftrightarrow CH_3 + C_2H_2$	$0.1807 \cdot 10^{11}$	0.00	0	h
68	$CH_2^{(3)} + C_2H_3 \leftrightarrow CH_3 + C_2H_2$	$0.1807 \cdot 10^{11}$	0.00	0	h
69	$CH_3 + C_2H_3 \leftrightarrow C_2H_2 + CH_4$	$0.3914 \cdot 10^9$	0.00	0	h
70	$CH_3 + C_2H_3 \leftrightarrow C_3H_6$	$0.1000 \cdot 10^8$	1.00	0	p
71	$CH_4 + C_2H_3 \leftrightarrow CH_3 + C_2H_4$	$0.1451 \cdot 10^{-2}$	4.02	2800	h
72	$C_2H_3 + C_2H_3 \leftrightarrow C_2H_2 + C_2H_4$	$0.8431 \cdot 10^{11}$	0.00	0	e
73	$C_2H_4 + M \leftrightarrow H_2 + C_2H_2 + M$	$0.7950 \cdot 10^{10}$	0.44	45000	h
74	$C_2H_4 + M \leftrightarrow H + C_2H_3 + M$	$0.2589 \cdot 10^{15}$	0.00	49000	e
75	$H + C_2H_4 + M \leftrightarrow C_2H_5 + M$	$0.8414 \cdot 10^3$	1.49	500	h
76	$H_2 + C_2H_4 \leftrightarrow H + C_2H_5$	$0.1018 \cdot 10^{11}$	0.00	34000	h
77	$CH_2^{(1)} + C_2H_4 \leftrightarrow H + CH_2CHCH_2$	$0.4529 \cdot 10^{11}$	0.00	-280	e
78	$CH_2^{(3)} + C_2H_4 \leftrightarrow H + CH_2CHCH_2$	$0.3192 \cdot 10^{11}$	0.00	2700	e
79	$CH_2^{(1)} + C_2H_4 + M \leftrightarrow C_3H_6 + M$	$0.5661 \cdot 10^8$	0.00	-280	e
80	$CH_2^{(3)} + C_2H_4 + M \leftrightarrow C_3H_6 + M$	$0.3192 \cdot 10^8$	0.00	2700	e
81	$CH_3 + C_2H_4 \leftrightarrow i\text{-}C_3H_7$	$0.4600 \cdot 10^2$	1.00	2200	p
82	$CH_3 + C_2H_4 \leftrightarrow n\text{-}C_3H_7$	$0.2200 \cdot 10^6$	1.00	2900	p
83	$C_2H_4 + C_2H_4 \leftrightarrow C_2H_3 + C_2H_5$	$0.4818 \cdot 10^{12}$	0.00	36000	h
84	$H + C_2H_5 \leftrightarrow C_2H_6$	$0.5440 \cdot 10^{11}$	0.16	0	q

85	$H_2 + C_2H_5 \leftrightarrow H + C_2H_6$	$0.3071 \cdot 10^{-2}$	3.60	4200	e
86	$CH_2^{(1)} + C_2H_5 \leftrightarrow CH_3 + C_2H_4$	$0.9033 \cdot 10^{10}$	0.00	0	h
87	$CH_2^{(3)} + C_2H_5 \leftrightarrow CH_3 + C_2H_4$	$0.1807 \cdot 10^{11}$	0.00	0	h
88	$CH_2^{(1)} + C_2H_5 \leftrightarrow H + C_3H_6$	$0.9033 \cdot 10^{10}$	0.00	0	h
89	$CH_2^{(3)} + C_2H_5 \leftrightarrow H + C_3H_6$	$0.1807 \cdot 10^{11}$	0.00	0	est.
90	$CH_3 + C_2H_5 \leftrightarrow CH_4 + C_2H_4$	$0.9033 \cdot 10^{9}$	0.00	0	e
91	$CH_4 + C_2H_5 \leftrightarrow CH_3 + C_2H_6$	$0.8618 \cdot 10^{-4}$	4.14	6300	h
92	$C_2H + C_2H_5 \leftrightarrow C_2H_2 + C_2H_4$	$0.1807 \cdot 10^{10}$	0.00	0	h
93	$C_2H + C_2H_5 \leftrightarrow CH_3 + C_3H_3$	$0.1813 \cdot 10^{11}$	0.00	0	h
94	$C_2H_2 + C_2H_5 \leftrightarrow C_2H + C_2H_6$	$0.2710 \cdot 10^{9}$	0.00	12000	h
95	$C_2H_3 + C_2H_5 \leftrightarrow C_2H_2 + C_2H_6$	$0.4818 \cdot 10^{9}$	0.00	0	h
96	$C_2H_4 + C_2H_5 \leftrightarrow C_2H_6 + C_2H_3$	$0.4878 \cdot 10^{-9}$	5.82	6000	e
97	$C_2H_5 + C_2H_5 \leftrightarrow C_2H_4 + C_2H_6$	$0.1385 \cdot 10^{10}$	0.00	0	e
98	$CH_2^{(1)} + C_2H_6 \leftrightarrow CH_3 + C_2H_5$	$0.3981 \cdot 10^{11}$	0.00	-280	i
99	$CH_2^{(3)} + C_2H_6 \leftrightarrow CH_3 + C_2H_5$	$0.1807 \cdot 10^{3}$	0.00	0	h
100	$H + C_3H_2 \leftrightarrow C_3H_3$	$0.7600 \cdot 10^{11}$	0.22	-44	r
101	$CH_2^{(1)} + C_3H_2 \leftrightarrow 2.0\ C_2H_2$	$0.1995 \cdot 10^{10}$	0.00	0	est.
102	$CH_2^{(3)} + C_3H_2 \leftrightarrow 2.0\ C_2H_2$	$0.1995 \cdot 10^{10}$	0.00	0	f
103	$H + C_3H_3 \leftrightarrow CH + C_2H_3$	$0.4348 \cdot 10^{11}$	0.00	0	s
104	$H + C_3H_3 \leftrightarrow H_2 + C_3H_2$	$0.1000 \cdot 10^{11}$	0.00	0	f
105	$H + C_3H_3 \leftrightarrow C_3H_4A$	$0.2002 \cdot 10^{11}$	0.21	-87	r
106	$H + C_3H_3 \leftrightarrow C_3H_4P$	$0.6473 \cdot 10^{11}$	0.10	-16	r
107	$C_3H_4P \leftrightarrow C_3H_4A$	$0.1700 \cdot 10^{15}$	0.00	34000	t
108	$H + C_3H_4A \leftrightarrow H_2 + C_3H_3$	$0.5012 \cdot 10^{4}$	2.00	3000	f
109	$H + C_3H_4P \leftrightarrow H_2 + C_3H_3$	$0.1995 \cdot 10^{12}$	2.00	7600	f
110	$H + C_3H_4A \leftrightarrow H + C_3H_4P$	$0.2512 \cdot 10^{11}$	0.00	0	f
111	$H + C_3H_4A \leftrightarrow CH_2CHCH_2$	$0.4000 \cdot 10^{10}$	0.00	1400	u
112	$H + C_3H_4P \leftrightarrow CH_2CHCH_2$	$0.1999 \cdot 10^{11}$	0.00	1200	v
113	$CH_3 + C_3H_4A \leftrightarrow CH_4 + C_3H_3$	$0.6607 \cdot 10^{-6}$	5.00	4200	f
114	$CH_3 + C_3H_4P \leftrightarrow CH_4 + C_3H_3$	$0.2188 \cdot 10^{-6}$	5.00	4200	f
115	$C_2H + C_3H_4P \leftrightarrow C_2H_2 + C_3H_3$	$0.9997 \cdot 10^{10}$	0.00	0	u
116	$H + CH_2CHCH_2 \leftrightarrow CH_3 + C_2H_3$	$0.1807 \cdot 10^{11}$	0.00	0	e
117	$H + CH_2CHCH_2 \leftrightarrow H_2 + C_3H_4A$	$0.1807 \cdot 10^{11}$	0.00	0	e
118	$H + CH_2CHCH_2 \leftrightarrow H_2 + C_3H_4P$	$0.1807 \cdot 10^{11}$	0.00	0	est.
119	$H + CH_2CHCH_2 \leftrightarrow C_3H_6$	$0.5701 \cdot 10^{11}$	0.18	-63	r
120	$H_2 + CH_2CHCH_2 \leftrightarrow H + C_3H_6$	$0.1084 \cdot 10^{3}$	2.40	9600	e
121	$CH_2^{(1)} + CH_2CHCH_2 \leftrightarrow C_2H_4 + C_2H_3$	$0.4818 \cdot 10^{11}$	0.00	0	g
122	$CH_2^{(3)} + CH_2CHCH_2 \leftrightarrow C_2H_4 + C_2H_3$	$0.7528 \cdot 10^{10}$	0.00	0	g
123	$CH_3 + CH_2CHCH_2 \leftrightarrow CH_4 + C_3H_4A$	$0.3009 \cdot 10^{10}$	-0.32	-66	g
124	$CH_3 + CH_2CHCH_2 \leftrightarrow CH_4 + C_3H_4P$	$0.3613 \cdot 10^{9}$	0.00	0	e
125	$CH_4 + CH_2CHCH_2 \leftrightarrow CH_3 + C_3H_6$	$0.3975 \cdot 10^{-1}$	3.40	12000	e
126	$C_2H + CH_2CHCH_2 \leftrightarrow C_2H_3 + C_3H_3$	$0.1204 \cdot 10^{23}$	0.00	0	g
127	$C_2H + CH_2CHCH_2 \leftrightarrow C_2H_2 + C_3H_4A$	$0.9033 \cdot 10^{20}$	0.00	0	g
128	$C_2H_3 + CH_2CHCH_2 \leftrightarrow C_2H_4 + C_3H_4A$	$0.2409 \cdot 10^{10}$	0.00	0	g
129	$C_2H_3 + CH_2CHCH_2 \leftrightarrow C_2H_2 + C_3H_6$	$0.4818 \cdot 10^{10}$	0.00	0	g

130	$C_2H_4 + CH_2CHCH_2 \leftrightarrow C_3H_6 + C_2H_3$	$0.3975 \cdot 10^{-1}$	3.40	13000	e
131	$C_2H_5 + CH_2CHCH_2 \leftrightarrow C_2H_6 + C_3H_4A$	$0.9635 \cdot 10^{9}$	0.00	-66	e
132	$C_2H_5 + CH_2CHCH_2 \leftrightarrow C_2H_4 + C_3H_6$	$0.2589 \cdot 10^{10}$	0.00	-66	e
133	$C_2H_6 + CH_2CHCH_2 \leftrightarrow C_3H_6 + C_2H_5$	$0.2349 \cdot 10^{0}$	3.30	10000	e
134	$CH_2CHCH_2 + CH_2CHCH_2 \leftrightarrow C_3H_6 + C_3H_4A$	$0.6022 \cdot 10^{8}$	0.00	0	e
135	$H + C_3H_6 \leftrightarrow i\text{-}C_3H_7$	$0.1319 \cdot 10^{11}$	0.00	780	g
136	$H + C_3H_6 \leftrightarrow n\text{-}C_3H_7$	$0.1319 \cdot 10^{11}$	0.00	1600	g
137	$CH_2^{(1)} + C_3H_6 \leftrightarrow CH_3 + CH_2CHCH_2$	$0.5239 \cdot 10^{11}$	0.00	0	g
138	$CH_2^{(3)} + C_3H_6 \leftrightarrow CH_3 + CH_2CHCH_2$	$0.7226 \cdot 10^{9}$	0.00	3100	g
139	$C_2H + C_3H_6 \leftrightarrow C_2H_3 + C_3H_4P$	$0.1210 \cdot 10^{11}$	0.00	0	g
140	$C_2H + C_3H_6 \leftrightarrow C_2H_2 + CH_2CHCH_2$	$0.3607 \cdot 10^{10}$	0.00	0	g
141	$C_2H_4 + C_3H_6 \leftrightarrow C_2H_3 + i\text{-}C_3H_7$	$0.7226 \cdot 10^{13}$	-0.65	37000	g
142	$C_2H_4 + C_3H_6 \leftrightarrow C_2H_3 + n\text{-}C_3H_7$	$0.6022 \cdot 10^{11}$	0.00	38000	g
143	$H + i\text{-}C_3H_7 \leftrightarrow H_2 + C_3H_6$	$0.3613 \cdot 10^{10}$	0.00	0	w
144	$H + n\text{-}C_3H_7 \leftrightarrow H_2 + C_3H_6$	$0.1813 \cdot 10^{10}$	0.00	0	w
145	$CH_2^{(1)} + i\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_2H_5$	$0.3115 \cdot 10^{11}$	0.00	0	est.
146	$CH_2^{(1)} + n\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_2H_5$	$0.2710 \cdot 10^{11}$	0.00	0	w
147	$CH_2^{(3)} + i\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_2H_5$	$0.3011 \cdot 10^{12}$	0.00	0	est.
148	$CH_2^{(3)} + n\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_2H_5$	$0.1807 \cdot 10^{11}$	0.00	0	w
149	$CH_2^{(1)} + i\text{-}C_3H_7 \leftrightarrow CH_3 + C_3H_6$	$0.1038 \cdot 10^{11}$	0.00	0	w
150	$CH_2^{(1)} + n\text{-}C_3H_7 \leftrightarrow CH_3 + C_3H_6$	$0.9033 \cdot 10^{10}$	0.00	0	w
151	$CH_2^{(3)} + i\text{-}C_3H_7 \leftrightarrow CH_3 + C_3H_6$	$0.3011 \cdot 10^{11}$	0.00	0	w
152	$CH_2^{(3)} + n\text{-}C_3H_7 \leftrightarrow CH_3 + C_3H_6$	$0.1807 \cdot 10^{10}$	0.00	0	w
153	$CH_3 + i\text{-}C_3H_7 \leftrightarrow CH_4 + C_3H_6$	$0.9408 \cdot 10^{8}$	0.68	0	w
154	$CH_3 + n\text{-}C_3H_7 \leftrightarrow CH_4 + C_3H_6$	$0.1145 \cdot 10^{11}$	-0.32	0	w
155	$C_2H + i\text{-}C_3H_7 \leftrightarrow C_2H_5 + C_3H_3$	$0.7250 \cdot 10^{10}$	0.00	0	est.
156	$C_2H + n\text{-}C_3H_7 \leftrightarrow C_2H_5 + C_3H_3$	$0.1210 \cdot 10^{11}$	0.00	0	w
157	$C_2H + i\text{-}C_3H_7 \leftrightarrow C_2H_2 + C_3H_6$	$0.3607 \cdot 10^{10}$	0.00	0	w
158	$C_2H + n\text{-}C_3H_7 \leftrightarrow C_2H_2 + C_3H_6$	$0.6022 \cdot 10^{10}$	0.00	0	w
159	$C_2H_3 + i\text{-}C_3H_7 \leftrightarrow C_2H_2 + C_3H_8$	$0.1520 \cdot 10^{12}$	-0.70	0	w
160	$C_2H_3 + n\text{-}C_3H_7 \leftrightarrow C_2H_2 + C_3H_8$	$0.1210 \cdot 10^{10}$	0.00	0	w
161	$C_2H_4 + i\text{-}C_3H_7 \leftrightarrow C_3H_6 + C_2H_5$	$0.2650 \cdot 10^{8}$	0.00	3300	w
162	$C_2H_4 + n\text{-}C_3H_7 \leftrightarrow C_3H_6 + C_2H_5$	$0.2650 \cdot 10^{7}$	0.00	3300	est.
163	$C_2H_5 + i\text{-}C_3H_7 \leftrightarrow C_2H_6 + C_3H_6$	$0.2300 \cdot 10^{11}$	-0.35	0	w
164	$C_2H_5 + n\text{-}C_3H_7 \leftrightarrow C_2H_6 + C_3H_6$	$0.1451 \cdot 10^{10}$	0.00	0	w
165	$C_2H_5 + i\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_3H_8$	$0.1844 \cdot 10^{11}$	-0.35	0	w
166	$C_2H_5 + n\text{-}C_3H_7 \leftrightarrow C_2H_4 + C_3H_8$	$0.1150 \cdot 10^{10}$	0.00	0	w
167	$CH_2CHCH_2 + i\text{-}C_3H_7 \leftrightarrow 2.0\ C_3H_6$	$0.2291 \cdot 10^{11}$	-0.35	-66	g
168	$CH_2CHCH_2 + n\text{-}C_3H_7 \leftrightarrow 2.0\ C_3H_6$	$0.1451 \cdot 10^{10}$	0.00	-66	g
169	$CH_2CHCH_2 + i\text{-}C_3H_7 \leftrightarrow C_3H_4A + C_3H_8$	$0.4600 \cdot 10^{10}$	-0.35	-66	g
170	$CH_2CHCH_2 + n\text{-}C_3H_7 \leftrightarrow C_3H_4A + C_3H_8$	$0.7226 \cdot 10^{9}$	0.00	-66	g
171	$i\text{-}C_3H_7 + i\text{-}C_3H_7 \leftrightarrow C_3H_6 + C_3H_8$	$0.2529 \cdot 10^{10}$	0.00	0	e
172	$i\text{-}C_3H_7 + n\text{-}C_3H_7 \leftrightarrow C_3H_6 + C_3H_8$	$0.1602 \cdot 10^{10}$	0.00	0	v
173	$n\text{-}C_3H_7 + n\text{-}C_3H_7 \leftrightarrow C_3H_6 + C_3H_8$	$0.1692 \cdot 10^{10}$	0.00	0	w
174	$C_3H_8 \leftrightarrow CH_3 + C_2H_5$	$0.1100 \cdot 10^{18}$	0.00	42000	a

175	$C_3H_8 \leftrightarrow H + i\text{-}C_3H_7$	$0.7200 \cdot 10^{15}$	-0.03	48000	p
176	$C_3H_8 \leftrightarrow H + n\text{-}C_3H_7$	$0.7600 \cdot 10^{16}$	-0.34	50000	p
177	$H + C_3H_8 \leftrightarrow H_2 + i\text{-}C_3H_7$	$0.8700 \cdot 10^{4}$	2.00	2300	p
178	$H + C_3H_8 \leftrightarrow H_2 + n\text{-}C_3H_7$	$0.5600 \cdot 10^{5}$	2.00	3900	p
179	$CH_2^{(1)} + C_3H_8 \leftrightarrow CH_3 + i\text{-}C_3H_7$	$0.4276 \cdot 10^{11}$	0.00	0	w
180	$CH_2^{(3)} + C_3H_8 \leftrightarrow CH_3 + i\text{-}C_3H_7$	$0.1506 \cdot 10^{-2}$	3.46	3800	w
181	$CH_2^{(1)} + C_3H_8 \leftrightarrow CH_3 + n\text{-}C_3H_7$	$0.1000 \cdot 10^{12}$	0.00	0	est.
182	$CH_2^{(3)} + C_3H_8 \leftrightarrow CH_3 + n\text{-}C_3H_7$	$0.9033 \cdot 10^{-3}$	3.65	3600	w
183	$CH_3 + C_3H_8 \leftrightarrow CH_4 + i\text{-}C_3H_7$	$0.1097 \cdot 10^{13}$	0.00	13000	j
184	$CH_3 + C_3H_8 \leftrightarrow CH_4 + n\text{-}C_3H_7$	$0.1097 \cdot 10^{13}$	0.00	13000	j
185	$C_2H + C_3H_8 \leftrightarrow C_2H_2 + i\text{-}C_3H_7$	$0.1210 \cdot 10^{10}$	0.00	0	w
186	$C_2H + C_3H_8 \leftrightarrow C_2H_2 + n\text{-}C_3H_7$	$0.3607 \cdot 10^{10}$	0.00	0	w
187	$C_2H_3 + C_3H_8 \leftrightarrow C_2H_4 + i\text{-}C_3H_7$	$0.1000 \cdot 10^{9}$	0.00	5200	j
188	$C_2H_3 + C_3H_8 \leftrightarrow C_2H_4 + n\text{-}C_3H_7$	$0.1000 \cdot 10^{9}$	0.00	5200	j
189	$C_2H_5 + C_3H_8 \leftrightarrow C_2H_6 + i\text{-}C_3H_7$	$0.1000 \cdot 10^{9}$	0.00	5200	j
190	$C_2H_5 + C_3H_8 \leftrightarrow C_2H_6 + n\text{-}C_3H_7$	$0.1000 \cdot 10^{9}$	0.00	5200	j
191	$CH_2CHCH_2 + C_3H_8 \leftrightarrow C_3H_6 + i\text{-}C_3H_7$	$0.7829 \cdot 10^{-1}$	3.30	8700	e
192	$CH_2CHCH_2 + C_3H_8 \leftrightarrow C_3H_6$	$0.2349 \cdot 10^{0}$	3.30	10000	e
193	$i\text{-}C_3H_7 + C_3H_8 \leftrightarrow n\text{-}C_3H_7 + C_3H_8$	$0.8430 \cdot 10^{-5}$	4.20	4400	w
194	$H_2 + 2\ H \leftrightarrow 2\ H_2$	$0.9791 \cdot 10^{11}$	-0.60	0	a
195	$C_3H_6 \leftrightarrow C_2H_2 + CH_4$	$0.3500 \cdot 10^{13}$	0.00	35000	x
196	$i\text{-}C_4H_{10} \leftrightarrow CH_3 + i\text{-}C_3H_7$	$0.2000 \cdot 10^{27}$	-3.50	40000	y
197	$H + i\text{-}C_4H_{10} \leftrightarrow H_2 + i\text{-}C_4H_9$	$0.3480 \cdot 10^{10}$	2.54	3400	y
198	$CH_3 + i\text{-}C_4H_{10} \leftrightarrow CH_4 + i\text{-}C_4H_9$	$0.1460 \cdot 10^{7}$	3.65	3600	y
199	$C_2H + i\text{-}C_4H_{10} \leftrightarrow C_2H_2 + i\text{-}C_4H_9$	$0.6020 \cdot 10^{10}$	0.00	0	y
200	$C_2H_3 + i\text{-}C_4H_{10} \leftrightarrow C_2H_4 + i\text{-}C_4H_9$	$0.1460 \cdot 10^{7}$	3.65	2600	y
201	$C_2H_5 + i\text{-}C_4H_{10} \leftrightarrow C_2H_6 + i\text{-}C_4H_9$	$0.1490 \cdot 10^{7}$	3.65	4600	y
202	$i\text{-}C_3H_7 + i\text{-}C_4H_{10} \leftrightarrow C_3H_8 + i\text{-}C_4H_9$	$0.3120 \cdot 10^{6}$	4.20	4400	y
203	$n\text{-}C_3H_7 + i\text{-}C_4H_{10} \leftrightarrow C_3H_8 + i\text{-}C_4H_9$	$0.1490 \cdot 10^{7}$	3.65	4600	y
204	$i\text{-}C_4H_9 + i\text{-}C_4H_9 \leftrightarrow i\text{-}C_4H_{10} + i\text{-}C_4H_8$	$0.7380 \cdot 10^{9}$	0.00	0	y
205	$i\text{-}C_4H_9 \leftrightarrow CH_3 + C_3H_6$	$0.2000 \cdot 10^{14}$	0.00	15000	y
206	$C_2H_2 + i\text{-}C_4H_9 \leftrightarrow C_3H_6 + CH_2CHCH_2$	$0.7230 \cdot 10^{9}$	0.00	4500	y
207	$CH_2 + i\text{-}C_4H_9 \leftrightarrow C_2H_4 + i\text{-}C_3H_7$	$0.1810 \cdot 10^{11}$	0.00	0	y
208	$C_2H_4 + i\text{-}C_4H_9 \leftrightarrow C_3H_6 + i\text{-}C_3H_7$	$0.3010 \cdot 10^{8}$	0.00	3100	y
209	$H + i\text{-}C_4H_9 \leftrightarrow H_2 + i\text{-}C_4H_8$	$0.9030 \cdot 10^{9}$	0.00	0	y
210	$CH_3 + i\text{-}C_4H_9 \leftrightarrow CH_4 + i\text{-}C_4H_8$	$0.9760 \cdot 10^{9}$	-0.32	0	y
211	$C_2H + i\text{-}C_4H_9 \leftrightarrow C_2H_2 + i\text{-}C_4H_8$	$0.6020 \cdot 10^{10}$	0.00	0	y
212	$C_2H_3 + i\text{-}C_4H_9 \leftrightarrow C_2H_4 + i\text{-}C_4H_8$	$0.8430 \cdot 10^{9}$	0.00	0	y
213	$C_2H_5 + i\text{-}C_4H_9 \leftrightarrow C_2H_6 + i\text{-}C_4H_8$	$0.8430 \cdot 10^{9}$	0.00	0	y
214	$i\text{-}C_3H_7 + i\text{-}C_4H_9 \leftrightarrow C_3H_8 + i\text{-}C_4H_8$	$0.3490 \cdot 10^{10}$	0.35	0	y
215	$n\text{-}C_3H_7 + i\text{-}C_4H_9 \leftrightarrow C_3H_8 + i\text{-}C_4H_8$	$0.7230 \cdot 10^{9}$	0.00	0	y
216	$C_2H_3 + i\text{-}C_4H_9 \leftrightarrow C_2H_2 + i\text{-}C_4H_{10}$	$0.8430 \cdot 10^{9}$	0.00	0	y
217	$C_2H_5 + i\text{-}C_4H_9 \leftrightarrow C_2H_4 + i\text{-}C_4H_{10}$	$0.8430 \cdot 10^{9}$	0.00	0	y
218	$i\text{-}C_3H_7 + i\text{-}C_4H_9 \leftrightarrow C_3H_6 + i\text{-}C_4H_{10}$	$0.1930 \cdot 10^{10}$	-0.35	0	y
219	$n\text{-}C_3H_7 + i\text{-}C_4H_9 \leftrightarrow C_3H_6 + i\text{-}C_4H_{10}$	$0.1450 \cdot 10^{10}$	0.00	0	y

220	$H + i\text{-}C_4H_8 \leftrightarrow CH_3 + C_3H_6$	$0.1720 \cdot 10^{11}$	0.00	1800	z

References:

a. D. L. Baulch et al, *J. Phys. Chem. Ref. Data*, 1994, **23**, 847
b. A. Bergeat et al, *J. Phys. Chem. A.*, 1999, **103**, 6360
c. J-C. Legrand et al, *Vacuum*, 1998, **50**, 491
d. S. Bauerle et al, *Ber. Bunsenges. Phys. Chem.*, 1995, **99**, 870
e. D. L. Baulch et al, *J. Phys. Chem. Ref. Data*, 2005, **34**, 757
f. J. H. Kiefer et al, *J. Phys. Chem. A.*, 1997, **101**, 4057
g. W. Tsang, *J. Phys. Chem. Ref. Data*, 1991, **20**, 221
h. W. Tsang and R. F. Hampson, *J. Phys. Chem. Ref. Data*, 1986, **15**, 1087
i. X. Yang et al, *J. Phys. Chem. A.*, 2009, **113**, 8307
j. M. D. Allendorf and R. J. Kee, *J. Electrochem. Soc.*, 1991, **138**, 841
k. D. L. Baulch et al, *J. Phys. Chem. Ref. Data*, 1992, **21**, 411
l. A. Rhallabi and Y. Catherine, *IEEE Trans. Plasma Sci.*, 1991, **19**, 270
m. C. D. Pintassilgo et al, *Plasma Sources Sci. Technol.*, 1999, **8**, 463
n. S. G. Davis et al, *J. Phys. Chem. A.*, 1999, **103**, 5889
o. E. W. Diau et al, *J. Chem. Phys.*, 1994, **101**, 3923
p. N. S. Titova et al, *Combust. Explos. Shock Waves*, 2011, **47**, 249
q. L. B. Harding et al, *J. Phys. Chem. A.*, 2005, **109**, 4646
r. L. B. Harding et al, *J. Phys. Chem. A.*, 2007, **111**, 3789
s. K. H. Homann and Ch. Wellmann, *Ber. Bunsenges. Phys. Chem.*, 1983, **87**, 609
t. T. Kakumoto et al, *J. Phys. Chem.*, 1987, **91**, 183
u. C. H. Wu and R. D. Kern, *J. Phys. Chem.*, 1987, **91**, 6291
v. J. Warnatz, in "*Combustion Chemistry*", W. C. Gardiner, Jr. ed., Springer-Verlag, 1984
w. W. Tsang, *J. Phys. Chem. Ref. Data*, 1988, **17**, 887
x. Y. Hidaka et al, *Int. J. Chem. Kinet.*, 1992, **24**, 761
y. W. Tsang, *J. Phys. Chem. Ref. Data*, 1990, **19**, 1
z. W. Tsang and J. A. Walker, *Symp. Int. Combust. Proc.*, 1989, **22**, 1015

Table S2 Decomposition of TMGa.

	Reaction	**A (m^3, mol, s)**	**n**	**Ea/R (K)**
1	$TMGa \rightarrow CH_3 + DMGa$	$0.1000 \cdot 10^{48}$	-9.18	39000
2	$CH_3 + DMGa \rightarrow TMGa$	$0.7130 \cdot 10^{29}$	-8.17	3600
3	$DMGa \rightarrow CH_3 + MMGa$	$0.7670 \cdot 10^{44}$	-9.80	17000
4	$CH_3 + MMGa \rightarrow DMGa$	$0.3040 \cdot 10^{28}$	-8.81	2300
5	$MMGa \rightarrow CH_3 + Ga$	$0.1680 \cdot 10^{31}$	-5.07	42000
6	$CH_3 + Ga \rightarrow MMGa$	$0.8930 \cdot 10^{15}$	-4.07	1300
7	$TMGa + NH_3 \rightarrow TMGaNH_3$	$0.2280 \cdot 10^{23}$	-8.31	1600
8	$TMGa + NH_3 \rightarrow CH_4 + Ga(CH_3)_2NH_2$	$0.1700 \cdot 10^{-7}$	2.00	10000
9	$DMGa + NH_3 \rightarrow DMGaNH_3$	$0.4080 \cdot 10^{19}$	-7.03	1600
10	$DMGa + NH_3 \rightarrow CH_4 + GaCH_3NH_2$	$0.5300 \cdot 10^{-6}$	1.56	10000
11	$MMGa + NH_3 \rightarrow MMGaNH_3$	$0.7950 \cdot 10^{13}$	-5.21	1100
12	$MMGa + NH_3 \rightarrow CH_4 + GaNH_2$	$0.8100 \cdot 10^{-6}$	1.30	8900
13	$CH_3 + NH_3 \leftrightarrow CH_4 + NH_2$	$0.3410 \cdot 10^{-8}$	2.51	5000
14	$H + TMGa \leftrightarrow CH_4 + DMGa$	$0.5000 \cdot 10^{2}$	0.00	5100
15	$H + DMGa \leftrightarrow CH_4 + MMGa$	$0.5000 \cdot 10^{11}$	0.00	5100
16	$TMGaNH_3 \leftrightarrow 2\ CH_3 + MMGa + NH_3$	$0.1330 \cdot 10^{45}$	-8.24	39000

Reference: D. Sengupta, S. Mazumder, W. Kuykendall and S. A. Lowry, *J. Cryst. Growth*, 2005, **279**, 369.

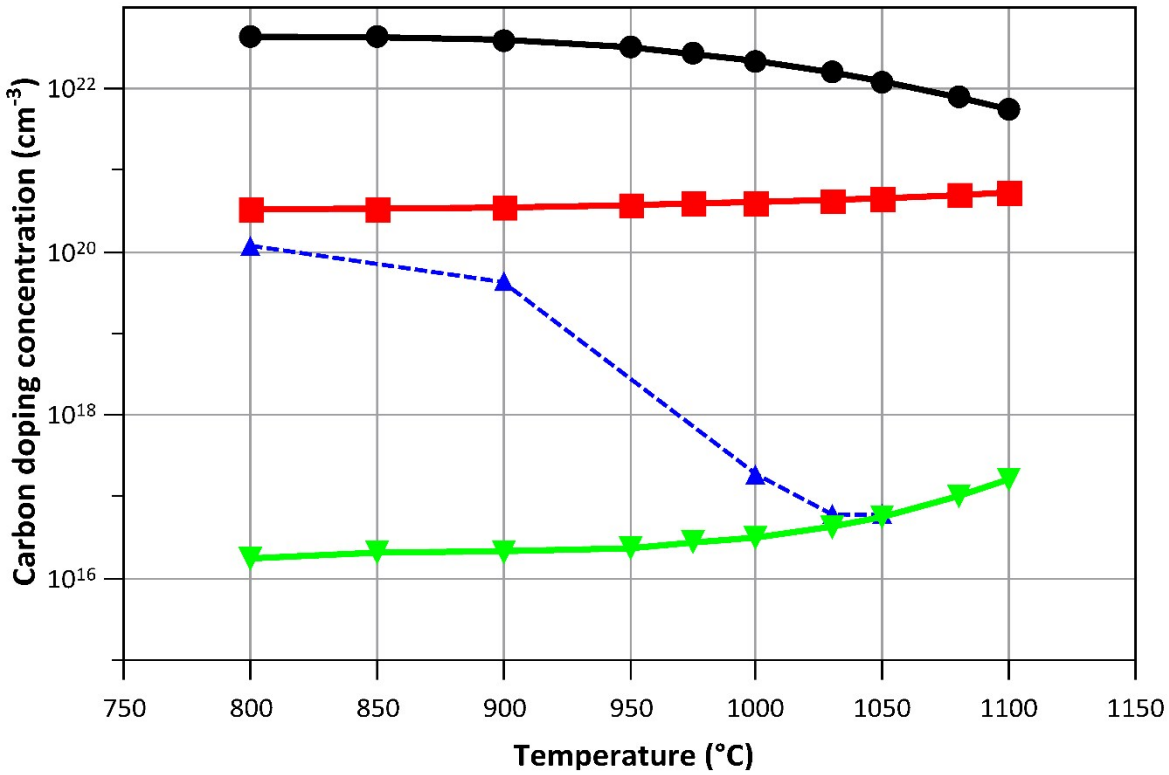

Fig. S6 Contribution to doping from different molecules as calculated by the model, without taking into account any removal of CH_3 groups: $GaCH_3$ (–●–), CH_3 (–■–) and C_2H_x (–♦–). Measured doping concentrations (--▲--) are shown for comparison.