Chemistry and kinetics of heterogeneous reaction mechanism for chemical vapor infiltration of pyrolytic carbon from propane

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This Supporting information document is divided in two parts:

- **Appendix A**: the nomenclature of 72 surface species;

-**Appendix B**: the detailed surface kinetic mechanism comprised of 277 reactions and related references.

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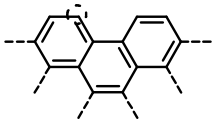
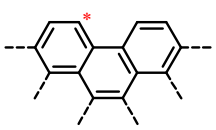
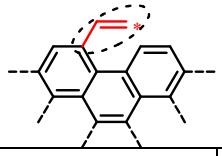
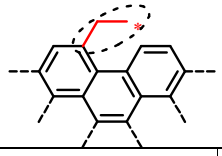
Appendix A: nomenclature of surface species and the number of sites every species occupied.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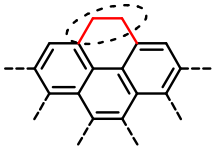				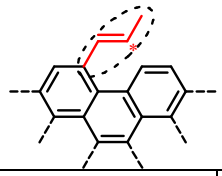		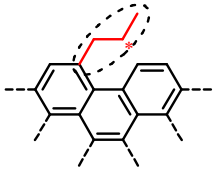	
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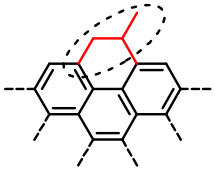		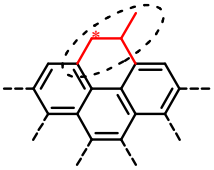		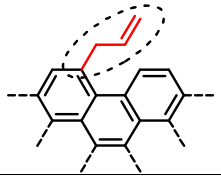		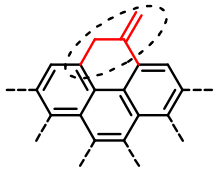	
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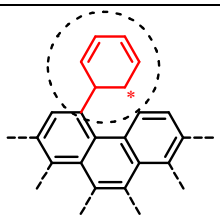		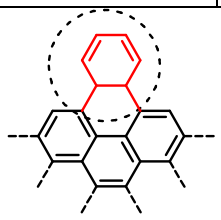		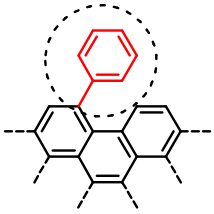		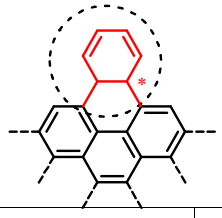	
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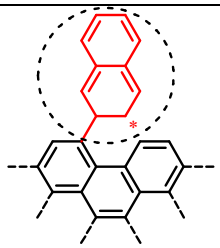		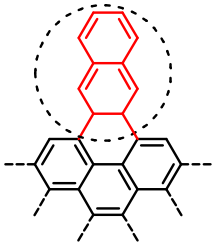		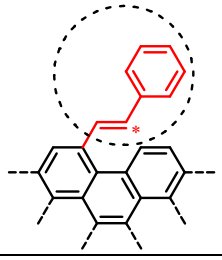		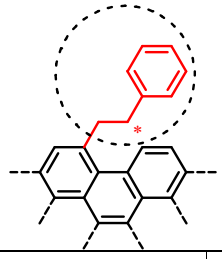	
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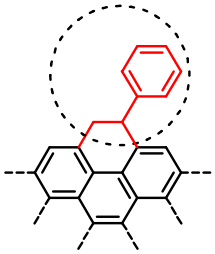		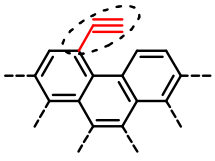		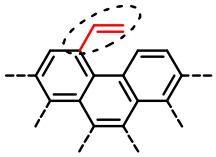		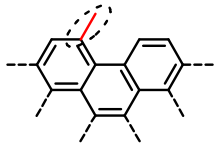	
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		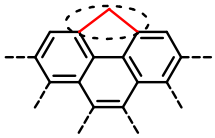		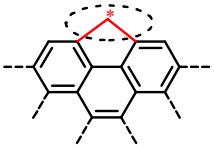		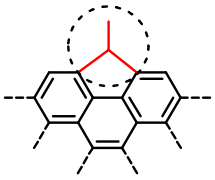	
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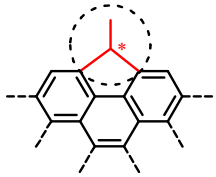		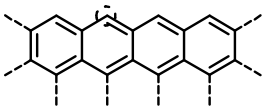		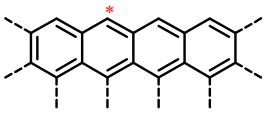		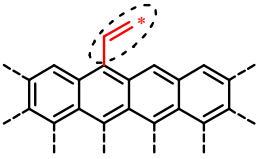	
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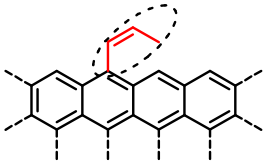		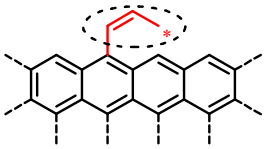		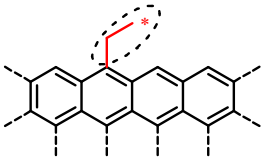		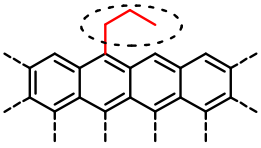	
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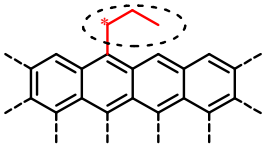		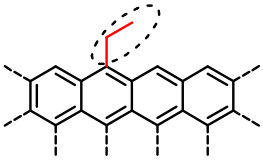		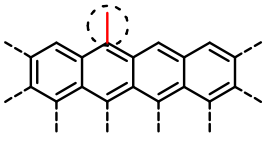		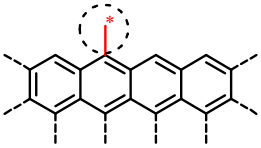	
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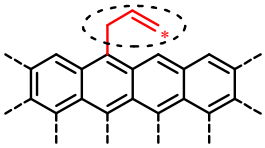		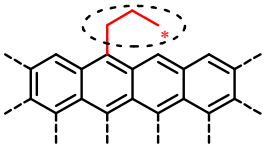		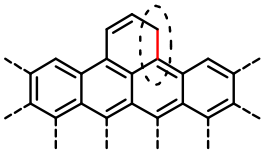		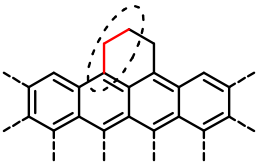	
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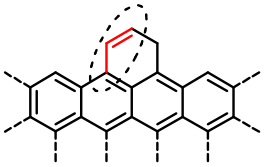		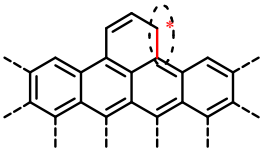		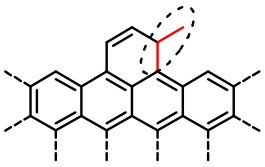		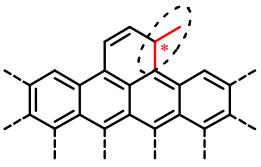	
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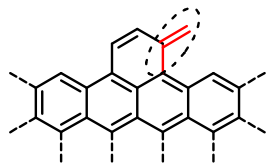		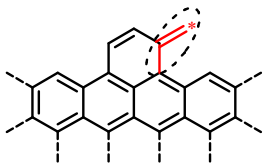		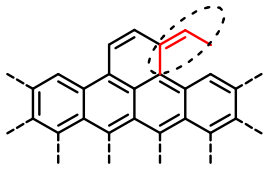		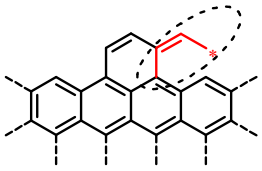	
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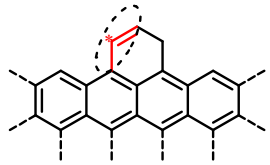		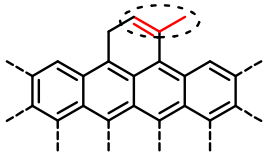		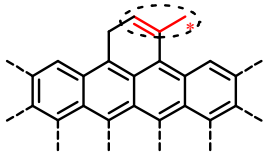		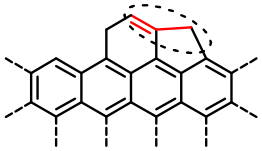	
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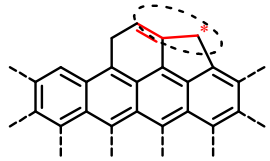
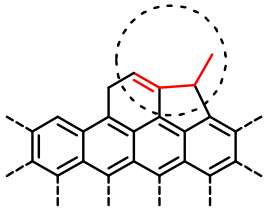
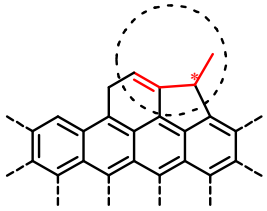
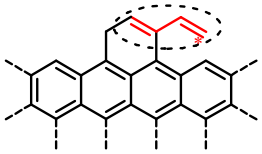
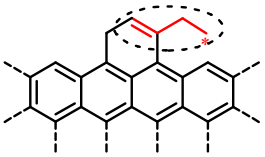
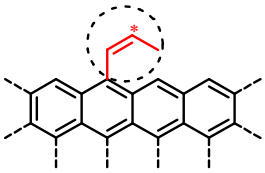
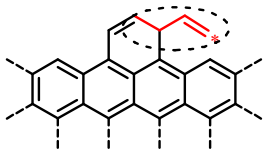
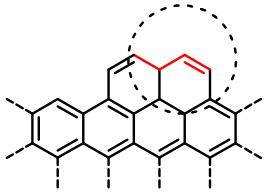
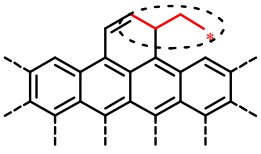
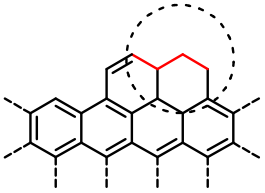
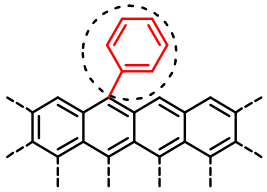
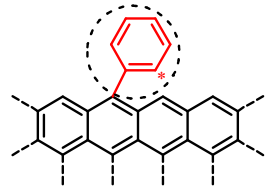
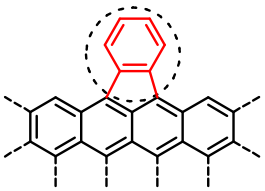
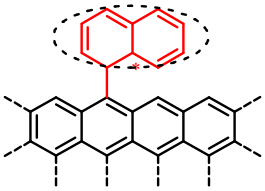
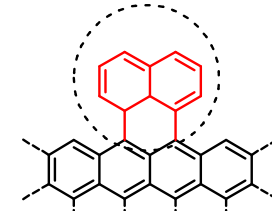
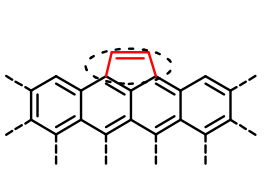
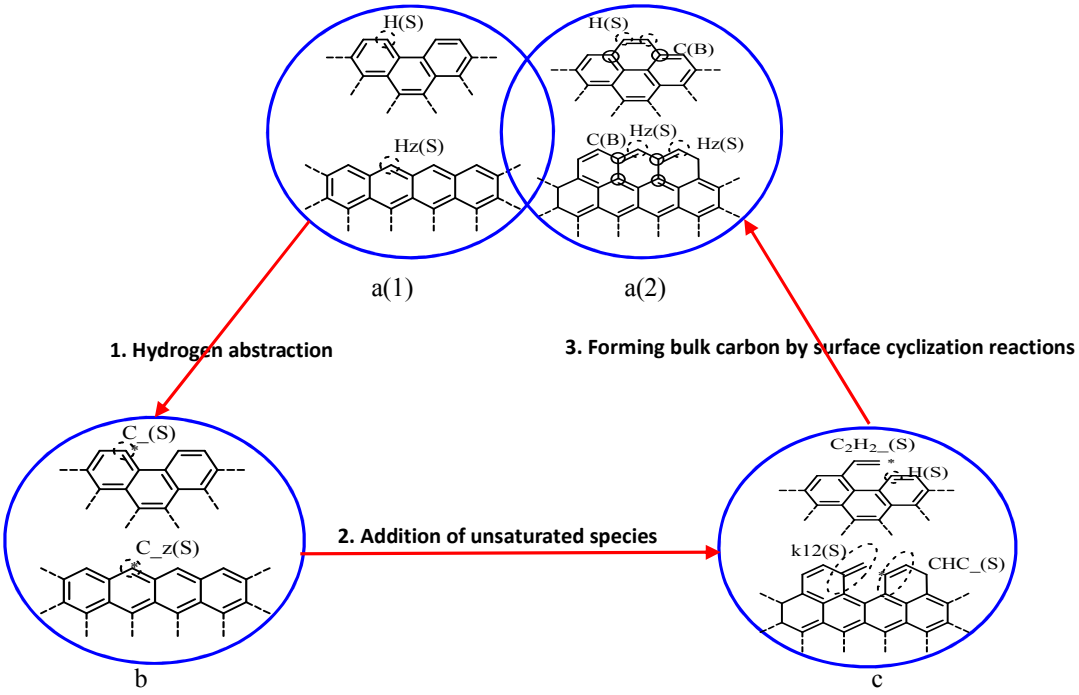
							
C3H2z(S)	2	C4H5z(S)	2	C4H4z(S)	2	k16(S)	1
							
k17(S)	1	k19(S)	1	k20(S)	1	k21(S)	2
							
k22(S)	1	k23(S)	2	k24(S)	1	k24_(S)	1
							
k25(S)	2	k26(S)	1	k27(S)	2	k28(S)	2

Appendix B: Detailed reaction pathways and related kinetic parameters

In the present work, a detailed heterogeneous reaction mechanism containing 72 surface species and 277 elementary surface reactions is proposed. Figure 2 describes the principal comprehension of the surface reaction mechanism for pyrocarbon deposition. We suppose the initial surface sites H(S) and Hz(S) each accounted for 50% of the total surface sites(Fig2.a(1)); These hydrogens occupying in the initial surface sites are abstracted by gas-phase radicals generated during the pyrolysis process, resulting in the formation of active carbon surface sites C_(S) and C_z(S) (Fig2.b); Addition of major aliphatic or aromatic unsaturated species on C_(S) or C_z(S) occurs lately, forming various kinds of radical surface sites(Fig2.c); New six-atom aromatic rings are created by surface cyclization reactions between these radical surface sites and neighboring H(S) or Hz(S), the sp2-like carbon of the new aromatic ring is viewed as bulk carbon C(B), and H(S) or Hz(S) occupies the outside part of the new ring(Fig2.a(2)). Through these successive steps, the surface sites are occupied by the initial surface sites H(S) and Hz(S). Subsequently, a new circle is moving forward from the a(1) again. A detailed description of the surface reaction mechanism referring to Lacroix et al [80], Heidi Bohm et al[81], Dong, G. L et al[82], and Koyo Norinaga et al[83] will be illustrated in the following.



1. Forming active carbon radical sites by hydrogen abstraction reactions

The heterogeneous surface reactions occur simultaneously with the homogeneous gas-phase reactions. Many gas-phase radical species (H, CH_3, C_2H_3, C_2H_5, C_3H_3, iC_4H_3, aC_3H_5, benzyl, indenyl) are very active, these radicals obtain hydrogen atoms by reacting with H(S) or Hz(S), which becomes C_(S) or C_z(S) by hydrogen

abstraction reactions. And the initiation reaction is also considered in the formation of C_(S) or C_z(S).

No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
1	H(S)+H => C_(S)+H_2	C_6H_6+H => C_6H_5+H_2	6.02E+08	1.8	68.55	ks=0.1kg[1]
2	C_(S)+H_2 => H(S)+H	C_6H_5+H_2 => C_6H_6+H	3.98E+12	0	32.98	ks=0.1kg[2]
3	H(S)+CH_3 => C_(S)+CH_4	C_6H_6+CH_3 => C_6H_5+CH_4	2.62E+13	0	80.67	ks=0.1kg[3]
4	C_(S)+CH_4 => H(S)+CH_3	C_6H_5+CH_4 => C_6H_6+CH_3	2.00E+12	0	35.97	ks=0.1kg[2]
5	H(S)+C_2H_3 => C_(S)+C_2H_4	C_6H_6+C_2H_3 => C_6H_5+C_2H_4	0.41	4.02	36.80	ks=0.1kg[4]
6	C_(S)+C_2H_4 => H(S)+C_2H_3	C_6H_5+C_2H_4 => C_6H_6+C_2H_3	9.45E-03	4.47	18.69	ks=0.1kg[4]
7	H(S)+C_2H_5 => C_(S)+C_2H_6	C_2H_4+C_2H_5 => C_2H_3+C_2H_6	632	3.13	75.24	ks=8.40E-03kg[5]
8	C_(S)+C_2H_6 => H(S)+C_2H_5	C_6H_5+C_2H_6 => C_6H_6+C_2H_5	2.09E+11	0	18.57	ks=0.1kg[6]
9	H(S)+C_3H_3 => C_(S)+PC_3H_4	C_6H_6+C_3H_3=> C_6H_5+PC_3H_4	6.30E+11	0	83.60	ks=0.1kg[7]
10	H(S)+I-C_4H_3 => C_(S)+C_4H_4	$C_4H_6$12+I-C_4H_3 =>I-$C_4H_5$1+ C_4H_4	2.00E+12	0	54.34	ks=5.40E-03kg[8]
11	C_(S)+C_4H_4 => H(S)+I-C_4H_3	C_2H_3+C_4H_4 => C_2H_4+I-C_4H_3	5.00E+11	0	68.20	ks=7.80E-03kg[9]
12	H(S)+AC_3H_5 => C_(S)+C_3H_6	C_5H_6+AC_3H_5 =>C_5H_5+C_3H_6	1.10E+11	0	23.01	ks=0.1kg[10]
13	C_(S)+C_3H_6 => H(S)+AC_3H_5	C_6H_5+C_3H_6 => C_6H_6+C_3H_5	1.36	3.82	6.01	ks=0.1kg[11]
14	H(S)+benzyl => C_(S)+toluene	C_6H_6+C_7H_7 => C_6H_5+C_7H_8	4.00E+08	0	0	ks=0.1kg[2]
15	C_(S)+toluene=>H(S)+benzyl	C_6H_5+C_7H_8 => C_6H_6+C_7H_7	7.94E+13	0	49.74	ks=0.1kg[2]
16	H(S)+indenyl=>C_(S)+indene	C_6H_6+C_7H_7 => C_6H_5+C_7H_8	4.00E+08	0	0	ks=0.1kg[2]
17	C_(S)+indene=>H(S)+indenyl	C_6H_5+C_7H_8 => C_6H_6+C_7H_7	7.94E+13	0	49.74	ks=0.1kg[2]
18	H(S) => C_(S)+H	C_6H_6 => C_6H_5+H	2.00E+17	0	459.80	ks=0.1kg[12]
19	C_(S)+H => H(S)	C_6H_5+H => C_6H_6	7.94E+13	0	0	ks=0.1kg[13]
20	Hz(S)+H => C_z(S)+H_2	C_6H_6+H => C_6H_5+H_2	6.02E+08	1.8	68.55	ks=0.1kg[1]
21	C_z(S)+H_2 => Hz(S)+H	C_6H_5+H_2 => C_6H_6+H	3.98E+12	0	32.98	ks=0.1kg[2]
22	Hz(S)+CH_3 => C_z(S)+CH_4	C_6H_6+CH_3 => C_6H_5+CH_4	2.62E+13	0	80.67	ks=0.1kg[3]
23	C_z(S)+CH_4 => Hz(S)+CH_3	C_6H_5+CH_4 => C_6H_6+CH_3	2.00E+12	0	35.97	ks=0.1kg[2]
24	Hz(S)+C_2H_3 => C_z(S)+C_2H_4	C_6H_6+C_2H_3 => C_6H_5+C_2H_4	0.41	4.02	36.80	ks=0.1kg[4]
25	C_z(S)+C_2H_4 => Hz(S)+C_2H_3	C_6H_5+C_2H_4 => C_6H_6+C_2H_3	9.45E-03	4.47	18.69	ks=0.1kg[4]
26	Hz(S)+C_2H_5 => C_z(S)+C_2H_6	C_2H_4+C_2H_5 => C_2H_3+C_2H_6	632	3.13	75.24	ks=8.40E-03kg[5]
27	C_z(S)+C_2H_6 => Hz(S)+C_2H_5	C_6H_5+C_2H_6 => C_6H_6+C_2H_5	2.09E+11	0	18.57	ks=0.1kg[6]
28	Hz(S)+C_3H_3 => C_z(S)+PC_3H_4	C_6H_6+C_3H_3=> C_6H_5+PC_3H_4	6.30E+11	0	83.60	ks=0.1kg[7]

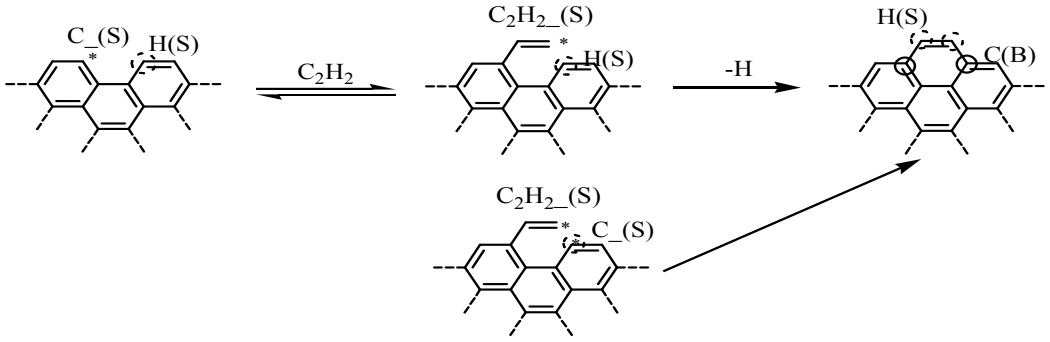
29	Hz(S)+I-C_4H_3 => C_z(S)+C_4H_4	$C_4H_6$12+I-C_4H_3 => C_4H_4+I-$C_4H_5$1	2.00E+12	0	54.34	ks=5.40E-03kg[8]
30	C_z(S)+C_4H_4 => Hz(S)+I-C_4H_3	C_2H_3+C_4H_4 => C_2H_4+I-C_4H_3	5.00E+11	0	68.20	ks=7.80E-03kg[9]
31	Hz(S)+AC_3H_5 => C_z(S)+C_3H_6	C_5H_6+AC_3H_5 =>C_5H_5+C_3H_6	1.10E+11	0	23.01	ks=0.1kg[10]
32	C_z(S)+C_3H_6 => Hz(S)+AC_3H_5	C_6H_5+C_3H_6 => C_6H_6+C_3H_5	1.36	3.82	6.01	ks=0.1kg[11]
33	Hz(S)+benzyl => C_z(S)+toluene	C_6H_6+C_7H_7 => C_6H_5+C_7H_8	4.00E+08	0	0	ks=0.1kg[2]
34	C_z(S)+toluene=>Hz(S)+benzyl	C_6H_5+C_7H_8 => C_6H_6+C_7H_7	7.94E+13	0	49.74	ks=0.1kg[2]
35	Hz(S)+indenyl=>C_z(S)+indene	C_6H_6+C_7H_7 => C_6H_5+C_7H_8	4.00E+08	0	0	ks=0.1kg[2]
36	C_z(S)+indene=>Hz(S)+indenyl	C_6H_5+C_7H_8 => C_6H_6+C_7H_7	7.94E+13	0	49.74	ks=0.1kg[2]
37	Hz(S) => C_z(S)+H	C_6H_6 => C_6H_5+H	2.00E+17	0	459.8	ks=0.1kg[12]
38	C_z(S)+H => Hz(S)	C_6H_5+H => C_6H_6	7.94E+13	0	0	ks=0.1kg[13]

The serial number of the surface reaction lists in the first column of the table. The surface reaction rate constant k= AT^nexp(-Ea/RT); the units of A are cm, mole, and s; the unit of T is K; and the units of Ea are kJ/mol; The last column of the table lists the values of surface reaction rate constant ks and related references.

2.Surface elementary reactions on armchair sites

2.1 Deposition of acetylene on armchair sites

As active carbon surface sites C_(S) are created on armchair sites, the four-carbon bays are immediately closed by acetylene addition on the basis of HACA model. When the acetylene molecular adsorbs on the C_(S), a radical surface site C_2H_2_(S) is formed. C_2H_2_(S) can react with neighboring H(S), leading to the formation of a new aromatic ring and a free hydrogen atom. The carbon atoms of the inside part of the new ring all surrounded by carbon atoms with the sp2-like hybrid orbital are considered as bulk carbon C(B). While the carbon atoms of the outside part are occupied by hydrogen atoms, viewed as H(S) surface species. And if the neighboring surface species of the C_2H_2_(S) is C_(S), cyclization reaction will occur without hydrogen abstraction. In these surface reactions, the number of sites included on the left-hand side of the reaction equals the number on the right-hand sites; these reactions conserve sites [84]. For lack of thermodynamic data of the surface species, all these surface reactions are listed in the irreversible format [84]. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.



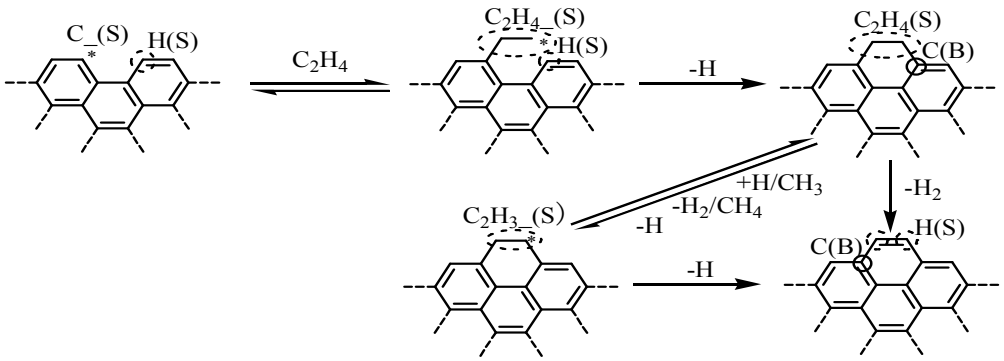
No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
39	C_(S)+C_2H_2=>C_2H_2_(S)	C_6H_5+C_2H_2=>Ethenyl,2-phenyl	2.69E+06	2.05	15.55	ks=0.1kg[14]
40	C_2H_2_(S) =>C_(S)+C_2H_2	Ethenyl,2-phenyl=>C_6H_5+C_2H_2	1.35E+14	0.34	191.02	ks=0.1kg[14]
41	C_2H_2_(S)+H(S) =>2C(B) +2H(S) +H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
42	C_2H_2_(S)+C_(S) =>2C(B)+2H(S)	N-C_6H_7=>C-C_6H_7	4.10E+24	-7.11	16.38	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

2.2 Deposition of ethylene on armchair sites

Analogous to the deposition of acetylene, the ethylene deposition pathway containing: (1) Adsorption of ethylene and desorption of ethylene from the surface; (2) Cyclization with a neighboring H(S).

And direct dehydrogenation or radical reactions are required for the formation of a new aromatic ring. It's worth noting that C_2H_4(S) occupies two sites owing to the cyclization reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

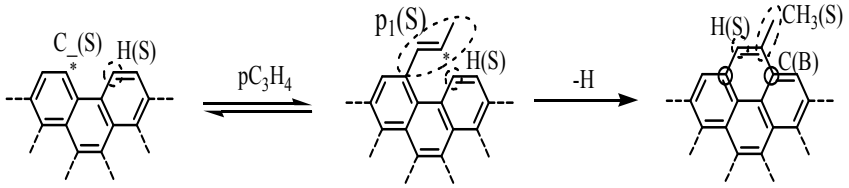


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
43	C_(S)+C_2H_4=>C_2H_4_(S)	1-Naphthalenyl +C_2H_4=>$C_{10}H_7C_2H_4$	3.00E+12	0	10.53	ks=0.1kg[16]
44	C_2H_4_(S) =>C_(S)+C_2H_4	Ethylbenzene=>Benzene+C_2H_4	1.15E+09	0	216.11	ks=0.1kg[17]
45	C_2H_4_(S)+ H(S) =>C(B)+C_2H_4(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
46	C_2H_4(S)+H=>C_2H_3_(S)+H_2	C_2H_4+H=>C_2H_3+H_2	3.55E+14	0	59.77	ks=4.10E-03kg[18]
47	C_2H_3_(S)+H_2=>C_2H_4(S)+H	C_2H_3+H_2 => C_2H_4+H	3.02E+04	2.63	35.72	ks=4.40E-03kg[5]
48	C_2H_4(S)+CH_3=>C_2H_3_(S)+CH_4	C_2H_4+CH_3=>C_2H_3+CH_4	4.16E+12	0	46.40	ks=8.00E-03kg[13]
49	C_2H_3_(S)+CH_4=>C_2H_4(S)+CH_3	C_2H_3+CH_4 => C_2H_4+CH_3	1.45	4.02	22.84	ks=8.20E-03kg[5]
50	C_2H_4(S)=>C_2H_3_(S)+H	C_2H_4 => C_2H_3+H	2.00E+16	0	459.8	ks=4.10E-03kg[20]
51	C_2H_3_(S)+H=>C_2H_4(S)	C_2H_3+H=> C_2H_4	3.88E+13	0.2	0	ks=4.10E-03kg[21]
52	C_2H_4(S) =>C(B) +2H(S) +H_2	1-3-Cyclohexadiene=>Benzene+H_2	2.51E+13	0	247.0	ks=0.1kg[22]
53	C_2H_3_(S) =>C(B) +2H(S)+H	Cyclohexdienyl => Benzene+H	1.60E+04	0	0	ks=0.1kg[23]

The same comments as shown above, Γ=1.45E-09.

2.3 Deposition of propine on armchair sites

Analogous to the deposition of acetylene, the propine deposition pathway containing: (1) Adsorption of propine and desorption of propine from the surface; (2) Cyclization with a neighboring H(S). Besides the new aromatic ring, a surface species $CH_3(S)$ is formed; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

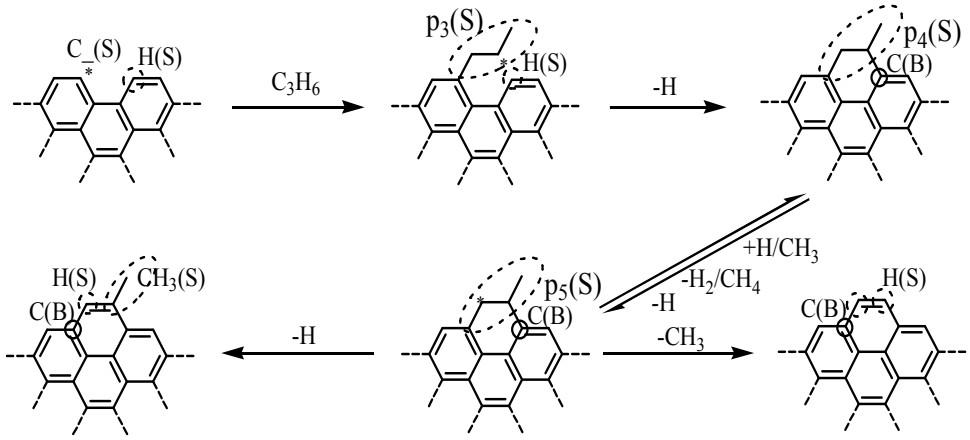


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
54	$C\_(S)+PC_3H_4$=>p1(S)	C_6H_5 +PC_3H_4 => Products	3.59E+04	2.55	11.53	ks=0.1kg[24]
55	p1(S)=>$C\_(S)+PC_3H_4$	1,2-pentadiene => $C_2H_4+PC_3H_4$	6.60E+12	0	242.86	ks=7.80E-03kg[25]
56	p1(S)+H(S)=>2C(B)+H(S)+CH_3(S)+ H	N-C_6H_7 => A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

2.4 Deposition of propene on armchair sites

Analogous to the deposition of acetylene, the propene deposition pathway containing: (1) Adsorption of propene from the surface; (2) Cyclization with a neighboring H(S). When the p4(S) occupying two sites is formed, hydrogen abstraction reaction with gas-phase radical H, CH_3 or initiation reaction occurs, leading to the formation of active surface site p5(S). Departure of a hydrogen atom and a methyl radical are considered for p5(S) consumption; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

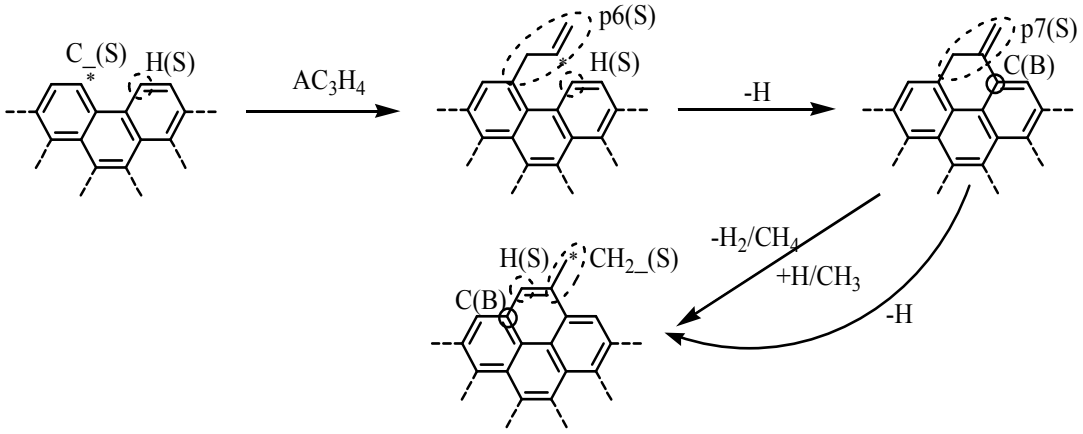


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
57	C_(S)+C_3H_6=>p3(S)	C_6H_5+C_3H_6=>$CH_3CHCH_2C_6H_5$	1.70E+04	2.47	3.07	ks=0.1kg[11]
58	p3(S) +H(S) =>C(B)+p4(S) +H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
59	p4(S)+H=>p5(S)+H_2	C_3H_6+H=>CH_3CHCH+H_2	7.83E+05	2.5	51.41	ks=3.00E-03kg[26]
60	p5(S)+H_2=>p4(S)+H	CH_2CHCH_2+H_2=>C_3H_6+H	1.08E+05	2.38	79.42	ks=2.80E-03kg[27]
61	p4(S)+CH_3=>p5(S)+CH_4	C_3H_6+CH_3=>n-Propyl +CH_4	9.00E-01	3.65	29.93	ks=6.40E-03kg[28]
62	p5(S)+CH_4=>p4(S)+CH_3	CH_3CHCH+CH_4=>C_3H_6+CH_3	3.99E+01	3.4	97.39	ks=5.70E-03kg[27]
63	p4(S)=>p5(S)+H	C_2H_4=>C_2H_3+H	2.00E+16	0	459.8	ks=4.10E-03kg[20]
64	p5(S)+H=>p4(S)	C_2H_3+H=>C_2H_4	3.88E+13	0.2	0	ks=4.10E-03kg[21]
65	p5(S)=>C(B)+H(S)+CH_3(S)+H	Cyclohexdienyl=>Benzene+H	1.60E+04	0	0	ks=0.1kg[23]
66	p5(S) =>C(B) + 2H(S) +CH_3	Toluene=>Phenyl+CH_3	5.00E+16	0	410	ks=0.1kg[29]

The same comments as shown above, Γ=1.45E-09.

2.5 Deposition of propadiene on armchair sites

Analogous to the deposition of acetylene, the propadiene deposition pathway containing: (1) Adsorption of propene from the surface; (2) Cyclization with a neighboring H(S). When p7(S) is formed, in the final step, a reaction consisting of a H-abstraction followed by an isomerization is written as a single reaction with kinetic rates corresponding to the H-abstraction reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

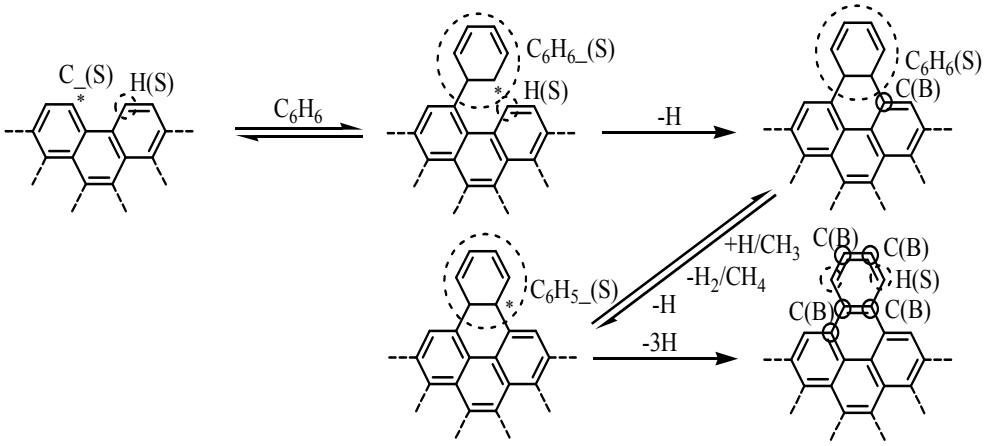


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
67	C_(S)+AC_3H_4=>p6(S)	C_6H_5 +AC_3H_4=>$C_6H_5CH_2CCH_2$	2.5E+12	0	25.92	ks=0.1kg[30]
68	p6(S)+H(S) =>C(B)+ p7(S) + H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
69	p7(S)+H=>C(B)+CH_2_(S)+H(S)+H_2	C_3H_6+H=>AC_3H_5+H_2	1.70E+05	2.5	10.39	ks=3.0E-03kg[26]
70	p7(S)+CH_3=>C(B)+CH_2_(S)+H(S)+CH_4	C_3H_6+CH_3=>AC_3H_5+CH_4	2.21E+00	3.5	23.78	ks=6.4E-03kg[27]
71	p7(S)=>C(B)+CH_2_(S)+H(S)+H	Cyclohexdienyl=>Benzene+H	1.60E+04	0	0	ks=0.1kg[23]

The same comments as shown above, Γ=1.45E-09.

2.6 Deposition of benzene on armchair sites

As active carbon surface sites C_(S) are created on armchair sites, the benzene molecular can adsorb on the site C_(S). Besides the addition of small unsaturated species, addition of small aromatic hydrocarbon, i.e. aryl-aryl combination, intramolecular dehydrocyclization are considered here[82]. When the C_6H_6(S) occupying two sites is formed, hydrogen abstraction reaction with gas-phase radical H, CH_3 or initiation reaction occurs, leading to the formation of active surface site C_6H_5_(S). The C_6H_5_(S) species is then transformed into bulk carbon C(B) by direct dehydrogenation reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

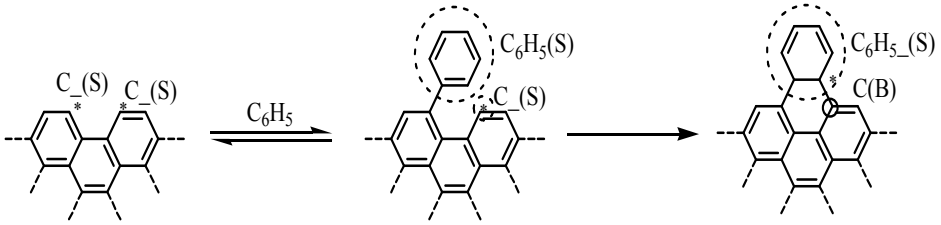


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
72	$C\_(S)+C_6H_6=>C_6H_6\_(S)$	Phenyl+Benzene=>Adduct	1.26E+12	0	45.14	ks=0.1kg[31]
73	$C_6H_6\_(S)=>C\_(S)+C_6H_6$	Ethylbenzene=>Benzene+C_2H_4	1.15E+09	0	216.11	ks=8.1E-03kg[17]
74	$C_6H_6\_(S)$ +H(S) =>C(B)+C_6H_6(S) +H	N-C_6H_7 =>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
75	$C_6H_6(S)+H=>C_6H_5\_(S)+H_2$	$C_6H_6+H=>C_6H_5+H_2$	6.02E+08	1.8	68.55	ks=0.1kg[1]
76	$C_6H_5\_(S)+H_2=>C_6H_6(S)+H$	$C_6H_5+H_2=>C_6H_6+H$	3.98E+12	0	32.98	ks=0.1kg[2]
77	$C_6H_6(S)+CH_3=>C_6H_5\_(S)+CH_4$	$C_6H_6+CH_3=>C_6H_5+CH_4$	2.62E+13	0	80.67	ks=0.1kg[3]
78	$C_6H_5\_(S)+CH_4=>C_6H_6(S)+CH_3$	$C_6H_5+CH_4=>C_6H_6+CH_3$	2.00E+12	0	35.97	ks=0.1kg[2]
79	$C_6H_6(S)=>C_6H_5\_(S)+H$	$C_6H_6=>C_6H_5+H$	2.00E+17	0	459.8	ks=0.1kg[12]
80	$C_6H_5\_(S)+H=>C_6H_6(S)$	$C_6H_5+H=>C_6H_6$	2.20E+14	0	0	ks=0.1kg[32]
81	$C_6H_5\_(S)=>5C(B)+2H(S)+3H$	1-3-Cyclohexdiene=>Benzene+H_2	2.51E+13	0	247	ks=0.1kg[22]

The same comments as shown above, Γ=1.45E-09.

2.7 Deposition of phenyl radicals on armchair sites

Analogous to the deposition of benzene, the phenyl radical adsorbs on the active carbon surface site C_(S), forming the surface site C_6H_5(S) without active, then through aryl-aryl combination and intramolecular cyclization with a neighboring C_(S), active surface site C_6H_5_(S) occupying two sites is formed; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

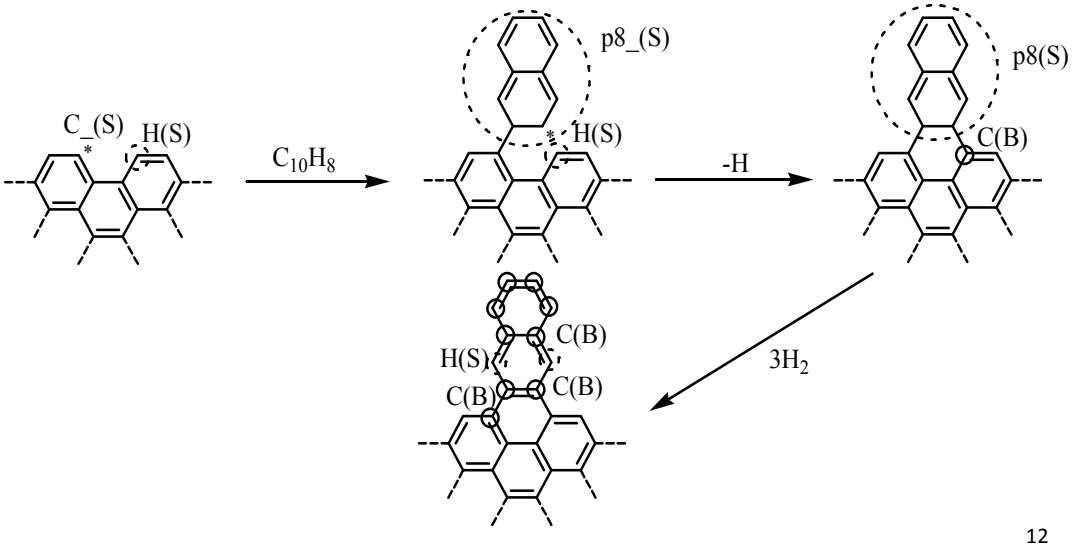


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
82	C_(S)+C_6H_5=>C_6H_5(S)	Phenyl+Phenyl=>Biphenyl	5.70E+12	0	0	ks=0.1kg[2]
83	C_6H_5(S)=>C_(S)+C_6H_5	Ethenyl,2-phenyl=>C_2H_2+C_6H_5	1.35E+14	0.34	191.03	ks=4.7E-03kg[14]
84	C_6H_5(S) + C_(S) => C(B) +C_6H_5_(S)	N-C_6H_7=>C-C_6H_7	4.10E+24	-7.11	16.38	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

2.8 Deposition of naphthalene on armchair sites

Analogous to the deposition of benzene, the naphthalene adsorbs on the active carbon surface site C_(S), forming the active surface site p8_(S), then through aryl-aryl combination and intramolecular dehydrocyclization with a neighboring H(S), surface site p8(S) occupying two sites is formed; these reactions conserve sites. The p8(S) species is then transformed into bulk carbon C(B) by direct dehydrogenation reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

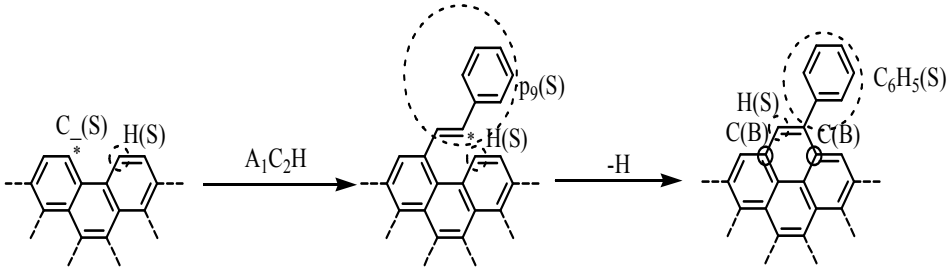


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
85	C_(S)+$C_{10}H_8$=>p8_(S)	C_6H_5+A1C_2H=>ethenyl,1,2-diphenyl	4.19E+04	2.74	14.68	ks=0.1kg[33]
86	p8_(S) + H(S) =>C(B)+p8(S) +H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
87	p8(S) =>9C(B) +2H(S) +3H_2		2.51E+13	0	246.76	[80]

The same comments as shown above, Γ=1.45E-09.

2.9 Deposition of phenylacetylene on armchair sites

Analogous to the deposition of acetylene, the phenylacetylene deposition pathway containing: (1) Adsorption of phenylacetylene on the surface; (2) Cyclization with a neighboring H(S). In this case, one C_6H_5(S), one H(S) and two C(B) are formed ; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

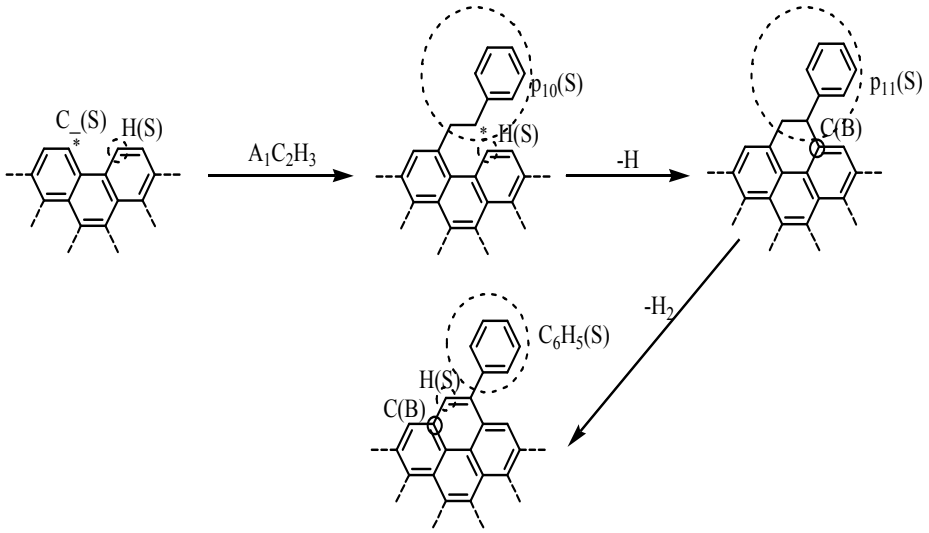


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
88	C_(S)+A1C2H=>p9(S)	C_6H_5+A1C_2H=>ethenyl,1,2-diphenyl	4.19E+04	2.74	14.68	ks=0.1kg[33]
89	P_9(S)+H(S) =>2C(B)+H(S) +C_6H_5(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

2.10 Deposition of styrene on armchair sites

Analogous to the deposition of acetylene, the phenylacetylene deposition pathway containing: (1) Adsorption of phenylacetylene on the surface; (2) Cyclization with a neighboring H(S). In this case, one C_6H_5(S), one H(S) and two C(B) are formed ; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

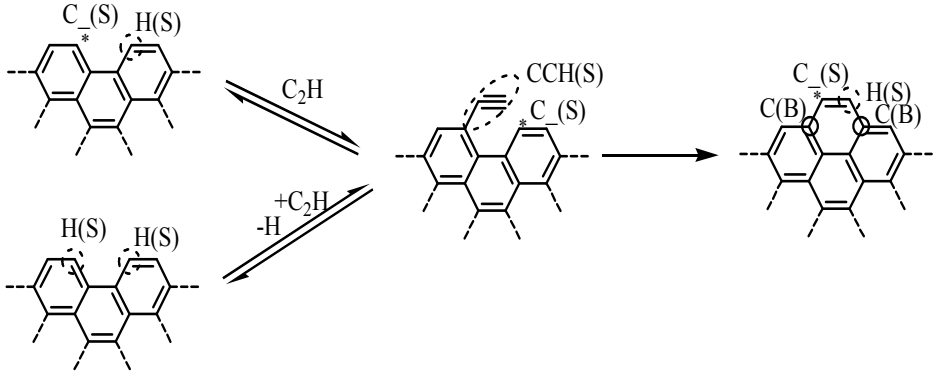


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
90	C_(S)+A1C_2H_3=>p10(S)	C_2H_2+Styrene=>Adduct	1.86E+11	0	142.96	ks=7.30E-03kg[34]
91	P10(S)+H(S) =>C(B)+p11(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
92	P11(S)=>C(B)+C_6H_5(S)+H(S)+H_2	1-3-Cyclohexadiene=>Benzene+H_2	2.51E+13	0	247	ks=0.1kg[22]

The same comments as shown above, Γ=1.45E-09.

2.11 Deposition of C_2H radicals on armchair sites

The C_2H radical may adsorb on the C_(S) site or react with H(S) followed by abstracting a hydrogen atom, forming surface site CCH(S). Unlike radical surface sites, CCH(S) is not so active. Therefore, CCH(S) will have the cyclization reaction with a neighboring C_(S), and one C_(S), one H(S), two C(B) are formed; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

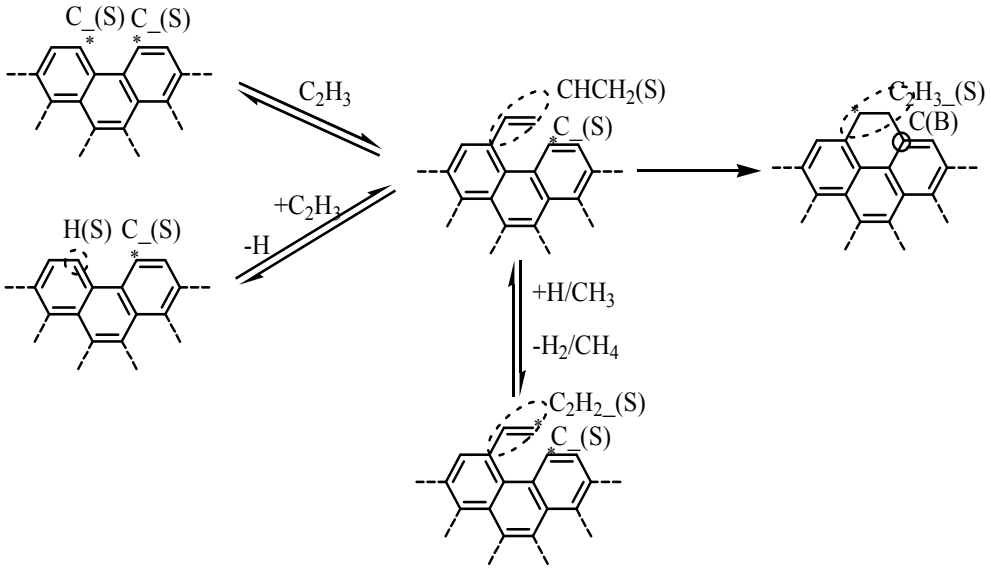


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
93	C_(S)+C_2H=>CCH(S)	C_2H_3+C_2H=>CH_2CHCCH	1.00E+14	0	0	ks=8.5E-03kg[35]
94	CCH(S)=>C_(S)+C_2H	1,3-Butadiene=>C_2H_3+C_2H_3	3.07E+12	0	278.39	ks=8.7E-03kg[36]
95	H(S)+C_2H=>CCH(S)+H	C_2H_4+C_2H=>CH_2CHCCH+H	1.21E+13	0	0	ks=8.6E-03kg[5]
96	CCH(S)+H=>H(S)+C_2H	CH_2CCHCH_3+H=>C_2H_4+C_2H_3	4.00E+11	0	0	ks=2.1E-03kg[36]
97	CCH(S)+C_(S) =>C_(S)+2C(B)+H(S)	N-C_6H_7=>C-C_6H_7	4.10E+24	-7.11	16.38	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

2.12 Deposition of C_2H_3 radicals on armchair sites

Analogous to the deposition of C_2H radical, the C_2H_3 radical may adsorb on the C_(S) site or react with H(S) followed by abstracting a hydrogen atom, forming surface site $CHCH_2$(S). Two consumption pathways of surface site $CHCH_2$(S) are considered here: (1) A hydrogen abstraction step by H/CH_3 radical, forming the radical surface site C_2H_2_(S); (2) Cyclization with a neighboring C_(S), one radical surface site C_2H_3_(S) and one C(B) are formed. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

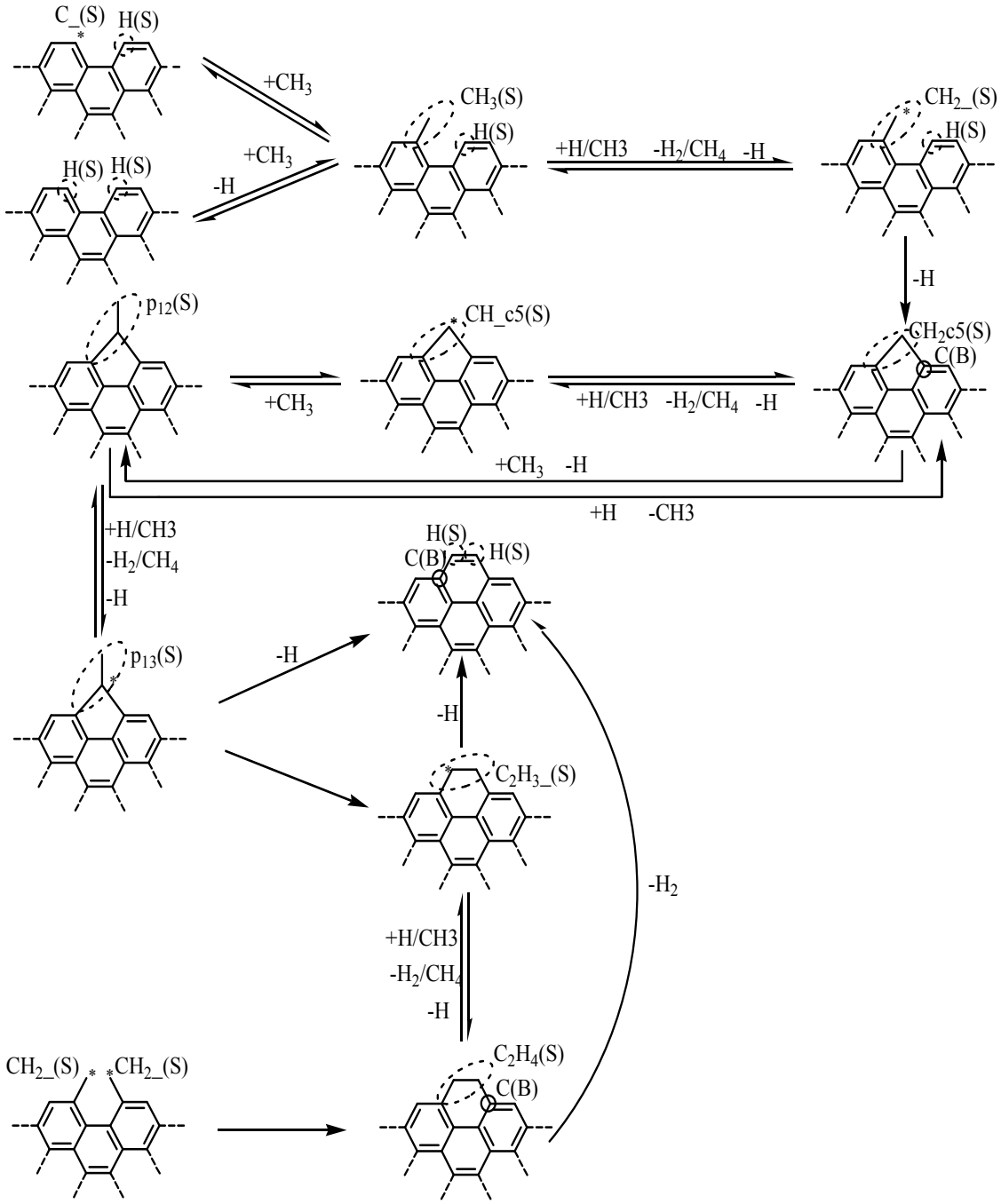


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
98	C_(S)+C_2H_3=>$CHCH_2$(S)	Benzene+C_2H_3=>Adduct	1.58E+11	0	12.54	ks=0.1kg[31]
99	$CHCH_2$(S)=>C_(S)+C_2H_3	1,3-Butadiene=>C_2H_3+C_2H_3	3.07E+12	0	278.39	ks=8.7E-03kg[36]
100	H(S)+C_2H_3=>$CHCH_2$(S)+H	Benzene+C_2H_3=>Styrene+H	7.94E+11	0	26.75	ks=0.1kg[37]
101	$CHCH_2$(S)+H=>H(S)+C_2H_3	CH_2CCHCH_3+H=>C_2H_4+C_2H_3	4.00E+11	0	0	ks=2.1E-03kg[36]
102	$CHCH_2$(S)+C_(S) =>C(B)+C_2H_3_(S)	N-C_6H_7=>C-C_6H_7	4.10E+24	-7.11	16.38	ks=kg/ Γ[15]
103	$CHCH_2$(S)+H=>C_2H_2_(S)+H_2	Styrene+H=>Ethenyl,1,2-phenyl+H_2	6.62E+05	2.53	51.00	ks=0.1kg[38]
104	C_2H_2_(S)+H_2=>$CHCH_2$(S)+H	C_2H_3+H_2=>C_2H_4+H	2.06E+12	0	34.75	ks=5.4E-03kg[39]
105	$CHCH_2$(S)+CH_3=>C_2H_2_(S)+CH_4	C_2H_4+CH_3=>C_2H_3+CH_4	4.16E+12	0	46.40	ks=8.0E-03kg[13]
106	C_2H_2_(S)+CH_4=>$CHCH_2$(S)+CH_3	CH_3CHCH+CH_4=>CH_3CHCH_2+CH_3	3.99E+01	3.4	97.39	ks=5.7E-03kg[27]

The same comments as shown above, Γ=1.45E-09.

2.13 Deposition of methyl radicals on armchair sites

The methyl radical may adsorb on the C_(S) site or react with H(S) followed by abstracting a hydrogen atom, forming the surface site CH_3(S). A hydrogen abstraction step by gas-phase radical H/CH_3 and initiation reaction are considered, leading to the formation of CH_2_(S), which reacts with a neighboring H(S) followed by a hydrogen abstraction, forming one 5-atom ring CH_2c5(S) and one C(B). Through hydrogen abstraction step by gas-phase radical H/CH3 and initiation reaction, the CH_2c5(S) turns into the surface species CH_c5(S). After addition of methyl on the radical surface site CH_c5(S) or addition of methyl on the surface site CH2c5(S) followed by a hydrogen abstraction, the surface species p12(S) is formed. A hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs, forming the radical surface site p13(S). Then the p13(S) transforms into 6-atom aromatic ring, i.e. (1) two H(S) and one C(B) followed by a hydrogen abstraction, (2) a radical surface species C_2H_3_(S). The C_2H_3_(S) may turn into two H(S) and one C(B) followed by a hydrogen abstraction as well. Here we also consider the cyclization reaction by two neighboring radical surface site CH_2_(S), forming one C_2H_4(S) and one C(B). The consumption pathway of surface species C_2H_4(S) illustrated below is already mentioned in the deposition of ethylene. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.


C_(S)
H(S)
+CH3
CH3(S)
H(S)
+H/CH3 -H2/CH4 -H
CH2_(S)
H(S)
H(S) H(S)
+CH3
-H
-H
p12(S)
CH_c5(S)
CH2c5(S)
C(B)
+CH3
+H/CH3 -H2/CH4 -H
+CH3 -H
+H -CH3
+H/CH3
-H2/CH4
-H
H(S)
C(B)
H(S)
p13(S)
-H
-H
C2H3_(S)
-H2
+H/CH3
-H2/CH4
-H
CH2_(S)
CH2_(S)
C2H4(S)
C(B)

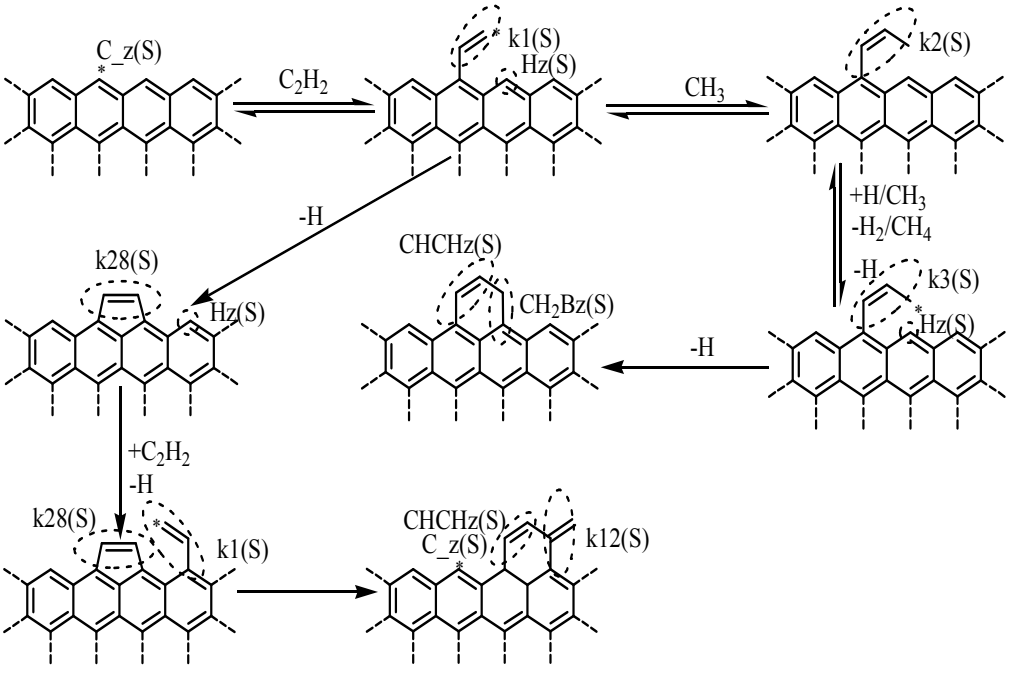
No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
107	C_(S)+CH_3=>CH_3(S)	Phenyl+CH3=>Toluene	1.38E+13	0	0.19	ks=0.1kg[40]
108	CH_3(S)=>C_(S)+CH_3	Toluene=>CH3+Phenyl	5.00E+16	0	409.64	ks=0.1kg[41]
109	H(S)+CH_3=>H+CH_3(S)	Benzene+CH3=>Toluene+H	1.20E+12	0	66.46	ks=0.1kg[42]
110	H+CH_3(S)=>H(S)+CH_3	Toluene+H=>Benzene+CH3	1.55E+13	0	24.21	ks=0.1kg[43]
111	CH_3(S)+H=>CH_2_(S)+H_2	Toluene+H=>Benzyl+H2	1.33E+15	0	62.28	ks=0.1kg[44]
112	CH_2_(S)+H_2=>CH_3(S)+H	Benzyl+H2=>Toluene+H	2.82E+12	0	60.61	ks=0.1kg[45]
113	CH_3(S)+CH_3=>CH_2_(S)+CH_4	CH_3CHCH_2+CH_3=>CH_2CHCH_2+CH_4	2.21E+00	3.5	23.75	ks=6.4E-03kg[27]
114	CH_2_(S)+CH_4=>CH_3(S)+CH_3	CH_2CHCH_2+CH_4=>CH_3CHCH_2+CH_3	3.99E+01	3.4	97.39	ks=5.7E-03kg[27]
115	CH_3(S)=>CH_2_(S)+H	Toluene=>Benzyl+H	6.31E+15	0	377.87	ks=0.1kg[46]
116	CH_2_(S)+H=>CH_3(S)	Benzyl+H=>Toluene	2.08E+14	0	0.36	ks=0.1kg[47]
117	2CH_2_(S)=>C_2H_4(S)+C(B)		5.61E+18	0.1	8.74	[80]
118	CH_2_(S)+H(S)=>CH_2c5(S)+H+C(B)	$CHCH_2CH_2CH_2CH_2$=>C_5H_8+H	6.90E-03	0	-17.63	ks=kg/ Γ[48]
119	CH_2c5(S)+H=>CH_c5(S)+H_2	Cyclopentane+H=>Cycolpentyl+H_2	2.41E+09	1.5	20.27	ks=0.1kg[49]
120	CH_c5(S)+H_2=>CH2c5(S)+H	CH_3CHCH_3+H_2=>C_3H_8+H	3.50E+01	3.28	36.22	ks=2.8E-03kg[28]
121	CH2c5(S)+CH_3=>CH_c5(S)+CH_4	C_5H_8+CH_3=>Cyclopentyl+CH_4	2.00E+11	0	35.97	ks=0.1kg[50]
122	CH_c5(S)+CH_4=>CH_2c5(S)+CH_3	iso-C_3H_7+CH_4=>C_3H_8+CH_3	7.23E-04	4.4	45.14	ks=5.7E-03kg[28]
123	CH_2c5(S)=>CH_c5(S)+H	C_3H_8=>iso-C_3H_7+H	6.31E+15	0	396.26	ks=2.5E-03kg[20]
124	CH_c5(S)+H=>CH_2c5(S)	iso-C_3H_7+H=>C_3H_8	2.00E+13	0	0	ks=2.5E-03kg[51]
125	CH_c5(S)+CH_3=>p12(S)	iso-C_3H_7+CH_3=>iso-C_4H_{10}	6.64E+14	-0.57	0	ks=5.5E-03kg[52]
126	p12(S)=>CH_c5(S)+CH_3	Methylcyclopentane=>C_5H_7+CH_3	1.26E+12	0	367.84	ks=0.1kg[53]
127	p12(S)+H=>p13(S)+H_2	iso-C_4H_{10}+H=>tert-C_4H_9+H_2	6.02E+05	2.4	10.80	ks=2.1E-03kg[54]
128	p13(S)+H_2=>P12(S)+H	tert-C_4H_9+H_2=>iso-C_4H_{10}+H	2.00E-02	4.24	37.46	ks=2.3E-03kg[54]
129	P12(S)+CH_3=>p13(S)+CH_4	iso-C_4H_{10}+CH_3=>tert-C_4H_9+CH_4	9.00E-01	3.46	19.19	ks=4.7E-03kg[54]
130	p13(S)+CH_4=>P12(S)+CH_3	tert-C_4H_9+CH_4=>iso-C_4H_{10}+CH_3	4.93E-07	5.38	49.742	ks=4.9E-03kg[54]
131	P12(S)=>p13(S)+H	C_3H_8=>iso-C_3H_7+H	6.31E+15	0	396.26	ks=2.5E-03kg[20]
132	p13(S)+H=>P12(S)	tert-C_4H_9+H=>iso-C_4H_{10}	5.20E+12	0.28	0	ks=2.1E-03kg[21]
133	p13(S)=>2C(B)+2H(S)+H		3.00E+13	0	215.27	[80]
134	p13(S)=>C_2H_3_(S)		5.54E+10	0	127.38	[80]
135	CH_2c5(S)+CH_3=>P12(S)+H	CH_4+CH_3=>C_2H_6+H	6.30E+01	0	0	ks=1.03E-02kg[55]
136	P12(S)+H=>CH_2c5(S)+CH_3	C_2H_6+H=>CH_3+CH_4	5.40E+04	0	48.59	ks=3.7E-03kg[55]

The same comments as shown above, Γ=1.45E-09.

3. Surface elementary reactions on zig-zag sites

3.1 Addition of three carbon atoms on zig-zag sites: C_2H_2+CH_3

When active carbon surface sites C_z(S) are created on zig-zag sites, addition of acetylene on C_z(S) occurs, forming the radical surface site k1(S). Unlike pyrocarbon deposition on armchair sites, three carbons are needed to form a non-aromatic six atoms ring. Two consumption pathways of k1(S) are considered: (1) Cyclization reaction with a neighboring Hz(S), forming the surface species k28(S) of a 5-atom ring[85,86]. Then isomerization reaction between k28(S) and a neighboring k1(S) occurs, leading to the elimination of a five-atom by formation of a six-atom ring. One k12(S), one CHCHz(S) and one C_z(S) are formed. (2) Addition of methyl on k1(S) occurs, forming the surface species k2(S). A hydrogen abstraction by gas-phase radical H/CH3 or initiation reaction occurs, forming the radical surface site k3(S). After the cyclization reaction between k3(S) and a neighboring Hz(S), one CHCHz(S) and one CH_2Bz(S) are formed. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

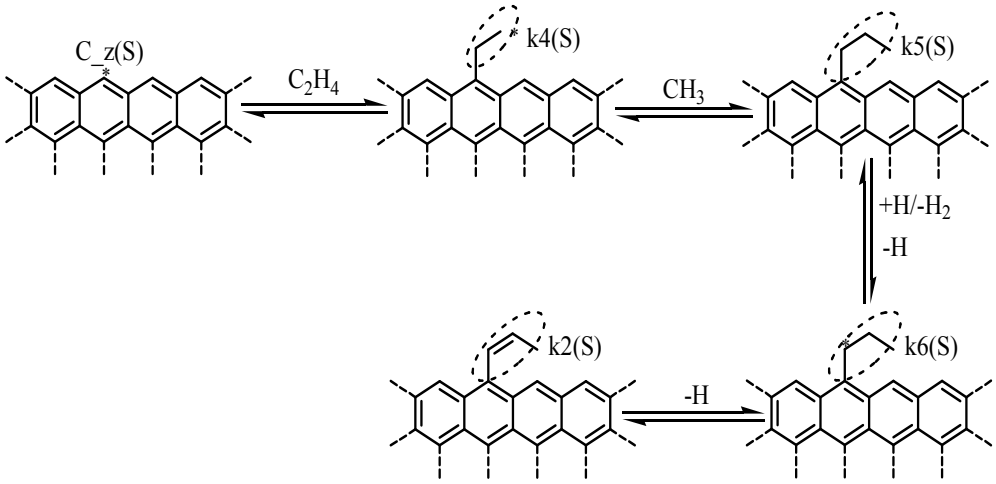


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
137	C_z(S)+C_2H_2=>k1(S)	C_6H_5+C_2H_2=>Products	2.69E+06	2.05	15.55	ks=0.1kg[14]
138	k1(S)=>C_z(S)+C_2H_2	Ethenyl,2-phenyl=>C_6H_5+C_2H_2	1.35E+14	0.34	191.03	ks=0.1kg[14]
139	k1(S)+CH_3=>k2(S)	C_2H_2+CH_3=>C_3H_5	1.61E+40	-8.58	84.85	ks=8.10E-03kg[56]
140	k2(S)=>k1(S)+CH_3	C_3H_5=>C_2H_2+CH_3	1.26E+13	0	585.2	ks=8.10E-03kg[20]
141	k2(S)+H=>k3(S)+H_2	CH_3CHCH_2+H=>CH_2CHCH_2+H_2	1.70E+05	2.5	10.38	ks=3.00E-03kg[26]
142	k3(S)+H_2=>k2(S)+H	CH_2CHCH_2+H_2=>CH_3CHCH_2+H	1.08E+05	2.38	79.42	ks=2.80E-03kg[27]
143	k2(S)+CH_3=>k3(S)+CH_4	CH_2CHCH_3+CH_3=>CH_2CHCH_2+CH_4	1.40E+11	0	36.47	ks=6.40E-03kg[57]
144	k3(S)+CH_4=>k2(S)+CH_3	CH_2CHCH_2+CH_4=>CH_3CHCH_2+CH_3	39.86	3.4	97.39	ks=5.70E-03kg[27]
145	k2(S)=>k3(S)+H	CH_3CHCH_2=>CH_2CHCH_2+H	2.5E+15	0	361.99	ks=2.60E-03kg[27]
146	k3(S)+H=>k2(S)	CH_2CHCH_2+H=>CH_3CHCH_2	5.83E+13	0.18	-0.52	ks=2.60E-03kg[58]
147	k3(S)+Hz(S)=>CH_2Bz(S)+CHCHz(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
148	k1(S)+Hz(S)=>k28(S)+H	$CHCH_2CH_2CH_2CH_2$=>C_5H_8+H	6.90E-03	0	-17.63	ks=kg/ Γ[59]
149	k1(S)+k28(S)=>k12(S)+CHCHz(S)+C_z(S)		3.00E+13	0	215.27	[80]

The same comments as shown above, Γ=1.45E-09.

3.2 Addition of three carbon atoms on zig-zag sites:C_2H_4+CH_3

When active carbon surface sites C_z(S) are created on zig-zag sites, addition of ethylene on C_z(S) occurs, forming the radical surface site k4(S). The methyl may adsorb on the radical surface site k4(S), forming the surface species k5(S). A hydrogen abstraction by gas-phase radical H or initiation reaction occurs, forming the radical surface site k6(S). Then the k6(S) may transform into k2(S) after a hydrogen abstraction by the initiation reaction, and the consumption of k2(S) is already mentioned above. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

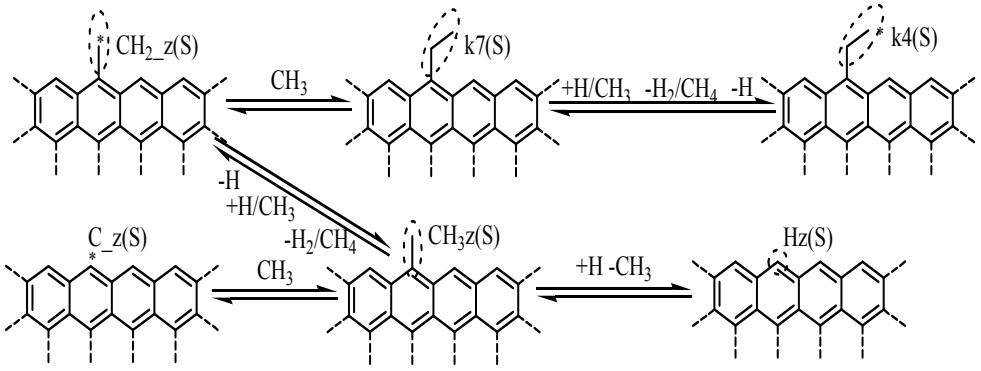


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
150	C_z(S)+C_2H_4=>k4(S)	C_6H_5+C_2H_4=>products	7.22E+06	1.62	12.38	ks=0.1kg[60]
151	k4(S)=>C_z(S)+C_2H_4	1-phenylethyl=>C_6H_5+C_2H_4	7.08E+14	0	181.83	ks=0.1kg[61]
152	k4(S)+CH_3=>k5(S)	CH_2CH_3+CH_3=>C_3H_8	1.93E+14	-0.32	0	ks=7.4E-03kg[62]
153	k5(S)=>k4(S)+CH_3	C_3H_8=>CH_2CH_3+CH_3	4.5E+16	0	337.74	ks=7.4E-03kg[63]
154	k5(S)+H=>k6(S)+H_2	C_3H_8+H=>C_3H_7+H_2	1.30E+06	2.4	18.69	ks=2.5E-03kg[64]
155	k6(S)+H_2=>k5(S)+H	C_3H_7+H_2=>C_3H_8+H	34.96	3.28	36.22	ks=2.8E-03kg[64]
156	k5(S)=>k6(S)+H	$CH_3CH_2CH_3$=>CH_3CHCH_3+H	6.31E+15	0	396.26	ks=2.5E-03kg[20]
157	k6(S)+H=>k5(S)	iso-C_3H_7+H=>C_3H_8	2.00E+13	0	0	ks=2.5E-03kg[51]
158	k6(S)=>k2(S)+H	iso-C_3H_7=>CH_3CHCH_2+H	1.11E+12	0.48	153.82	ks=3.0E-03kg[65]
159	k2(S)+H=>k6(S)	CH_3CHCH_2+H=>iso-C_3H_7	4.24E+11	0.51	5.14	ks=3.0E-03kg[65]

The same comments as shown above, Γ=1.45E-09.

3.3 Addition of three carbon atoms on zig-zag sites: CH_3+CH_3+CH_3

The methyl may adsorb on the active surface carbon site C_z(S), forming the surface species CH_3z(S). The CH_3z(S) reacts with a hydrogen atom followed by a methyl abstraction, turning into the surface species Hz(S). On the other hand, the CH_3z(S) turns into the radical surface site CH_2_z(S) by gas-phase radical H/CH_3 or initiation reaction. The methyl may adsorb on the CH_2_z(S), which is transformed into the surface species k7(S). A hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs, forming the radical surface site k4(S). The consumption of k4(S) is already mentioned above. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

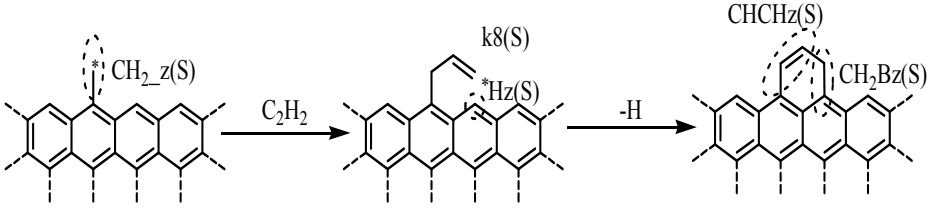


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
160	CH_2_z(S)+CH_3=>k7(S)	Benzyl+CH_3=>$C_6H_5CH_2CH_3$	1.19E+13	0	0.92	ks=0.1kg[47]
161	k7(S)=>CH_2_z(S)+CH_3	$C_6H_5CH_2CH_3$=>Benzyl+CH_3	2.09E+16	0	322.28	ks=0.1kg[47]
162	k7(S)+H=>k4(S)+H_2	CH_3CH_3+H=>CH_2CH_3+H_2	1.2E+14	0	34.39	ks=3.7E-03kg[42]
163	k4(S)+H_2=>k7(S)+H	CH_2CH_3+H_2=>CH_3CH_3+H	3.98E+13	0	96.56	ks=4.0E-03kg[66]
164	k7(S)+CH_3=>k4(S)+CH_4	CH_3CH_3+CH_3=>CH_2CH_3+CH_4	2E+13	0	56.43	ks=7.3E-03kg[67]
165	k4(S)+CH_4=>k7(S)+CH_3	CH_2CH_3+CH_4=>CH_3CH_3+CH_3	0.09	4.14	52.67	ks=7.6E-03kg[5]
166	k7(S)=>k4(S)+H	CH_3CH_3=>CH_2CH_3+H	8.96E+20	-1.23	426.36	ks=3.7E-03kg[68]
167	k4(S)+H=>k7(S)	CH_3CH_2+H=>CH_3CH_3	5.44E+13	0.16	0	ks=3.7E-03kg[21]
168	C_z(S)+CH_3=>CH_3z(S)	CH_3+C_6H_5=>$C_6H_5CH_3$	1.38E+13	0	0.19	ks=0.1kg[40]
169	CH_3z(S)=>C_z(S)+CH_3	$C_6H_5CH_3$=>C_6H_5+CH_3	5E+16	0	409.64	ks=0.1kg[29]
170	Hz(S)+CH_3=>H+CH_3z(S)	C_6H_6+CH_3=>$C_6H_5CH_3$+H	1.2E+12	0	66.46	ks=0.1kg[42]
171	H+CH_3z(S)=>Hz(S)+CH_3	$C_6H_5CH_3$+H=>C_6H_6+CH_3	9.50E+05	2	3.95	ks=0.1kg[69]
172	CH_3z(S)+H=>CH_2_z(S)+H_2	$C_6H_5CH_3$+H=>$C_6H_5CH_2$+H_2	1.33E+15	0	62.28	ks=0.1kg[44]
173	CH_2_z(S)+H_2=>CH_3z(S)+H	$C_6H_5CH_2$+H_2=>$C_6H_5CH_3$+H	2.82E+12	0	60.61	ks=0.1kg[45]
174	CH_3z(S)+CH_3=>CH_2_z(S)+CH_4	$C_6H_5CH_3$+CH_3=>$C_6H_5CH_2$+CH_4	2.51E+10	0	28.99	ks=0.1kg[50]
175	CH_2_z(S)+CH_4=>CH_3z(S)+CH_3	$CHCH_2$+CH_4=>C_2H_4+CH_3	1.45	4.02	22.84	ks=8.2E-03kg[5]
176	CH_3z(S)=>CH_2_z(S)+H	$C_6H_5CH_3$=>$C_6H_5CH_2$+H	6.31E+15	0	377.87	ks=0.1kg[46]
177	CH_2_z(S)+H=>CH_3z(S)	$C_6H_5CH_2$+H=>$C_6H_5CH_3$	2.08E+14	0	0.36	ks=0.1kg[47]

The same comments as shown above, Γ=1.45E-09.

3.4 Addition of three carbon atoms on zig-zag sites: CH_3+C_2H_2

We illustrate another consumption pathway of the radical surface site CH_2_z(S) here. Addition of acetylene on the CH_2_z(S) forms a radical surface site k8(S). Then after a cyclization reaction between k8(S) and a neighboring Hz(S), one surface species CHCHz(S) and one CH_2Bz(S) are formed. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

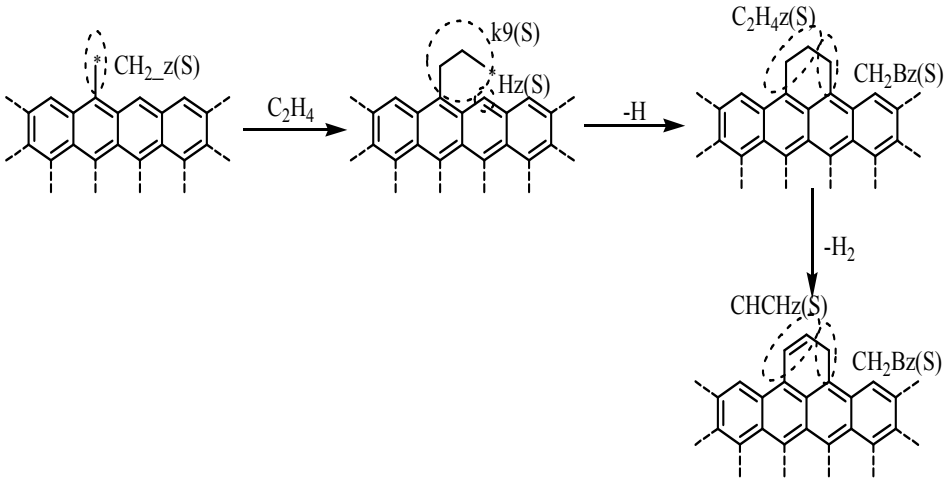


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
178	$CH_2\_z(S)+C_2H_2=>k8(S)$	C_2H_2+Benzyl=>Products	2.04E+06	1.84	51.83	ks=0.1kg[70]
179	$k8(S)+Hz(S)=>CH_2Bz(S)+CHCHz(S)+H$	$nC_6H_7=>A1+H$	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

3.5 Addition of three carbon atoms on zig-zag sites: $CH_3+C_2H_4$

We illustrate another consumption pathway of the radical surface site $CH_2\_z(S)$ here. Addition of ethylene on the $CH_2\_z(S)$ forms a radical surface site k9(S). Then after a cyclization reaction between k9(S) and a neighboring Hz(S), one surface species $C_2H_4z(S)$ and one $CH_2Bz(S)$ are formed. Through direct dehydrogenation reaction, the $C_2H_4z(S)$ turns into CHCHz(S). These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.



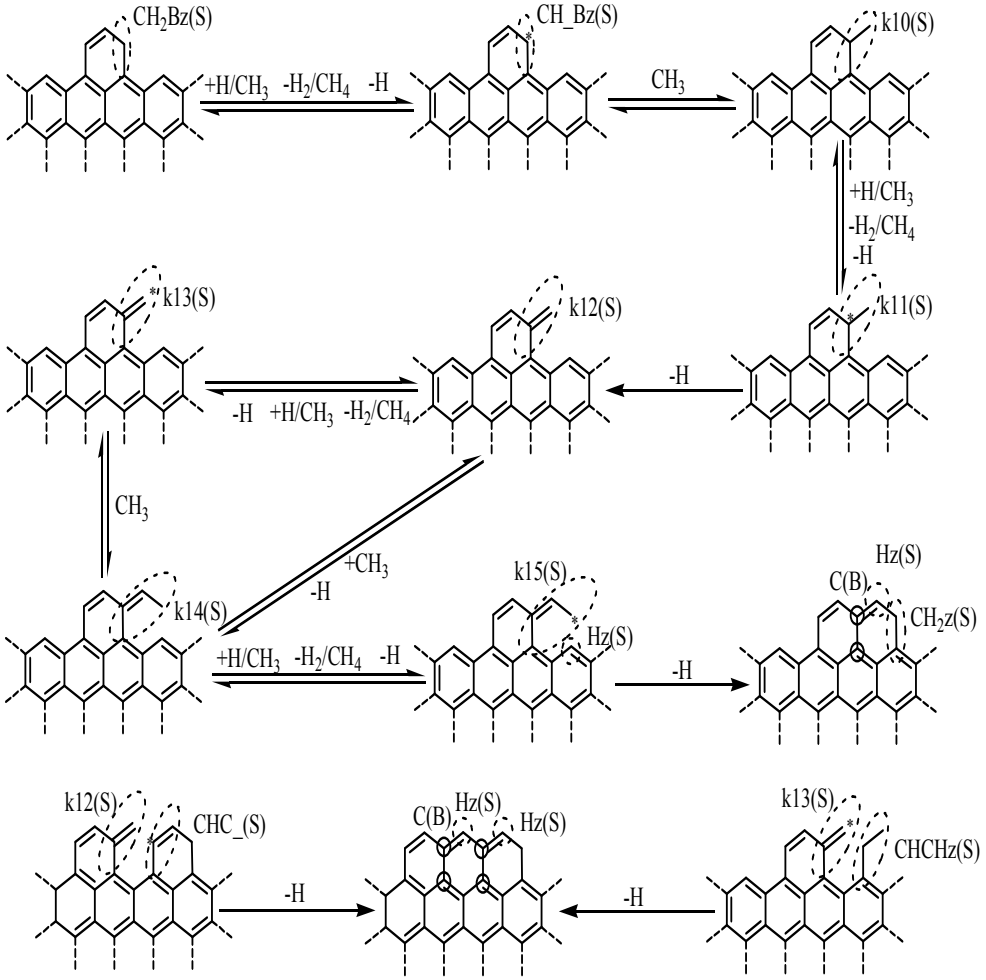
No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
180	$CH_2\_z(S)+C_2H_4=>k9(S)$	$CH_3+C_2H_4=>n\text{-}C_3H_7$	1.76E+04	2.48	25.62	ks=1.1E-02kg[65]
181	$k9(S)+Hz(S)=>CH_2Bz(S)+C_2H_4z(S)+H$	$nC_6H_7=>A1+H$	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
182	$C_2H_4z(S)=>CHCHz(S)+H_2$	$C_2H_4=>C_2H_2+H_2$	9.16E+16	0	313.92	ks=4.5E-03kg[71]

The same comments as shown above, Γ=1.45E-09.

3.6 Consumption of $CH_2Bz(S)$ sites

A non-aromatic six atoms ring is formed by the cyclization reaction, one of which is the surface species $CH_2Bz(S)$. A hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs on the $CH_2Bz(S)$, forming the radical surface site CH_Bz(S). The methyl may adsorb on the intermediate CH_Bz(S), forming the surface species k10(S). Then a hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs on the k10(S), forming the radical surface site k11(S). The k12(S) is formed by the hydrogen abstraction of the k11(S). Three consumption pathways are considered here: firstly, a hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs, the radical surface site k13(S) is formed; secondly,

addition of the methyl followed by a hydrogen abstraction occurs, forming the surface species k14(S); thirdly, cyclization reaction between the k12(S) and a neighboring CHC_(S) occurs, two Hz(S) and four C(B) are formed. Two consumption pathways of k13(S) are considered here: addition of the methyl occurs, the surface species k14(S) is formed; cyclization reaction between k13(S) and a neighboring CHCHz(S) occurs, two Hz(S) and four C(B) are formed. A hydrogen abstraction by gas-phase radical H/CH_3 occurs on the k14(S), forming an intermediate k15(S). The k15(S) may react with a neighboring Hz(S) by cyclization reaction, one Hz(S), one CH_2z(S) and two C(B) are formed. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.



No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
183	$CH_2Bz(S)+H=>CH\_Bz(S)+H_2$	$Cyclohexane+H=>H_2+Cycolhexyl$	2.80E+12	0	0	ks=0.1kg[72]
184	$CH\_Bz(S)+H_2=>CH_2Bz(S)+H$	$CH_2CHCH_2+H_2=>CH_3CHCH_2+H$	1.08E+05	2.38	79.42	ks=2.8E-03kg[27]
185	$CH_2Bz(S)+CH_3=>CH\_Bz(S)+CH_4$	$C_3H_6+CH_3=>C_3H_5+CH_4$	2.21E+00	3.5	23.75	ks=6.4E-03kg[27]
186	$CH\_Bz(S)+CH_4=>CH_2Bz(S)+CH_3$	$C_3H_5+CH_4=>C_3H_6+CH_3$	3.99E+01	3.4	97.39	ks=5.7E-03kg[27]
187	$CH_2Bz(S)=>CH\_Bz(S)+H$	$Benzyl=>C_7H_6+H$	8.20E+14	0	337.33	ks=0.1kg[44]

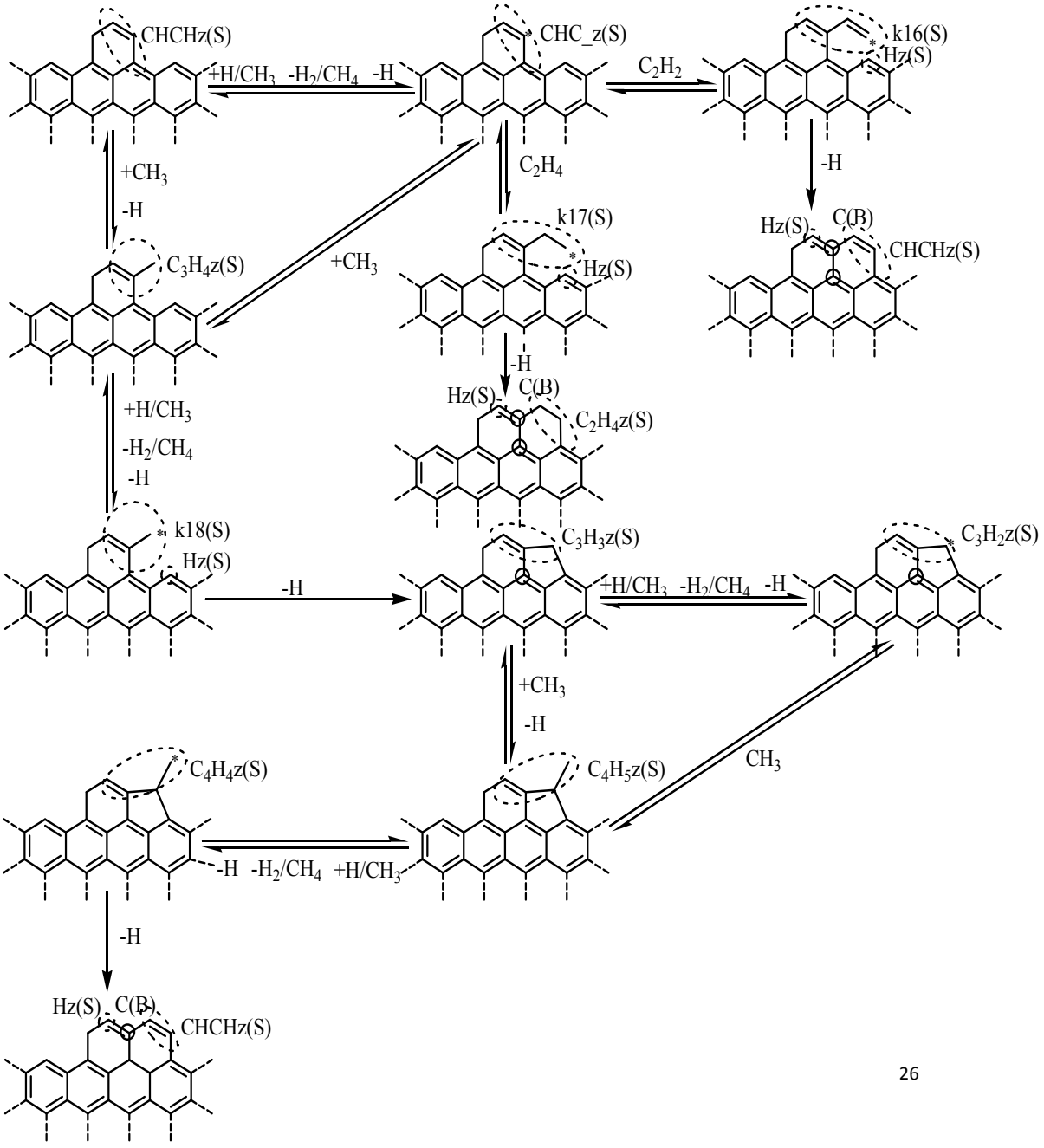
188	CH_Bz(S)+H=>CH_2Bz(S)	C_3H_5+H=>C_3H_6	5.83E+13	0.18	-0.52	ks=2.6E-03kg[58]
189	CH_Bz(S)+CH_3=>k10(S)	CH_2CHCH_2+CH_3=>1-C_4H_8	1.02E+14	-0.32	-0.55	ks=5.6E-03kg[27]
190	k10(S)=>CH_Bz(S)+CH_3	1-C_4H_8=>CH_2CHCH_2+CH_3	1.00E+16	0	304.72	ks=4.8E-03kg[20]
191	k10(S)+H=>k11(S)+H_2	C_3H_8+H=>iso-C_3H_7+H_2	1.30E+06	2.4	18.69	ks=2.5E-03kg[28]
192	k11(S)+H_2=>k10(S)+H	iso-C_3H_7+H_2=>C_3H_8+H	3.50E+01	3.28	36.22	ks=2.8E-03kg[28]
193	k10(S)+CH_3=>k11(S)+CH_4	1-C_4H_8+CH_3=>$CH_2CHCHCH_3$+CH_4	2.50E+11	0	34.80	ks=4.8E-03kg[51]
194	k11(S)+CH_4=>k10(S)+CH_3	iso-C_3H_7+CH_4=>C_3H_8+CH_3	7.23E-04	4.4	45.14	ks=5.7E-03kg[28]
195	k10(S)=>k11(S)+H	1-C_4H_8=>$CH_2CHCHCH_3$+H	1.26E+15	0	344.85	ks=2.20E-03kg[20]
196	k11(S)+H=>k10(S)	iso-C_3H_7+H=>C_3H_8	2.00E+13	0	0	ks=2.5E-03kg[51]
197	k11(S)=>k12(S)+H	iso-C_3H_7=>CH_3CHCH_2+H	1.11E+12	0.48	153.82	ks=3.0E-03kg[65]
198	k12(S)+H=>k13(S)+H_2	CH_3CHCH_2+H=>CH_3CHCH+H_2	7.83E+05	2.5	51.41	ks=3.0E-03kg[26]
199	k13(S)+H_2=>k12(S)+H	$CH_2CHCHCH$+H_2=>1,3-Butadiene+H	3.98E+09	0.5	15.45	ks=2.5E-03kg[73]
200	k12(S)+CH_3=>k13(S)+CH_4	1,3-Butadiene+CH_3=>$CH_2CHCHCH$+CH_4	7.00E+13	0	77.33	ks=4.8E-03kg[36]
201	k13(S)+CH_4=>k12(S)+CH_3	C_2H_3+CH_4=>C_2H_4+CH_3	1.45E+00	4.02	22.84	ks=8.20E-03kg[5]
202	k12(S)+CH_3=>k14(S)+H	C_2H_4+CH_3=>CH_3CHCH_2+H	1.70E+00	0	0	ks=8.0E-03kg[74]
203	k14(S)+H=>k12(S)+CH_3	CH_3CHCH_2+H=>C_2H_4+CH_3	4.52E+12	0	0	ks=3.0E-03kg[75]
204	k13(S)+CH_3=>k14(S)	C_2H_3+CH_3=>CH_3CHCH_2	7.23E+13	0	0	ks=8.0E-03kg[76]
205	k14(S)=>k13(S)+CH_3	CH_3CHCH_2=>C_2H_3+CH_3	1.10E+21	-1.2	408.80	ks=8.0E-03kg[27]
206	k14(S)+H=>k15(S)+H_2	CH_3CHCH_2+H=>CH_2CHCH_2+H_2	1.70E+05	2.5	10.38	ks=3.0E-03kg[26]
207	k15(S)+H_2=>k14(S)+H	CH_2CHCH_2+H_2=>CH_3CHCH_2+H	1.08E+05	2.38	79.42	ks=3.8E-03kg[27]
208	k14(S)+CH_3=>k15(S)+CH_4	CH_3CHCH_2+CH_3=>CH_2CHCH_2+CH_4	2.21E+00	3.5	23.75	ks=6.4E-03kg[27]
209	k15(S)+CH_4=>k14(S)+CH_3	CH_2CHCH_2+CH_4=>CH_3CHCH_2+CH_3	3.99E+01	3.4	97.39	ks=5.70E-03kg[27]
210	k14(S)=>k15(S)+H	CH_3CHCH_2=>CH_2CHCH_2+H	2.50E+15	0	361.99	ks=2.6E-03kg[27]
211	k15(S)+H=>k14(S)	CH_2CHCH_2+H=>CH_3CHCH_2	5.83E+13	0.18	-0.5225	ks=2.6E-03kg[58]
212	k15(S)+Hz(S)=>2C(B)+Hz(S)+CH_2Bz(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
213	k12(S)+CHC_z(S)=>4C(B)+2Hz(S) +H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
214	k13(S)+CHCHz(S) =>4C(B) +2Hz(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]

The same comments as shown above, Γ=1.45E-09.

3.7 Consumption of CHCHz(S) sites

A non-aromatic six atoms ring is formed by the cyclization reaction, one of which is the surface species CHCHz(S). Two consumption pathway of CHCHz(S) are considered here: a hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs on the CHCHz(S), forming the radical surface site CHC_z(S); addition of methyl followed by a hydrogen abstraction occurs, forming the surface species C_3H_4z(S). Three consumption pathways of the intermediate CHC_z(S) are considered here: firstly, addition of methyl occurs, forming the C_2H_4z(S); secondly, addition of acetylene occurs, forming the radical surface site k16(S), and the k16(S) transforms into one Hz(S), one CHCHz(S) and two C(B) by cyclization reaction between k16(S) and a neighboring Hz(S); thirdly, addition of ethylene occurs, forming the radical surface site k17(S), and the k17(S) transforms into one Hz(S), one C2H4z(S) and two C(B) by cyclization reaction between k17(S) and a neighboring

Hz(S). A hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs on the $C_3H_4z(S)$, forming the radical surface site k18(S). The intermediate k18(S) reacts with a neighboring Hz(S) by cyclization reaction, forming the $C_3H_3z(S)$ of a new five-atom ring. Two consumption pathways of $C_3H_3z(S)$ are considered here: a hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs, forming the radical surface site $C_3H_2z(S)$; addition of the methyl followed by a hydrogen abstraction occurs, forming the surface species $C_4H_5z(S)$. And the $C_3H_2z(S)$ can also transform into $C_4H_5z(S)$ by the methyl addition. Through a hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction, the surface species $C_4H_5z(S)$ turns into the radical surface site $C_4H_4z(S)$. Then isomerization reaction of the intermediate $C_4H_4z(S)$ occurs, one Hz(S), one CHCHz(S) and one C(B) are formed, leading to the elimination of a five-atom ring by the formation of a six-atom ring. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

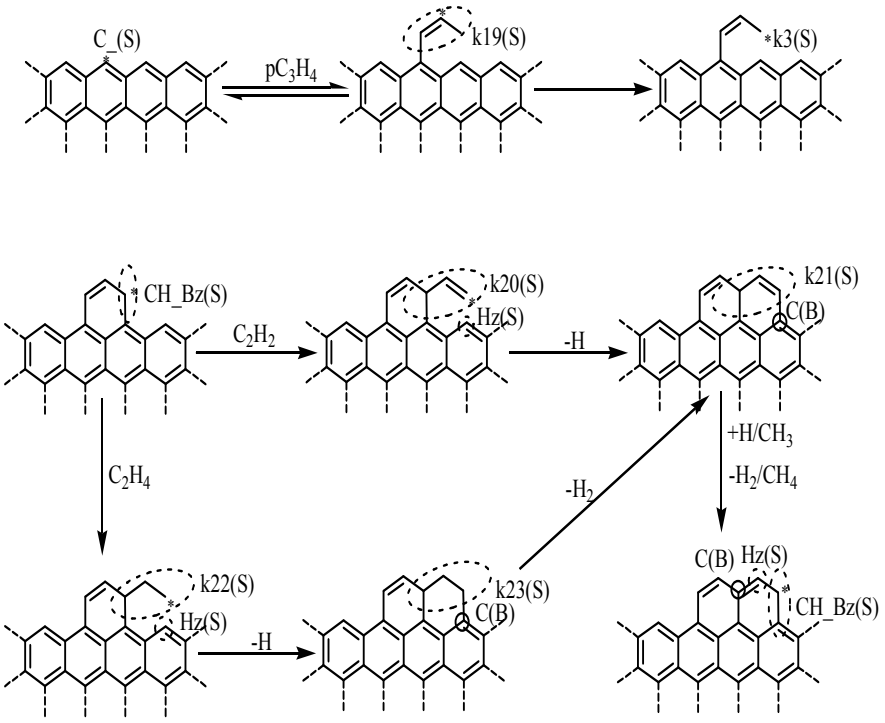


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
215	CHCHz(S)+H=>CHC_z(S)+H_2	C_3H_6+H=>C_3H_5+H_2	7.83E+05	2.5	51.41	ks=3.0E-03kg[26]
216	CHC_z(S)+H_2=>CHCHz(S)+H	CCH+H_2=>C_2H_2+H	2.36E+05	2.57	1.08	ks=4.6E-03kg[76]
217	CHCHz(S)+CH_3=>CHC_z(S)+CH_4	C_3H_6+CH_3=>C_3H_5+CH_4	6.10E-01	0	29.99	ks=6.4E-03kg[27]
218	CHC_z(S)+CH_4=>CHCHz(S)+CH_3	CH_2CH+CH_4=>C_2H_4+CH_3	1.45E+00	4.02	22.84	ks=8.2E-03kg[5]
219	CHCHz(S)+CH_3=>C_3H_4z(S)+H	Benzene+CH_3=>Toluene+H	1.20E+12	0	66.46	ks=0.1kg[42]
220	C_3H_4z(S)+H=>CHCHz(S)+CH_3	Toluene+H=>Benzene+CH_3	1.55E+13	0	24.21	ks=0.1kg[43]
221	CHCHz(S)=>CHC_z(S)+H	C_2H_4=>C_2H_3+H	2.00E+16	0	459.8	ks=4.1E-03kg[20]
222	CHC_z(S)+H=>CHCHz(S)	C_2H_3+H=>C_2H_4	3.88E+13	0.2	0	ks=4.1E-03kg[21]
223	CHC_z(S)+C_2H_2=>k16(S)	C_2H_3+C_2H_2=>CH_2CHCHCH	5.40E+09	0	0	ks=8.6E-03kg[35]
224	k16(S)=>CHC_z(S)+C_2H_2	CH_2CHCHCH=>C_2H_3+C_2H_2	1.00E+14	0	183.50	ks=8.6E-03kg[20]
225	k16(S)+Hz(S)=>2C(B)+Hz(S)+CHCHz(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
226	CHC_z(S)+C_2H_4=>k17(S)	C_2H_3+C_2H_4=>CH_2CHCH$_2$CH$_2$	2.00E+11	0	8.39	ks=8.9E-03kg[31]
227	k17(S)=>CHC_z(S)+C_2H_4	N-C_4H_9=>C_2H_4+C_2H_5	3.58E+12	0.46	123.31	ks=8.3E-03kg[65]
228	k17(S)+Hz(S)=>2C(B)+Hz(S)+C_2H_4z(S)+H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
229	CHC_z(S)+CH_3=>C_3H_4z(S)	C_3H_5+CH_3=>1-C_4H_8	1.02E+14	-0.32	-0.55	ks=5.6E-03kg[27]
230	C_3H_4z(S)=>CHC_z(S)+CH_3	Toluene=>CH_3+Phenyl	5.00E+16	0	409.64	ks=0.1kg[41]
231	C_3H_4z(S)+H=>k18(S)+H_2	Toluene+H=>Benzyl+H_2	1.33E+15	0	62.28	ks=0.1kg[44]
232	k18(S)+H_2=>C_3H_4z(S)+H	Benzyl+H_2=>Toluene+H	2.82E+12	0	60.61	ks=0.1kg[45]
233	C_3H_4z(S)+CH_3=>k18(S)+CH_4	Toluene+CH_3=>Benzyl+CH_4	2.51E+10	0	28.99	ks=0.1kg[50]
234	k18(S)+CH_4=>C_3H_4z(S)+CH_3	C_3H_5+CH_4=>C_3H_6+CH_3	3.99E+01	3.4	97.39	ks=5.7E-03kg[27]
235	C_3H_4z(S)=>k18(S)+H	Toluene=>Benzyl+H	3.10E+15	0	372.86	ks=0.1kg[13]
236	k18(S)+H=>C_3H_4z(S)	Benzyl+H=>Toluene	2.59E+14	0	0	ks=0.1kg[13]
237	k18(S) + Hz(S) =>C(B)+ C_3H_3z(S) + H	$CHCH_2CH_2CH_2CH_2$=>C_5H_8+H	6.90E-03	0	-17.63	ks=kg/ Γ[48]
238	C_3H_3z(S)+H=>C_3H_2z(S)+H_2	C_5H_{10}+H=>Cycolpentyl+H_2	2.41E+09	1.5	20.27	ks=0.1kg[49]
239	C_3H_2z(S)+H_2=>C_3H_3z(S)+H	iso-C_3H_7+H_2=>C_3H_8+H	3.50E+01	3.28	36.22	ks=2.8E-03kg[64]
240	C_3H_3z(S)+CH_3=>C_3H_2z(S)+CH_4	C_5H_{10}+CH_3=>Cyclopentyl+CH_4	2.00E+11	0	35.97	ks=0.1kg[50]
241	C_3H_2z(S)+CH_4=>C_3H_3z(S)+CH_3	iso-C_3H_7+CH_4=>C_3H_8+CH_3	7.32E-04	4.4	45.14	ks=5.7E-03kg[64]
242	C_3H_3z(S)=>C_3H_2z(S)+H	C_3H_8=>iso-C_3H_7+H	6.31E+15	0	411.31	ks=2.5E-03kg[20]
243	C_3H_2z(S)+H=>C_3H_3z(S)	iso-C_3H_7+H=>C_3H_8	2.00E+13	0	0	ks=2.5E-03kg[51]
244	C_3H_3z(S)+CH_3=>C_4H_5z(S)+H	CH_4+CH_3=>C_2H_6+H	6.30E+01	0	0	ks=1.03E-02kg[55]
245	C_4H_5z(S)+H=>C_3H_3z(S)+CH_3	C_2H_6+H=>CH_4+CH_3	5.40E+04	0	48.59	ks=3.7E-03kg[55]
246	C_3H_2z(S)+CH_3=>C_4H_5z(S)	iso-C_3H_7+CH_3=>iso-C_4H_{10}	6.64E+14	-0.57	0	ks=5.5E-03kg[62]
247	C_4H_5z(S)=>C_3H_2z(S)+CH_3	Methylcyclopentane=>Cyclopentyl+CH_3	1.26E+12	0	367.84	ks=0.1kg[53]
248	C_4H_5z(S)+H=>C_4H_4z(S)+H_2	iso-C_4H_{10}+H=>tert-C_4H_9+H_2	6.02E+05	2.4	10.80	ks=2.1E-03kg[54]
249	C_4H_4z(S)+H_2=>C_4H_5z(S)+H	tert-C_4H_9+H_2=>iso-C_4H_{10}+H	2.00E-02	4.24	37.46	ks=2.3E-03kg[54]
250	C_4H_5z(S)+CH_3=>C_4H_4z(S)+CH_4	iso-C_4H_{10}+CH_3=>tert-C_4H_9+CH_4	3.60E+00	3.46	19.18	ks=4.7E-03kg[77]
251	C_4H_4z(S)+CH_4=>C_4H_5z(S)+CH_3	tert-C_4H_9+CH_4=>iso-C_4H_{10}+CH_3	4.93E-07	5.38	49.74	ks=4.9E-03kg[54]
252	C_4H_5z(S)=>C_4H_4z(S)+H	C_3H_8=>iso-C_3H_7+H	6.31E+15	0	396.26	ks=2.5E-03kg[20]
253	C_4H_4z(S)+H=>C_4H_5z(S)	tert-C_4H_9+H=>iso-C_4H_{10}	5.20E+12	0.28	0	ks=2.1E-03kg[21]
254	C_4H_4z(S) =>C(B)+Hz(S) +CHCHz(S) +H		3.00E+13	0	215.27	[80]

The same comments as shown above, Γ=1.45E-09.

3.8 Addition of three carbon atoms on zig-zag sites: propyne deposition

When active carbon surface sites C_z(S) are created on zig-zag sites, addition of propyne on C_z(S) occurs, forming the radical surface site k19(S). An isomerization step of the intermediate k19(S) occurs, leading to the formation of the radical surface site k3(S). The consumption of the intermediate k3(S) is already mentioned above. Here we focus on the consumption of the intermediate CH_Bz(S): (1) addition of acetylene on the CH_Bz(S) occurs, forming the radical surface site k20(S), which may react with a neighboring Hz(S) by cyclization reaction. One k21(S) and one C(B) are formed in this process. A hydrogen abstraction by gas-phase radical H/CH_3 occurs on the k21(S), forming one Hz(S), one C(B) and one radical surface site CH_Bz(S); (2) addition of ethylene on the CH_Bz(S) occurs, forming the radical surface site k22(S), which may react with a neighboring Hz(S) by cyclization reaction. One k23(S) and one C(B) are formed in this process. Then the k23(S) may transform into k21(S) by direct dehydrogenation reaction. These reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

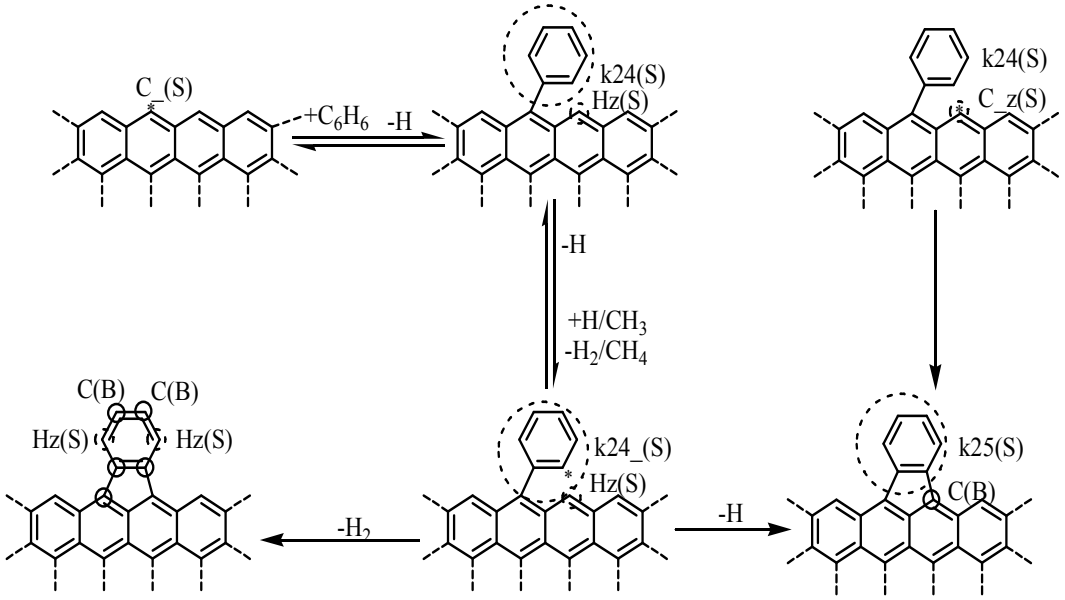


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
255	C_z(S)+PC3H4=>k19(S)	C_6H_5+CH_3CCH=>Products	3.59E+04	2.55	11.53	ks=0.1kg[24]
256	k19(S)=>C_z(S)+PC3H4	$CH_2CCHCH_2CH_3$=>C_2H_4+CH_3CCH	6.60E+12	0	242.86	ks=7.8E-03kg[78]
257	k19(S)=>k3(S)	$C_6H_5(CH_3)CHC$=>$C_6H_5C_3H_4$	1.00E+10	0	0	ks=0.1kg[38]
258	CH_Bz(S)+C_2H_2=>k20(S)	C_2H_2+Benzyl=>Products	2.04E+06	1.84	51.83	ks=0.1kg[70]
259	k20(S) + Hz(S) => k21(S) +C(B) + H	N-C_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
260	k21(S) + H =>C(B)+Hz(S)+H_2+ CH_Bz(S)	C_6H_6+H=>C_6H_5+H_2	6.02E+08	1.8	68.6	ks=0.1kg[1]
261	k21(S)+CH3=>C(B)+Hz(S)+CH4+CH_Bz(S)	C_6H_6+CH_3=>C_6H_5+CH_4	2.00E+12	0	35.97	ks=0.1kg[2]
262	CH_Bz(S)+C_2H_4=>k22(S)	ethyl,2-phenyl+C_2H_4=>$C_6H_5CH_2CH_2CH_2CH_2$	5.11E+12	0	49.74	ks=0.1kg[79]
263	k22(S) + Hz(S) => C(B) +H +k23(S)	nC_6H_7=>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
264	k23(S) =>k21(S) +H_2	1,3-C_6H_8=>C_6H_6+H_2	2.51E+13	0	246.62	ks=0.1kg[22]

The same comments as shown above, Γ=1.45E-09.

3.9 Deposition of benzene on zig-zag sites

Analogous to the deposition of benzene on the armchair site, the benzene adsorbs on the active carbon surface site C_z(S), forming the surface species k24(S) without active, then through aryl-aryl combination and intramolecular cyclization with a neighboring C_(S), active surface site k25(S) occupying two sites is formed; these reactions conserve sites. A hydrogen abstraction by gas-phase radical H/CH_3 or initiation reaction occurs, forming the radical surface site k24_(S), then through aryl-aryl combination and intramolecular dehydrocyclization with a neighboring Hz(S), surface site k25(S) occupying two sites is formed. The k24_(S) species transforms into bulk carbon C(B) by direct dehydrogenation reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.

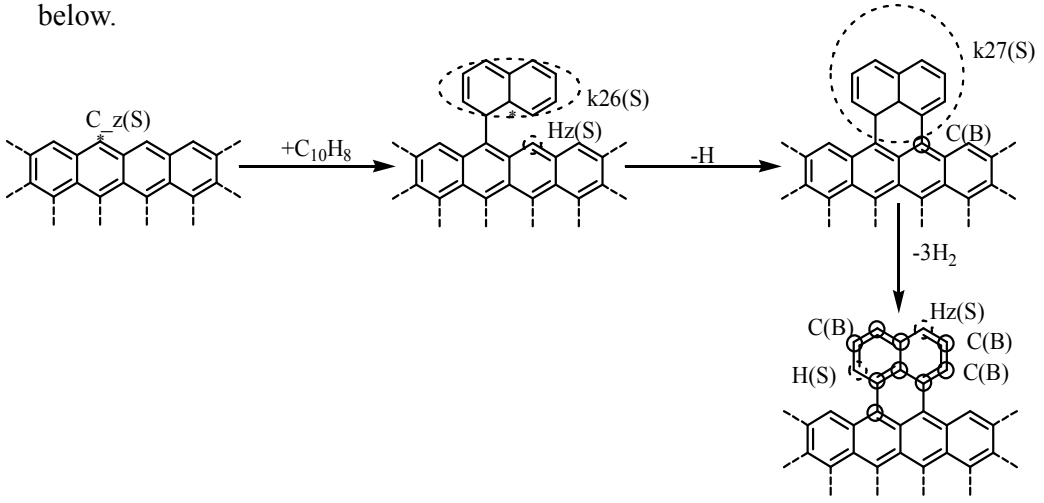


No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
265	C_z(S)+C_6H_6=>k24(S)+H	C_6H_5+C_6H_6=>Biphenyl+H	3.16E+12	0	35.59	ks=0.1kg[37]
266	k24(S)+C_z(S)=>C(B)+k25(S)+H	N-C_6H_7 =>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
267	k24(S)+H=>k24_(S)+H_2	C_6H_6+H=>C_6H_5+H_2	6.02E+08	1.8	68.55	ks=0.1kg[1]
268	k24_(S)+H_2=>k24(S)+H	C_6H_5+H_2=>C_6H_6+H	3.98E+12	0	32.98	ks=0.1kg[2]
269	k24(S)+CH_3=>k24_(S)+CH_4	C_6H_6+CH_3=>C_6H_5+CH_4	2.62E+13	0	80.67	ks=0.1kg[3]
270	k24_(S)+CH_4=>k24(S)+CH_3	C_6H_5+CH_4=>C_6H_6+CH_3	2E+12	0	35.97	ks=0.1kg[2]
271	k24(S)=>k24_(S)+H	C_6H_6=>C_6H_5+H	2E+17	0	459.8	ks=0.1kg[12]
272	k24_(S)+H=>k24(S)	C_6H_5+H=>C_6H_6	2.20E+14	0	0	ks=0.1kg[32]
273	k24_(S)+Hz(S)=>C(B)+k25(S)+H	N-C_6H_7 =>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
274	k25(S)=>5C(B)+2Hz(S)+H_2	1-3-Cyclohexadiene=>Benzene+H_2	2.51E+13	0	247	ks=0.1kg[22]

The same comments as shown above, Γ=1.45E-09.

3.10 Deposition of naphthalene on zig-zag sites

Analogous to the deposition of naphthalene on armchair site, the naphthalene adsorbs on the active carbon surface site C_z(S), forming the radical surface site k26(S), then through aryl-aryl combination and intramolecular dehydrocyclization with a neighboring Hz(S), the surface species k27(S) occupying two sites is formed; The k27(S) then transforms into Hz(S), H(S) and bulk carbon C(B) by direct dehydrogenation reaction; these reactions conserve sites. Detailed reaction pathway and the related surface reactions with corrected kinetic parameters are illustrated below.



No.	Surface reaction	Prototype gas-phase reaction	A	n	Ea	values for ks and references
275	C_z(S)+$C_{10}H_8$=>k26(S)	Phenyl+Phenylacetylene=>ethenyl,1,2-diphenyl	4.19E+04	2.74	14.68	ks=0.1kg[33]
276	k26(S)+Hz(S)=>C(B)+k27(S)+H	N-C_6H_7 =>A1+H	8.40E+21	-4.22	47.46	ks=kg/ Γ[15]
277	k27(S)=>9C(B)+H(S)+Hz(S)+3H_2		2.51E+13	0	246.76	[80]

The same comments as shown above, Γ=1.45E-09.

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