Supplementary Information

Reaction Mechanism Reduction for Ozone-Enhanced CH_4/Air Combustion by a Combination of Directed Relation Graph with Error Propagation, Sensitivity Analysis and Quasi-Steady State Assumption

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Table S1. The ozone-enhanced CH_4 combustion skeletal mechanism

Species in skeletal mechanism						
H_2	H	O	O_2	OH	H_2O	HO_2
CH_2	$CH_2(S)$	CH_3	CH_4	CO	CO_2	HCO
CH_3O	C_2H_4	C_2H_5	C_2H_6	N	NO	HCN
AR	O_3	CH	CH_2O	N_2		

No.	Elementary Reaction[1]	A	b	E	No.	Elementary Reaction [1]	A	b	E
1	$2O+M=O_2+M$[2]	1.20E+17	-1	0	65	$HO_2+CH_2=OH+CH_2O$	2.00E+13	0	0
2	$O+H+M=OH+M$[2]	5.00E+17	-1	0	66	$HO_2+CH_3=O_2+CH_4$	1.00E+12	0	0
3	$O+H_2=H+OH$	3.87E+04	2.7	6260	67	$HO_2+CH_3=OH+CH_3O$	3.78E+13	0	0
4	$O+HO_2=OH+O_2$	2.00E+13	0	0	68	$HO_2+CO=OH+CO_2$	1.50E+14	0	23600
5	$O+CH=H+CO$	5.70E+13	0	0	69	$CH+O_2=O+HCO$	6.71E+13	0	0
6	$O+CH_2=H+HCO$	8.00E+13	0	0	70	$CH+H_2=H+CH_2$	1.08E+14	0	3110
7	$O+CH_2(S)=H_2+CO$	1.50E+13	0	0	71	$CH+H_2O=H+CH_2O$	5.71E+12	0	-755
8	$O+CH_2(S)=H+HCO$	1.50E+13	0	0	72	$CH+CH_4=H+C_2H_4$	6.00E+13	0	0
9	$O+CH_3=H+CH_2O$	5.06E+13	0	0	73	$CH+CO_2=HCO+CO$	1.90E+14	0	15792
10	$O+CH_4=OH+CH_3$	1.02E+09	1.5	8600	74	$CH_2+O_2=>OH+H+CO$	5.00E+12	0	1500
11	$O+CO(+M)=CO_2(+M)$[2]	1.80E+10	0	2385	75	$CH_2+H_2=H+CH_3$	5.00E+05	2	7230
12	$O+HCO=OH+CO$	3.00E+13	0	0	76	$CH_2+CH_3=H+C_2H_4$	4.00E+13	0	0
13	$O+HCO=H+CO_2$	3.00E+13	0	0	77	$CH_2+CH_4=2CH_3$	2.46E+06	2	8270
14	$O+CH_2O=OH+HCO$	3.90E+13	0	3540	78	$CH_2(S)+N_2=CH_2+N_2$	1.50E+13	0	600
15	$O+CH_3O=OH+CH_2O$	1.00E+13	0	0	79	$CH2(S)+O_2=H+OH+CO$	2.80E+13	0	0
16	$O+C_2H_4=CH_3+HCO$	1.25E+07	1.8	220	80	$CH_2(S)+O_2=CO+H_2O$	1.20E+13	0	0

Table S1. *Cont.*

17	$O+C_2H_5=CH_3+CH_2O$	2.24E+13	0	0	81	$CH_2(S)+H_2=CH_3+H$	7.00E+13	0	0
18	$O+C_2H_6=OH+C_2H_5$	8.98E+07	1.9	5690	82	$CH_2(S)+H_2O=CH_2+H_2O$	3.00E+13	0	0
19	$O_2+CO=O+CO_2$	2.50E+12	0	47800	83	$CH_2(S)+CH_3=H+C_2H_4$	1.20E+13	0	-570
20	$O_2+CH_2O=HO_2+HCO$	1.00E+14	0	40000	84	$CH_2(S)+CH_4=2CH_3$	1.60E+13	0	-570
21	$H+O_2+M=HO_2+M^2$	2.80E+18	-0.9	0	85	$CH_2(S)+CO=CH_2+CO$	9.00E+12	0	0
22	$H+2O_2=HO_2+O_2$	2.08E+19	-1.2	0	86	$CH_2(S)+CO_2=CH_2+CO_2$	7.00E+12	0	0
23	$H+O_2+H_2O=HO_2+H_2O$	1.13E+19	-0.8	0	87	$CH_2(S)+CO_2=CO+CH_2O$	1.40E+13	0	0
24	$H+O_2+N_2=HO_2+N_2$	2.60E+19	-1.2	0	88	$CH_2(S)+C_2H_6=CH_3+C_2H_5$	4.00E+13	0	-550
25	$H+O_2=O+OH$	2.65E+16	-0.7	17041	89	$CH_3+O_2=O+CH_3O$	3.56E+13	0	30480
26	$2H+M=H_2+M^2$	1.00E+18	-1	0	90	$CH_3+O_2=OH+CH_2O$	2.31E+12	0	20315
27	$2H+H_2=2H_2$	9.00E+16	-0.6	0	91	$2CH_3(+M)=C_2H_6(+M)^2$	6.77E+16	-1.2	654
28	$2H+H_2O=H_2+H_2O$	6.00E+19	-1.2	0	92	$2CH_3=H+C_2H_5$	6.84E+12	0.1	10600
29	$2H+CO_2=H_2+CO_2$	5.50E+20	-2	0	93	$CH_3+HCO=CH_4+CO$	2.65E+13	0	0
30	$H+OH+M=H_2O+M^2$	2.20E+22	-2	0	94	$CH_3+CH_2O=HCO+CH_4$	3.32E+03	2.8	5860
31	$H+HO_2=O+H_2O$	3.97E+12	0	671	95	$CH_3+C_2H_6=C_2H_5+CH_4$	6.14E+06	1.7	10450
32	$H+HO_2=O_2+H_2$	4.48E+13	0	1068	96	$HCO+H_2O=H+CO+H_2O$	1.50E+18	-1	17000
33	$H+HO_2=2OH$	8.40E+13	0	635	97	$HCO+M=H+CO+M^2$	1.87E+17	-1	17000
34	$H+CH_2(+M)=CH_3(+M)^2$	6.00E+14	0	0	98	$HCO+O_2=HO_2+CO$	1.34E+13	0	400
35	$H+CH_2(S)=CH+H_2$	3.00E+13	0	0	99	$CH_3O+O_2=HO_2+CH_2O$	4.28E-13	7.6	-3530
36	$H+CH_3(+M)=CH_4(+M)^2$	1.39E+16	-0.5	536	100	$C_2H_5+O_2=HO_2+C_2H_4$	8.40E+11	0	3875
37	$H+CH_4=CH_3+H_2$	6.60E+08	1.6	10840	101	$N+NO=N_2+O$	2.70E+13	0	355
38	$H+HCO(+M)=CH_2O(+M)^2$	1.09E+12	0.5	-260	102	$N+O_2=NO+O$	9.00E+09	1	6500
39	$H+HCO=H_2+CO$	7.34E+13	0	0	103	$N+OH=NO+H$	3.36E+13	0	385
40	$H+CH_2O(+M)=CH_3O(+M)^2$	5.40E+11	0.5	2600	104	$CH+N_2=HCN+N$	3.12E+09	0.9	20130
41	$H+CH_2O=HCO+H_2$	5.74E+07	1.9	2742	105	$CH+NO=HCN+O$	4.10E+13	0	0
42	$H+CH_3O=H_2+CH_2O$	2.00E+13	0	0	106	$CH+NO=N+HCO$	2.46E+13	0	0
43	$H+CH_3O=OH+CH_3$	1.50E+12	0.5	-110	107	$CH_2+NO=OH+HCN$	2.90E+14	-0.7	760
44	$H+CH_3O=CH_2(S)+H_2O$	2.62E+14	-0.2	1070	108	$CH_2(S)+NO=OH+HCN$	2.90E+14	-0.7	760
45	$H+C_2H_4(+M)=C_2H_5(+M)^2$	5.40E+11	0.5	1820	109	$CH_3+NO=HCN+H_2O$	9.60E+13	0	28800
46	$H+C_2H_5(+M)=C_2H_6(+M)^2$	5.21E+17	-1	1580	110	$CH_3+N=HCN+H_2$	3.70E+12	0.1	-90
47	$H+C_2H_5=H_2+C_2H_4$	2.00E+12	0	0	111	$N+CO_2=NO+CO$	3.00E+12	0	11300
48	$H+C_2H_6=C_2H_5+H_2$	1.15E+08	1.9	7530	112	$O+CH_3=>H+H_2+CO$	3.37E+13	0	0
49	$H_2+CO(+M)=CH_2O(+M)^2$	4.30E+07	1.5	79600	113	$OH+HO_2=O_2+H_2O$	5.00E+15	0	17330
50	$OH+H_2=H+H_2O$	2.16E+08	1.5	3430	114	$OH+CH_3=>H_2+CH_2O$	8.00E+09	0.5	-1755
51	$2OH=O+H_2O$	3.57E+04	2.4	-2110	115	$CH+H_2(+M)=CH_3(+M)^2$	1.97E+12	0.4	-370
52	$OH+HO_2=O_2+H_2O$	1.45E+13	0	-500	116	$CH_2+O_2=>2H+CO_2$	5.80E+12	0	1500
53	$OH+CH=H+HCO$	3.00E+13	0	0	117	$CH_2+O_2=O+CH_2O$	2.40E+12	0	1500
54	$OH+CH_2=H+CH_2O$	2.00E+13	0	0	118	$CH_2(S)+H_2O=>H_2+CH_2O$	6.82E+10	0.2	-935
55	$OH+CH_2=CH+H_2O$	1.13E+07	2	3000	119	$2O_2+O=>O_3+O_2$	3.26E+19	-2.1	0
56	$OH+CH_2(S)=H+CH_2O$	3.00E+13	0	0	120	$O_2+O+N_2=>O_3+N_2$	1.60E+14	-0.4	-1391
57	$OH+CH_3=CH_2+H_2O$	5.60E+07	1.6	5420	121	$O_2+2O=>O_3+O$	2.28E+15	-0.5	-1391

Table S1. *Cont.*

58	$OH+CH_3=CH_2(S)+H_2O$	6.44E+17	-1.3	1417	122	$O_2+O+O_3=>2O_3$	1.67E+15	-0.5	-1391
59	$OH+CH_4=CH_3+H_2O$	1.00E+08	1.6	3120	123	$O_3+H=O_2+OH$	8.43E+13	0	934
60	$OH+CO=H+CO_2$	4.76E+07	1.2	70	124	$O_3+H=O+HO_2$	4.52E+11	0	0
61	$OH+HCO=H_2O+CO$	5.00E+13	0	0	125	$O_3+OH=O_2+HO_2$	1.85E+11	0	831
62	$OH+CH_2O=HCO+H_2O$	3.43E+09	1.2	-447	126	$O_3+HO_2=OH+2O_2$	6.62E+09	0	994
63	$OH+CH_3O=H_2O+CH_2O$	5.00E+12	0	0	127	$O_3+O=2O_2$	4.82E+12	0	4094
64	$OH+C_2H_6=C_2H_5+H_2O$	3.54E+06	2.1	870	128	$O_3+CH_3=CH_3O+O_2$	5.83E+10	0	0

[1] The rate constants are in form of $k = AT^n\exp(-E/RT)$ (cal, cm^3, mol, s)

[2] Third-body enhancement coefficients: (1) H_2/2.4，H_2O/15.4，CH_4/2，CO/1.75，CO_2/3.6，C_2H_6/3；(2) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/6；(11) H_2/2，O_2/6，H_2O/6，CH_4/2，CO/1.5，CO_2/3.5，C_2H_6/3；(21) O_2/0，H_2O/0，CO/0.75，CO_2/1.5，C_2H_6/1.5，N_2/0；(26) H_2/0，H_2O/0，CH_4/2，CO_2/0，C_2H_6/3；(30) H_2/0.73，H_2O/3.65，CH_4/2，C_2H_6/3；(34) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(36) H_2/2，H_2O/6，CH_4/3，CO/1.5，CO_2/2，C_2H_6/3；(38) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(40) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(45) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(46) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(49) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(91) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(97) H_2/2，H_2O/0，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3；(115) H_2/2，H_2O/6，CH_4/2，CO/1.5，CO_2/2，C_2H_6/3。

Table S2. The reaction rate of each overall reaction and species

The reaction rate of each overall reaction:

*W[1] = - 0.5*w[2] + w[3] + 1.5*w[4] + 0.5*w[5] - 0.5*w[6] - w[7] + 0.5*w[8] - 0.5*w[9] + w[10] - 0.5*w[12] - 0.5*w[14] - w[15] + 0.5*w[16] + 0.5*w[17] + w[18] - 2*w[20] - 2*w[21] - 2*w[22] - 2*w[23] - 2*w[24] - 0.5*w[25] - 1.5*w[26] - 1.5*w[27] - 1.5*w[28] - 1.5*w[29] + w[30] + 2.5*w[31] + 0.5*w[32] + w[33] - 1.5*w[35] - 1.5*w[36] - 1.5*w[39] + 0.5*w[40] - 1.5*w[41] - 2*w[42] - 0.5*w[43] - 0.5*w[44] - 1.5*w[46] - 1.5*w[47] + 1.5*w[49] + 2.5*w[50] + 1.5*w[51] + 3.0*w[52] + w[53] + w[56] + w[57] + 2.5*w[59] + 0.5*w[60] + w[61] + w[62] + 0.5*w[63] + 2.5*w[64] + w[65] + 0.5*w[66] + 1.5*w[67] + 1.5*w[68] + 0.5*w[69] + 2.5*w[70] + 1.5*w[72] + 0.5*w[73] - w[74] + 1.5*w[75] - w[76] + 1.5*w[77] + w[78] + w[80] + 2.5*w[81] + w[82] + 2.5*w[84] + w[85] + w[86] + 0.5*w[87] + 2.5*w[88] - w[90] - 2.5*w[91] - w[92] - 1.5*w[93] - 1.5*w[94] - 2*w[98] - 2.5*w[99] - 2*w[100] + 0.5*w[102] + w[103] - 1.5*w[107] - 0.5*w[108] - 0.5*w[109] - 2*w[110] + 0.5*w[111] - 2*w[112] + 3.0*w[113] - 1.5*w[114] + 2.5*w[115] - 0.5*w[116] - 0.5*w[117] - 1.5*w[118] - 0.5*w[123] - 2*w[124] - 1.5*w[125] + 1.5*w[126]*

*W[2] = - 0.5*w[2] + 0.5*w[4] + 0.5*w[5] - 0.5*w[6] + 0.5*w[8] - 0.5*w[9] - 0.5*w[12] - 0.5*w[14] - w[15] + 0.5*w[16] + 0.5*w[17] - w[20] - w[21] - w[22] - w[23] - w[24] - 0.5*w[25] - 0.5*w[26] - 0.5*w[27] - 0.5*w[28] - 0.5*w[29] + w[30] + 1.5*w[31] + 0.5*w[32] - 0.5*w[35] - 0.5*w[36] - 0.5*w[39] + 0.5*w[40] - 0.5*w[41] - w[42] - 0.5*w[43] - 0.5*w[44] - 0.5*w[46] - 0.5*w[47] + 0.5*w[49] + 1.5*w[50] + 1.5*w[51] + 2*w[52] + w[53] + w[56] + w[57] + 1.5*w[59] + 0.5*w[60] + w[61] + w[62] + 0.5*w[63] + 1.5*w[64] + 0.5*w[66] + 0.5*w[67] + 0.5*w[68] + 0.5*w[69] + 1.5*w[70] + 0.5*w[72] + 0.5*w[73] - w[74] + 0.5*w[75] - w[76] + 0.5*w[77] + w[78] + w[80] + 1.5*w[81] + w[82] + 1.5*w[84] + w[85] + w[86] + 0.5*w[87] + 1.5*w[88] - w[90] - 1.5*w[91] - w[92] - 0.5*w[93] - 0.5*w[94] - w[98] - 1.5*w[99] - w[100] + 0.5*w[102] + w[103] - 1.5*w[107] - 0.5*w[108] - 0.5*w[109] - w[110] + 0.5*w[111] - w[112] + 2*w[113] - 0.5*w[114] + 1.5*w[115] - 0.5*w[116] - 0.5*w[117] - 0.5*w[118] - 0.5*w[123] - w[124] - 0.5*w[125] + 0.5*w[126]*

*W[3] = w[5] - w[9] + w[10] + w[16] + 2*w[18] + w[34] - w[35] - w[36] + w[37] + w[43] + w[45] - 2*w[46] - w[47] + 2*w[48] + w[53] - w[55] - w[57] - w[58] + w[59] + 2*w[64] - w[66] - w[67] + w[69] + w[70] + w[71] + w[72] + w[73] + w[75] - w[76] + 2*w[77] + w[81] - w[83] + 2*w[84] + 3.0*w[88] - w[89] - w[90] - 3.0*w[91] - w[92] - w[93] - w[94] + w[95] - w[100] + w[102] + w[103] - w[107] - w[108] - 2*w[109] - w[110] + w[111] - w[112] - w[114] + 2*w[115] - w[128]*

Table S2. *Cont.*

$W[4] = w[4] - w[10] - w[15] - w[18] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[36] - w[37] + w[40] - w[42] - w[43] + w[46] - w[48] + w[50] + w[51] + 2*w[52] + w[55] + w[57] + w[58] + w[61] + w[62] + w[65] + 2*w[66] + 2*w[67] + w[68] - w[71] - w[72] - w[77] + w[80] - w[84] - w[88] + w[89] + w[91] + w[93] + w[94] - w[98] - 2*w[99] - w[100] + w[109] + 2*w[113] - w[118] - w[124] - w[125] + w[126] + w[128]$
$W[5] = w[4] - w[6] - w[10] - w[15] - w[18] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] - w[34] + w[36] - w[37] + w[40] - w[42] - w[43] + w[46] - w[48] + w[50] + w[51] + 2*w[52] - w[54] + 2*w[57] + w[58] + w[61] + w[62] + 2*w[66] + 2*w[67] + w[68] + w[70] - w[71] - w[72] - w[74] - w[75] - w[76] - 2*w[77] + w[78] + w[80] + w[82] - w[84] + w[85] + w[86] - w[88] + w[89] + w[91] + w[93] + w[94] - w[98] - 2*w[99] - w[100] - w[107] + w[109] + 2*w[113] - w[116] - w[117] - w[118] - w[124] - w[125] + w[126] + w[128]$
$W[6] = - w[9] + w[10] + w[16] + w[18] + w[34] - w[36] + w[37] + w[43] + w[45] - w[46] - w[47] + w[48] - w[57] - w[58] + w[59] + w[64] - w[66] - w[67] + w[75] - w[76] + 2*w[77] + w[81] - w[83] + 2*w[84] + 2*w[88] - w[89] - w[90] - 2*w[91] - w[92] - w[93] - w[94] - w[100] - w[109] - w[110] - w[112] - w[114] + w[115] - w[128]$
$W[7] = 2*w[4] - 2*w[6] - w[9] - w[14] - w[15] + w[17] - 3.0*w[20] - 2*w[21] - 2*w[22] - 2*w[23] - 2*w[24] + 2*w[30] + 4.0*w[31] + 2*w[32] + 2*w[33] + w[38] + w[40] - w[41] - w[42] + w[49] + 2*w[50] + 2*w[51] + 4.0*w[52] - w[54] + w[56] + 2*w[57] + 2*w[59] + 2*w[61] + w[62] + w[63] + 2*w[64] + w[65] + 2*w[66] + 2*w[67] + 2*w[68] + 2*w[70] - w[71] - 2*w[74] - 2*w[76] + 2*w[78] + 2*w[80] + 2*w[81] + 2*w[82] + 2*w[84] + 2*w[85] + 2*w[86] + w[87] + 2*w[88] - w[90] - 2*w[91] - 2*w[92] - w[94] - 2*w[98] - 3.0*w[99] - 2*w[100] + w[102] + w[103] - w[106] - 2*w[107] - w[110] + w[111] - 2*w[112] + 4.0*w[113] - w[114] + 2*w[115] - 2*w[116] - w[117] - w[118] - 2*w[124] - 2*w[125] + 2*w[126]$
$W[8] = w[4] - w[6] - w[9] - w[15] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[40] - w[42] + w[50] + w[51] + 2*w[52] - w[54] + w[57] + w[59] + w[61] + w[62] + w[64] + w[66] + w[67] + w[68] + w[70] - w[71] - w[74] - w[76] + w[78] + w[80] + w[81] + w[82] + w[84] + w[85] + w[86] + w[88] - w[90] - w[91] - w[92] - w[98] - 2*w[99] - w[100] - w[107] - w[110] - w[112] + 2*w[113] - w[114] + w[115] - w[116] - w[117] - w[118] - w[124] - w[125] + w[126]$
$W[9] = w[4] + w[5] - w[6] + w[7] + w[8] - w[9] - w[15] + w[16] + w[17] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[40] - w[42] - w[44] + w[50] + w[51] + 2*w[52] + w[53] - w[54] - w[55] + w[56] + w[57] - w[58] + w[59] + w[61] + w[62] + w[64] + w[66] + w[67] + w[68] + w[69] + 2*w[70] + w[73] - w[74] - 2*w[76] + 2*w[78] + w[79] + 2*w[80] + 2*w[81] + 2*w[82] + 2*w[84] + 2*w[85] + 2*w[86] + w[87] + 2*w[88] - w[90] - 2*w[91] - 2*w[92] - w[98] - 2*w[99] - w[100] + w[102] + w[103] - 2*w[107] - w[109] - w[110] + w[111] - w[112] + 2*w[113] - w[114] + 2*w[115] - w[116] - w[117] - w[124] - w[125] + w[126]$
$W[10] = - w[102] - w[103] + w[104] + w[105] + w[106] + w[107] + w[108] + w[109] - w[111]$
$W[11] = - 0.5*w[2] + 1.5*w[4] + 0.5*w[5] - 0.5*w[6] + 0.5*w[8] - 0.5*w[9] - 0.5*w[12] - 0.5*w[14] - w[15] + 0.5*w[16] + 0.5*w[17] - 2*w[20] - 2*w[21] - 2*w[22] - 2*w[23] - 2*w[24] - 0.5*w[25] - 0.5*w[26] - 0.5*w[27] - 0.5*w[28] - 0.5*w[29] + w[30] + 2.5*w[31] + 1.5*w[32] + w[33] - 0.5*w[35] - 0.5*w[36] - 0.5*w[39] + 0.5*w[40] - 0.5*w[41] - w[42] - 0.5*w[43] - 0.5*w[44] - 0.5*w[46] - 0.5*w[47] + 0.5*w[49] + 1.5*w[50] + 1.5*w[51] + 3.0*w[52] + w[53] + w[56] + w[57] + 1.5*w[59] + 0.5*w[60] + w[61] + w[62] + 0.5*w[63] + 1.5*w[64] + w[65] + 1.5*w[66] + 1.5*w[67] + 1.5*w[68] + 0.5*w[69] + 1.5*w[70] + 0.5*w[72] + 0.5*w[73] - w[74] + 0.5*w[75] - w[76] + 0.5*w[77] + w[78] + w[80] + 1.5*w[81] + w[82] + 1.5*w[84] + w[85] + w[86] + 0.5*w[87] + 1.5*w[88] - w[90] - 1.5*w[91] - w[92] - 0.5*w[93] - 0.5*w[94] - 2*w[98] - 2.5*w[99] - 2*w[100] + 0.5*w[102] + w[103] - 1.5*w[107] - 0.5*w[108] - 0.5*w[109] - w[110] + 0.5*w[111] - w[112] + 3.0*w[113] - 0.5*w[114] + 1.5*w[115] - 0.5*w[116] - 0.5*w[117] - 0.5*w[118] - w[119] - w[120] - w[121] - w[122] + 0.5*w[123] - w[124] - 0.5*w[125] + 2.5*w[126] + w[127] + w[128]$

Table S2. *Cont.*

$W[12] = - 0.5*w[2] + 1.5*w[4] + 0.5*w[5] - 0.5*w[6] + 0.5*w[8] - 0.5*w[9] - 0.5*w[12] - 0.5*w[14] - w[15] + 0.5*w[16] + 0.5*w[17] - 2*w[20] - 2*w[21] - 2*w[22] - 2*w[23] - 2*w[24] - 0.5*w[25] - 0.5*w[26] - 0.5*w[27] - 0.5*w[28] - 0.5*w[29] + w[30] + 2.5*w[31] + 1.5*w[32] + w[33] - 0.5*w[35] - 0.5*w[36] - 0.5*w[39] + 0.5*w[40] - 0.5*w[41] - w[42] - 0.5*w[43] - 0.5*w[44] - 0.5*w[46] - 0.5*w[47] + 0.5*w[49] + 1.5*w[50] + 1.5*w[51] + 3.0*w[52] + w[53] + w[56] + w[57] + 1.5*w[59] + 0.5*w[60] + w[61] + w[62] + 0.5*w[63] + 1.5*w[64] + w[65] + 1.5*w[66] + 1.5*w[67] + 1.5*w[68] + 0.5*w[69] + 1.5*w[70] + 0.5*w[72] + 0.5*w[73] - w[74] + 0.5*w[75] - w[76] + 0.5*w[77] + w[78] + w[80] + 1.5*w[81] + w[82] + 1.5*w[84] + w[85] + w[86] + 0.5*w[87] + 1.5*w[88] - w[90] - 1.5*w[91] - w[92] - 0.5*w[93] - 0.5*w[94] - 2*w[98] - 2.5*w[99] - 2*w[100] + 0.5*w[102] + w[103] - 1.5*w[107] - 0.5*w[108] - 0.5*w[109] - w[110] + 0.5*w[111] - w[112] + 3.0*w[113] - 0.5*w[114] + 1.5*w[115] - 0.5*w[116] - 0.5*w[117] - 0.5*w[118] - 0.5*w[123] - 2*w[124] - 1.5*w[125] + 1.5*w[126]$

$W[13] = - w[1] - 0.5*w[2] - 0.5*w[4] - 0.5*w[5] - 0.5*w[6] - w[7] - 0.5*w[8] - 0.5*w[9] - 0.5*w[12] - 0.5*w[14] - w[15] - 0.5*w[16] - 0.5*w[17] + w[19] + 0.5*w[25] - 0.5*w[26] - 0.5*w[27] - 0.5*w[28] - 0.5*w[29] + 0.5*w[31] - 0.5*w[32] - 0.5*w[35] - 0.5*w[36] - 0.5*w[39] + 0.5*w[40] - 0.5*w[41] - w[42] - 0.5*w[43] - 0.5*w[44] - 0.5*w[46] - 0.5*w[47] + 0.5*w[49] + 0.5*w[50] + 0.5*w[51] + 0.5*w[59] + 0.5*w[60] - 0.5*w[63] + 0.5*w[64] - 0.5*w[66] + 0.5*w[67] + 0.5*w[68] + 0.5*w[69] + 0.5*w[70] + 0.5*w[72] - 0.5*w[73] + 0.5*w[75] + 0.5*w[77] + 0.5*w[81] + 0.5*w[84] - 0.5*w[87] + 0.5*w[88] + w[89] - 0.5*w[91] - 0.5*w[93] - 0.5*w[94] - 0.5*w[99] + 0.5*w[102] - 0.5*w[107] - 0.5*w[108] - 0.5*w[109] - w[110] - 0.5*w[111] - w[112] - 0.5*w[114] + 0.5*w[115] + 0.5*w[116] + 0.5*w[117] - 0.5*w[118] - 0.5*w[123] - 0.5*w[125] - 0.5*w[126] - w[127]$

$W[14] = w[4] - w[15] - w[18] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[40] - w[42] - w[43] + w[46] - w[48] + w[50] + w[51] + 2*w[52] + w[55] + w[57] + w[58] + w[59] + w[61] + w[62] + w[65] + w[66] + 2*w[67] + w[68] - w[71] + w[80] - w[88] + w[89] + w[91] - w[95] - w[98] - 2*w[99] - w[100] + w[109] + 2*w[113] - w[118] - w[124] - w[125] + w[126] + w[128]$

$W[15] = w[4] - w[5] - w[7] - w[12] - w[13] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] - w[39] + w[44] + w[49] + w[50] + w[51] + 2*w[52] + w[55] + w[57] + w[58] + w[59] + w[62] + w[63] + w[64] + w[65] + w[66] + w[67] + w[68] - w[71] - w[74] - w[79] - w[93] - w[96] - w[97] - 2*w[98] - w[99] - w[100] + w[109] - w[112] + 2*w[113] - w[116] - w[118] - w[124] - w[125] + w[126]$

$W[16] = w[4] - w[11] - w[13] - w[19] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[44] + w[50] + w[51] + 2*w[52] + w[55] + w[57] + w[58] + w[59] - w[60] + w[61] + w[62] + w[63] + w[64] + w[65] + w[66] + w[67] - w[71] + w[73] + w[80] + w[87] - w[98] - w[99] - w[100] + w[109] + w[111] + 2*w[113] - w[116] - w[118] - w[124] - w[125] + w[126]$

$W[17] = - w[102] - w[103] + w[106] - w[110] - w[111]$

$W[18] = w[4] - w[15] - w[20] - w[21] - w[22] - w[23] - w[24] + w[30] + 2*w[31] + w[32] + w[33] + w[40] - w[42] - w[43] + w[50] + w[51] + 2*w[52] + w[55] + w[57] + w[58] + w[59] + w[61] + w[62] + w[64] + w[65] + w[66] + 2*w[67] + w[68] - w[71] + w[80] + w[89] - w[98] - 2*w[99] - w[100] + w[109] + 2*w[113] - w[118] - w[124] - w[125] + w[126] + w[128]$

The reaction rate of each substance:

$R[H_2] = - W[1] - W[4] + W[12] + W[18]$

$R[H] = + W[1] - W[3] - W[7] + W[12] - W[14] - W[15] - W[17] + W[18]$

$R[O] = - W[1] + W[10] + W[11] + 2*W[13] + W[16] - W[18]$

$R[O_2] = + W[8] - W[9] + W[11] - W[13] - W[18]$

$R[OH] = + W[1] - 3*W[2] + W[9]$

$R[H_2O] = + W[2] - W[12] + W[18]$

$R[HO_2] = + W[2] - W[12]$

$R[CH] = - W[3] + W[6] - W[10] - W[14] + W[18]$

$R[CH_2] = - W[4] + W[5]$

$R[CH_2(S)] = + W[3] + W[5] - W[9]$

Table S2. *Cont.*

$R[CH_3] = + W[6]$

$R[CH_4] = + W[4] - W[14]$

$R[CO] = - W[15] + W[16]$

$R[CO_2] = - W[16] + W[18]$

$R[HCO] = - W[7] + W[9] + W[15]$

$R[CH_2O] = + W[7] - 2*W[8] + W[17]$

$R[C_2H_4] = - W[5] - W[6] + W[8]$

$R[C_2H_6] = + W[14] - W[18]$

$R[NO] = - W[10] - W[17]$

$R[HCN] = + W[10] - W[17]$

$R[N_2] = + W[17]$

$R[O_3] = - W[11] + W[12]$

Chemical reaction rate of quasi-steady substance:

$R[N] = - w[101] - w[102] - w[103] + w[104] + w[106] - w[110] - w[111] = 0$

$R[C_2H_5] = - w[17] + w[18] + w[45] - w[46] - w[47] + w[48] + w[64] + w[88] + w[95] - w[100] = 0$

$R[CH_3O] = - w[15] + w[40] – w[42] – w[43] – w[44] – w[63] + w[67] + w[89] – w[99] + w[128] = 0$

W[i] represented reaction rate in the *i* step of the overall reaction, *w[i]* represented the reaction rate in the *i* step elementary reaction of the skeleton mechanism in Table 3.