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基于特征值分析的正癸烷骨架和总包简化机理

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Skeletal and Reduced Mechanisms of *n*-Decane Simplified with Eigenvalue Analysis

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表 S1　正癸烷骨架反应机理

Table S1　Skeletal mechanism of *n*-decane

No.	Reactions	*A*/(mol-cm-sec-K)	*b*	*E*/(cal·mol^{-1})
1	$H+O_2=OH+O$	9.76×10^{13}	0	14842.3
2	$O+H_2=OH+H$	5.12×10^{4}	2.7	6285.9
3	$OH+H_2=H_2O+H$	1.02×10^{8}	1.6	3298.3
4	$2OH=H_2O+O$	1.51×10^{9}	1.1	100.4
5	$H+O_2+M=HO_2+M$	3.54×10^{18}	-0.8	0
6	$HO_2+H=2OH$	1.69×10^{14}	0	874.8
7	$HO_2+H=H_2+O_2$	4.28×10^{13}	0	1410.1
8	$HO_2+OH=H_2O+O_2$	2.89×10^{13}	0	-501.9
9	$HO_2+H=H_2O+O$	3.01×10^{13}	0	1720.8
10	$HO_2+O=OH+O_2$	3.19×10^{13}	0	0
11	$2HO_2=H_2O_2+O_2$	5.20×10^{12}	0	1539.2
12	$H_2O_2+H=H_2O+OH$	1.02×10^{13}	0	3585.1
13	$H_2O_2+H=HO_2+H_2$	1.69×10^{12}	0	3752.4
14	$H_2O_2+O=OH+HO_2$	6.62×10^{11}	0	3967.5
15	$H_2O_2+OH=H_2O+HO_2$	3.94×10^{12}	0	1331.3
16	$H_2O_2(+M)=2OH(+M)$	2.49×10^{20}	-1.7	52376.8
17	$2H+M=H_2+M$	1.86×10^{18}	-1	0
18	$H+OH+M=H_2O+M$	2.21×10^{22}	-2	0
19	$2O+M=O_2+M$	2.86×10^{17}	-1	0
20	$CO+OH=CO_2+H$	8.97×10^{6}	1.5	-740.9
21	$CO+HO_2=CO_2+OH$	1.51×10^{14}	0	23637.7
22	$CO+O(+M)=CO_2(+M)$	1.80×10^{10}	0	2380.5
23	$CO+O_2=CO_2+O$	2.51×10^{12}	0	47801.2
24	$HCO+M=CO+H+M$	7.00×10^{14}	0	16802.1
25	$HCO+H=CO+H_2$	9.03×10^{13}	0	0
26	$HCO+O=CO+OH$	3.01×10^{13}	0	0
27	$HCO+O=CO_2+H$	3.01×10^{13}	0	0

28	$HCO+OH=CO+H_2O$	1.02×10^{15}	0	0
29	$HCO+O_2=CO+HO_2$	3.01×10^{12}	0	0
30	$2HCO=CH_2O+CO$	3.01×10^{13}	0	0
31	$CH_2O+H\rightarrow HCO+H_2$	1.26×10^{8}	1.6	2165.4
32	$CH_2O+OH\rightarrow HCO+H_2O$	3.43×10^{9}	1.2	-454.1
33	$CH_2O+M\rightarrow HCO+H+M$	1.62×10^{36}	-5.5	96696.9
34	$CH_2O+O_2=HCO+HO_2$	6.02×10^{13}	0	40631
35	$2CH_3=C_2H_5+H$	3.16×10^{13}	0	14675
36	$2CH_3(+M)\rightarrow C_2H_6(+M)$	1.81×10^{13}	0	0
37	$2CH_3\rightarrow C_2H_4+H_2$	1.00×10^{14}	0	32026.8
38	$CH_3+O=CH_2O+H$	8.43×10^{13}	0	0
39	$CH_3+OH=CH_2OH+H$	2.64×10^{19}	-1.8	8068.8
40	$CH_3+OH=CH_3O+H$	5.74×10^{12}	-0.2	13929.2
41	$CH_3+HO_2=CH_3O+OH$	3.78×10^{13}	0	0
42	$CH_3+HO_2=CH_4+O_2$	1.00×10^{12}	0	0
43	$CH_3+O_2=CH_2O+OH$	3.30×10^{11}	0	8938.8
44	$CH_3+H(+M)=CH_4(+M)$	2.11×10^{14}	0	0
45	$CH_3O+M\rightarrow CH_2O+H+M$	5.42×10^{13}	0	13503.8
46	$CH_3O+H=CH_2O+H_2$	1.80×10^{13}	0	0
47	$CH_3O+O_2=CH_2O+HO_2$	2.17×10^{10}	0	1744.7
48	$CH_3O+O=CH_3+O_2$	1.50×10^{13}	0	0
49	$CH_3O+O=CH_2O+OH$	1.40×10^{12}	0	0
50	$CH_2OH+M\rightarrow CH_2O+H+M$	5.00×10^{13}	0	25095.6
51	$CH_2OH+H\rightarrow CH_2O+H_2$	3.00×10^{13}	0	0
52	$CH_2OH+O_2=CH_2O+HO_2$	1.00×10^{13}	0	7170.2
53	$CH_4+H=CH_3+H_2$	1.30×10^{4}	3	8030.6
54	$CH_4+O=CH_3+OH$	7.23×10^{8}	1.6	8484.7
55	$CH_4+OH=CH_3+H_2O$	1.56×10^{7}	1.8	2772.5
56	$CH_4+HO_2=CH_3+H_2O_2$	9.03×10^{12}	0	24639.1
57	$OH+CH_3(+M)=CH_3OH(+M)$	6.02×10^{13}	0	0
58	$CH_3OH+H=CH_2OH+H_2$	4.00×10^{13}	0	6094.6

59	$CH_3OH+H=CH_3O+H_2$	4.00×10^{12}	0	6094.6
60	$CH_3OH+O=CH_2OH+OH$	1.00×10^{13}	0	4684.5
61	$CH_3OH+OH=CH_2OH+H_2O$	3.55×10^{4}	2.6	-884.3
62	$CH_3OH+CH_3=CH_4+CH_2OH$	9.00×10^{12}	0	9823.1
63	$CH_3OH+HO_2\rightarrow CH_2OH+H_2O_2$	6.20×10^{12}	0	19383.4
64	$CH_2OH+H_2O_2\rightarrow CH_3OH+HO_2$	1.00×10^{7}	1.7	11448.4
65	$HCCO+O\rightarrow 2CO+H$	1.00×10^{14}	0	0
66	$HCCO+O_2=HCO+CO_2$	8.13×10^{11}	0	855.6
67	$HCCO+O_2=2CO+OH$	8.13×10^{11}	0	855.6
68	$C_2H_2+O_2=HCCO+OH$	2.00×10^{8}	1.5	30114.7
69	$C_2H_2+O=HCCO+H$	5.06×10^{6}	2.1	1570.3
70	$CH_2CO+H=CH_3+CO$	4.20×10^{13}	0	3848
71	$CH_2CO+O=HCO+CHO$	2.30×10^{12}	0	693.1
72	$CH_2CO+OH=CH_2O+HCO$	1.00×10^{13}	0	0
73	$C_2H_3(+M)=C_2H_2+H(+M)$	2.00×10^{14}	0	39744.3
74	$C_2H_3+H=C_2H_2+H_2$	1.20×10^{13}	0	0
75	$C_2H_3+O=C_2H_2+OH$	1.00×10^{13}	0	0
76	$C_2H_3+OH=C_2H_2+H_2O$	2.00×10^{13}	0	0
77	$C_2H_3+O=CH_3+CO$	1.00×10^{13}	0	0
78	$C_2H_3+O_2=CH_2O+HCO$	1.70×10^{29}	-5.3	6493.8
79	$C_2H_3+O_2=CH_2CHO+O$	3.50×10^{14}	-0.6	5258.1
80	$C_2H_3+O_2=C_2H_2+HO_2$	5.19×10^{15}	-1.3	3307.8
81	$C_2H_3+O_2=C_2H_2+HO_2$	2.12×10^{-6}	6	9474.2
82	$CH_3CO=CH_3+CO$	2.32×10^{26}	-5	17949.3
83	$CH_3CO+H=CH_2CO+H_2$	2.00×10^{13}	0	0
84	$CH_3CO+CH_3=C_2H_6+CO$	5.00×10^{13}	0	0
85	$CH_3CHO+M\rightarrow CH_3+HCO+M$	7.00×10^{15}	0	81931.2
86	$CH_3CHO+H=CH_3CO+H_2$	2.10×10^{9}	1.2	2414
87	$CH_3CHO+H=CH_2CHO+H_2$	2.00×10^{9}	1.2	2414
88	$CH_3CHO+O=CH_3CO+OH$	5.00×10^{12}	0	1816.4
89	$CH_3CHO+O=CH_2CHO+OH$	8.00×10^{11}	0	1816.4

90	$CH_3CHO+OH=CH_3CO+H_2O$	2.30×10^{10}	0.7	-1123.3
91	$CH_3CHO+HO_2=CH_3CO+H_2O_2$	3.00×10^{12}	0	11950.3
92	$CH_3CHO+O_2=CH_3CO+HO_2$	4.00×10^{13}	0	39268.6
93	$CH_3CHO+CH_3=CH_3CO+CH_4$	2.00×10^{-6}	5.5	2461.8
94	$C_2H_4+M=C_2H_2+H_2+M$	3.50×10^{16}	0	71462.7
95	$C_2H_4+M\rightarrow C_2H_3+H+M$	7.30×10^{17}	0	96558.3
96	$C_2H_4+H=C_2H_3+H_2$	5.40×10^{14}	0	14914
97	$C_2H_4+OH=C_2H_3+H_2O$	3.00×10^{13}	0	3011.5
98	$C_2H_4+O=CH_3+HCO$	1.36×10^{7}	1.9	178.8
99	$C_2H_5(+M)\rightarrow C_2H_4+H(+M)$	8.20×10^{13}	0	39914
100	$C_2H_4+H(+M)\rightarrow C_2H_5(+M)$	3.98×10^{9}	1.3	1290.6
101	$C_2H_5+CH_3=C_2H_4+CH_4$	1.14×10^{12}	0	0
102	$C_2H_5+O_2=C_2H_4+HO_2$	1.02×10^{10}	0	-2186.9
103	$C_2H_5+O=CH_2O+CH_3$	6.62×10^{13}	0	0
104	$C_2H_6+H=C_2H_5+H_2$	1.40×10^{9}	1.5	7433.1
105	$C_2H_6+O=C_2H_5+OH$	1.00×10^{9}	1.5	5831.7
106	$C_2H_6+OH=C_2H_5+H_2O$	7.20×10^{6}	2	860.4
107	$C_2H_6+CH_3=C_2H_5+CH_4$	1.50×10^{-7}	6	6070.8
108	$C_2H_6+HO_2=C_2H_5+H_2O_2$	1.70×10^{13}	0	20530.6
109	$C_2H_6+O_2=C_2H_5+HO_2$	6.00×10^{13}	0	51864.2
110	$C_2H_2+HCCO=C_3H_3+CO$	1.00×10^{11}	0	2987.6
111	$C_3H_3+O=C_2H_2+CO+H$	1.40×10^{14}	0	0
112	$C_3H_3+O_2=HCO+CH_2CO$	3.01×10^{10}	0	2868.1
113	$C_3H_3+O=C_2H_3+CO$	3.80×10^{13}	0	0
114	$C_3H_4+M\rightarrow C_3H_3+H+M$	2.00×10^{18}	0	79923.5
115	$C_3H_4+H=C_3H_3+H_2$	2.00×10^{7}	2	4995.2
116	$C_3H_4+CH_3=C_3H_3+CH_4$	2.00×10^{11}	0	7696
117	$C_3H_4+OH=C_3H_3+H_2O$	2.00×10^{7}	2	999
118	$C_3H_4+H=C_3H_5$	2.00×10^{12}	0	2700.8
119	$C_3H_4=p\text{-}C_3H_4$	1.20×10^{15}	0	92311.2
120	$p\text{-}C_3H_4+H=C_2H_2+CH_3$	1.30×10^{5}	2.5	999

121	p-C_3H_4+OH=C_3H_3+H_2O	2.00×10^{7}	2	999
122	p-C_3H_4+CH_3=C_3H_3+CH_4	1.50	3.5	5592.7
123	C_3H_5+H=C_3H_4+H_2	3.33×10^{12}	0	0
124	C_3H_5+O_2=C_3H_4+HO_2	6.00×10^{11}	0	10014.3
125	C_3H_6→C_2H_3+CH_3	3.15×10^{15}	0	85803.1
126	C_3H_6+H=C_3H_5+H_2	5.00×10^{12}	0	1505.7
127	C_3H_6+OH=C_3H_5+H_2O	4.00×10^{12}	0	0
128	C_3H_6+CH_3=C_3H_5+CH_4	8.96×10^{12}	0	8508.6
129	C_3H_6+O=C_2H_4+CH_2O	5.90×10^{13}	0	5019.1
130	C_3H_6+O=C_2H_5+HCO	3.60×10^{12}	0	0
131	C_3H_6+OH=C_2H_5+CH_2O	7.90×10^{12}	0	0
132	n-C_3H_7=CH_3+C_2H_4	9.60×10^{13}	0	31022.9
133	n-C_3H_7=H+C_3H_6	1.25×10^{14}	0	37022
134	n-C_3H_7+O_2=C_3H_6+HO_2	1.00×10^{12}	0	4995.2
135	i-C_3H_7=C_3H_6+H	6.30×10^{13}	0	36926.4
136	i-C_3H_7=C_2H_4+CH_3	2.00×10^{10}	0	29517.2
137	i-C_3H_7+O_2=C_3H_6+HO_2	1.00×10^{12}	0	4995.2
138	C_2H_5+CH_3=C_3H_8	7.00×10^{12}	0	0
139	C_3H_8+H=i-C_3H_7+H_2	1.00×10^{14}	0	8341.3
140	C_3H_8+H=n-C_3H_7+H_2	1.30×10^{14}	0	9703.6
141	C_3H_8+O=i-C_3H_7+OH	2.60×10^{13}	0	4469.4
142	C_3H_8+O=n-C_3H_7+OH	3.00×10^{13}	0	5760
143	C_3H_8+OH=i-C_3H_7+H_2O	2.80×10^{12}	0	860.4
144	C_3H_8+OH=n-C_3H_7+H_2O	3.70×10^{12}	0	1649.1
145	C_3H_8+HO_2→i-C_3H_7+H_2O_2	2.00×10^{12}	0	17017.2
146	i-C_3H_7+H_2O_2→C_3H_8+HO_2	4.16×10^{11}	0	7433.1
147	C_3H_8+HO_2→n-C_3H_7+H_2O_2	1.70×10^{13}	0	20482.8
148	n-C_3H_7+H_2O_2→C_3H_8+HO_2	2.33×10^{12}	0	9823.1
149	C_3H_8+CH_3→CH_4+i-C_3H_7	1.30×10^{12}	0	11615.7
150	i-C_3H_7+CH_4→CH_3+C_3H_8	1.01×10^{13}	0	18570.8
151	CH_3+C_3H_8→CH_4+n-C_3H_7	4.00×10^{11}	0	9512.4

152	n-C_3H_7+CH_4→CH_3+C_3H_8	3.12×10^{12}	0	16467.5
153	C_3H_8+O_2→i-C_3H_7+HO_2	4.00×10^{13}	0	47538.2
154	i-C_3H_7+HO_2→C_3H_8+O_2	2.08×10^{12}	0	0
155	C_3H_8+O_2→n-C_3H_7+HO_2	4.00×10^{13}	0	47538.2
156	n-C_3H_7+HO_2→C_3H_8+O_2	2.08×10^{12}	0	0
157	C_3H_8+CH_3O→n-C_3H_7+CH_3OH	3.00×10^{11}	0	7002.9
158	n-C_3H_7+CH_3OH→C_3H_8+CH_3O	1.22×10^{10}	0	9201.7
159	C_3H_8+CH_3O→i-C_3H_7+CH_3OH	3.00×10^{11}	0	7002.9
160	i-C_3H_7+CH_3OH→C_3H_8+CH_3O	1.22×10^{10}	0	9201.7
161	C_4H_2+OH=C_2H_2+HCCO	1.50×10^{13}	0	0
162	C_2H_2+C_2H_3=C_4H_4+H	1.60×10^{13}	0	25095.6
163	C_2H_2+C_2H_3=u-C_4H_5	1.20×10^{12}	0	0
164	C_4H_4+H=s-C_4H_5	5.50×10^{12}	0	2390.1
165	C_4H_4+H=u-C_4H_5	5.50×10^{12}	0	2390.1
166	s-C_4H_5+H=C_4H_4+H_2	2.00×10^{13}	0	0
167	u-C_4H_5+H=C_4H_4+H_2	2.00×10^{13}	0	0
168	u-C_4H_5+M=s-C_4H_5+M	1.00×10^{14}	0	0
169	u-C_4H_5+O_2→C_2H_3+2HCO	1.00×10^{12}	0	2007.7
170	s-C_4H_5+O_2→C_2H_3+CO+CH_2O	1.00×10^{12}	0	2007.7
171	C_4H_6→2C_2H_3	4.03×10^{19}	-1	98231.4
172	C_2H_3+C_2H_4=C_4H_6+H	1.00×10^{11}	0	7289.7
173	C_3H_3+CH_3→C_4H_6	2.00×10^{12}	0	0
174	C_4H_6→C_3H_3+CH_3	1.00×10^{12}	0	59512.4
175	C_4H_6+H=u-C_4H_5+H_2	3.00×10^{7}	2	13001.9
176	C_4H_6+H=s-C_4H_5+H_2	3.00×10^{7}	2	5999
177	C_4H_6+OH=u-C_4H_5+H_2O	2.00×10^{7}	2	4995.2
178	C_4H_6+OH=s-C_4H_5+H_2O	2.00×10^{7}	2	2007.7
179	C_4H_6+O=C_2H_4+CH_2CO	1.00×10^{12}	0	0
180	C_4H_6+O=CH_2O+C_3H_4	1.00×10^{12}	0	0
181	C_4H_6+OH=C_2H_5+CH_2CO	1.00×10^{12}	0	0
182	C_4H_6+OH=CH_2O+C_3H_5	2.00×10^{12}	0	0

183	$C_4H_6+OH=C_2H_3+CH_3CHO$	5.00×10^{12}	0	0
184	$C_4H_7=C_4H_6+H$	1.20×10^{14}	0	49330.8
185	$C_4H_7=C_2H_4+C_2H_3$	1.00×10^{11}	0	37022
186	$H+C_4H_7=C_4H_6+H_2$	3.16×10^{12}	0	0
187	$C_4H_7+O_2=C_4H_6+HO_2$	1.00×10^{11}	0	0
188	$2C_4H_7=C_4H_6+p\text{-}C_4H_8$	3.16×10^{12}	0	0
189	$C_4H_7+CH_3=C_4H_6+CH_4$	1.00×10^{13}	0	0
190	$C_4H_7+C_2H_3=C_4H_6+C_2H_4$	4.00×10^{12}	0	0
191	$C_4H_7+C_2H_5=C_4H_6+C_2H_6$	4.00×10^{12}	0	0
192	$C_4H_7+C_2H_5=p\text{-}C_4H_8+C_2H_4$	5.00×10^{11}	0	0
193	$C_4H_7+C_3H_5=C_4H_6+C_3H_6$	4.00×10^{13}	0	0
194	$C_3H_5+CH_3=p\text{-}C_4H_8$	1.00×10^{13}	0	0
195	$p\text{-}C_4H_8\rightarrow C_2H_3+C_2H_5$	2.00×10^{18}	-1	96845.1
196	$p\text{-}C_4H_8\rightarrow H+C_4H_7$	4.11×10^{18}	-1	97442.6
197	$p\text{-}C_4H_8+H=C_4H_7+H_2$	5.00×10^{13}	0	3895.8
198	$p\text{-}C_4H_8+O=CH_3CHO+C_2H_4$	2.50×10^{12}	0	0
199	$p\text{-}C_4H_8+O=CH_3+C_2H_5+CO$	1.62×10^{13}	0	860.4
200	$p\text{-}C_4H_8+O=C_3H_6+CH_2O$	7.23×10^{5}	2.3	-1051.6
201	$p\text{-}C_4H_8+O=C_4H_7+OH$	1.30×10^{13}	0	4493.3
202	$p\text{-}C_4H_8+OH=CH_3CHO+C_2H_5$	1.00×10^{11}	0	0
203	$p\text{-}C_4H_8+OH=CH_3+C_2H_6+CO$	1.00×10^{10}	0	0
204	$p\text{-}C_4H_8+OH=n\text{-}C_3H_7+CH_2O$	6.50×10^{12}	0	0
205	$p\text{-}C_4H_8+OH=C_4H_7+H_2O$	1.75×10^{13}	0	6955.1
206	$p\text{-}C_4H_8+CH_3=C_4H_7+CH_4$	1.00×10^{11}	0	7313.6
207	$p\text{-}C_4H_8+O_2\rightarrow C_4H_7+HO_2$	4.00×10^{12}	0	40009.6
208	$p\text{-}C_4H_8+HO_2=C_4H_7+H_2O_2$	1.00×10^{11}	0	17065
209	$p\text{-}C_4H_8+C_2H_5=C_4H_7+C_2H_6$	1.00×10^{11}	0	8006.7
210	$p\text{-}C_4H_8+C_3H_5\rightarrow C_4H_7+C_3H_6$	8.00×10^{10}	0	12404.4
211	$p\text{-}C_4H_9=C_2H_5+C_2H_4$	2.50×10^{13}	0	28824.1
212	$p\text{-}C_4H_9=p\text{-}C_4H_8+H$	1.26×10^{13}	0	38623.3
213	$p\text{-}C_4H_9+O_2=p\text{-}C_4H_8+HO_2$	1.00×10^{12}	0	2007.7

214	$C_5H_9 \rightarrow C_3H_5+C_2H_4$	2.50×10^{13}	0	30019.1
215	$C_5H_9 \rightarrow C_2H_3+C_3H_6$	2.50×10^{13}	0	30019.1
216	$p\text{-}C_5H_{10}=C_2H_5+C_3H_5$	3.16×10^{16}	0	80927.3
217	$p\text{-}C_5H_{10}+H \rightarrow C_5H_9+H_2$	2.80×10^{13}	0	4015.3
218	$p\text{-}C_5H_{10}+O \rightarrow C_5H_9+OH$	2.54×10^{5}	2.6	-1123.3
219	$p\text{-}C_5H_{10}+OH \rightarrow C_5H_9+H_2O$	6.80×10^{13}	0	3059.3
220	$p\text{-}C_5H_{10}+CH_3 \rightarrow C_5H_9+CH_4$	1.00×10^{11}	0	7313.6
221	$p\text{-}C_6H_{12} \rightarrow n\text{-}C_3H_7+C_3H_5$	3.16×10^{16}	0	80927.3
222	$p\text{-}C_6H_{12}+H \rightarrow C_4H_7+C_2H_4+H_2$	2.80×10^{7}	2	7696
223	$p\text{-}C_6H_{12}+H \rightarrow C_3H_5+C_3H_6+H_2$	8.00×10^{6}	2	4995.2
224	$p\text{-}C_6H_{12}+H \rightarrow p\text{-}C_4H_8+C_2H_3+H_2$	8.00×10^{6}	2	4995.2
225	$p\text{-}C_6H_{12}+O \rightarrow C_4H_7+C_2H_4+OH$	5.00×10^{13}	0	7863.3
226	$p\text{-}C_6H_{12}+O \rightarrow C_3H_5+C_3H_6+OH$	2.80×10^{13}	0	5210.3
227	$p\text{-}C_6H_{12}+O \rightarrow p\text{-}C_4H_8+C_2H_3+OH$	2.80×10^{13}	0	5210.3
228	$p\text{-}C_6H_{12}+OH \rightarrow C_4H_7+C_2H_4+H_2O$	4.30×10^{9}	1.1	1816.4
229	$p\text{-}C_6H_{12}+OH \rightarrow C_3H_5+C_3H_6+H_2O$	1.30×10^{9}	1.3	693.1
230	$p\text{-}C_6H_{12}+OH \rightarrow p\text{-}C_4H_8+C_2H_3+H_2O$	1.30×10^{9}	1.3	693.1
231	$p\text{-}C_6H_{13} \rightarrow p\text{-}C_4H_9+C_2H_4$	2.50×10^{13}	0	28776.3
232	$p\text{-}C_7H_{14} \rightarrow p\text{-}C_4H_9+C_3H_5$	3.16×10^{16}	0	80927.3
233	$p\text{-}C_7H_{14}+H \rightarrow 3C_2H_4+CH_3$	7.20×10^{12}	2	2896.8
234	$p\text{-}C_7H_{14}+H \rightarrow C_3H_6+C_2H_5+C_2H_4$	7.20×10^{12}	1.3	1298.8
235	$p\text{-}C_7H_{14}+H \rightarrow C_2H_4+C_4H_6+H_2+CH_3$	5.80×10^{4}	2.5	289.2
236	$p\text{-}C_7H_{14}+OH \rightarrow C_2H_4+C_4H_6+H_2O+CH_3$	3.00×10^{6}	2	-1505.7
237	$p\text{-}C_7H_{14}+HO_2 \rightarrow H_2O_2+C_2H_4+C_4H_6+CH$	6.40×10^{3}	2.6	12380.5
238	$p\text{-}C_7H_{14}+C_2H_5 \rightarrow C_2H_6+C_2H_4+C_4H_6+CH_3$	1.40	3.5	4330.8
239	$p\text{-}C_7H_{14}+O \rightarrow OH+C_2H_4+C_4H_6+CH_3$	9.20×10^{10}	0.7	3824.1
240	$p\text{-}C_7H_{15}+O_2 \rightarrow p\text{-}C_7H_{14}+HO_2$	3.20×10^{12}	0	4995.2
241	$p\text{-}C_7H_{15} \rightarrow p\text{-}C_5H_{10}+C_2H_5$	4.00×10^{13}	0	28776.3
242	$p\text{-}C_7H_{15} \rightarrow p\text{-}C_4H_8+n\text{-}C_3H_7$	2.00×10^{13}	0	28776.3
243	$p\text{-}C_7H_{15} \rightarrow p\text{-}C_6H_{12}+CH_3$	2.00×10^{13}	0	30970.4
244	$p\text{-}C_7H_{15} \rightarrow p\text{-}C_4H_9+C_3H_6$	2.00×10^{13}	0	28776.3

245	s-$C_{10}H_{21}$→p-C_7H1_5+C_3H_6	1.50×10^{13}	0	28274.4
246	t-$C_{10}H_{21}$→C_6H_{13}+p-C_4H_8	1.50×10^{13}	0	28274.4
247	$C_{10}H_{22}$→C_4H_9+C_6H_{13}	3.10×10^{16}	0	84335.6
248	$C_{10}H_{22}$→n-C_3H_7+C_7H_{15}	3.10×10^{16}	0	84335.6
249	$C_{10}H_{22}$+O_2→t-$C_{10}H_{21}$+HO_2	3.00×10^{14}	0	47562.1
250	$C_{10}H_{22}$+O_2→s-$C_{10}H_{21}$+HO_2	3.00×10^{14}	0	47562.1
251	$C_{10}H_{22}$+OH→t-$C_{10}H_{21}$+H_2O	1.30×10^{07}	2	-764.8
252	$C_{10}H_{22}$+OH→s-$C_{10}H_{21}$+H_2O	1.30×10^{07}	2	-764.8
253	$C_{10}H_{22}$+HO_2→t-$C_{10}H_{21}$+H_2O_2	4.00×10^{13}	0	17017.2
254	$C_{10}H_{22}$+HO_2→s-$C_{10}H_{21}$+H_2O_2	4.00×10^{13}	0	17017.2
255	$C_{10}H_{22}$+CH_3→t-$C_{10}H_{21}$+CH_4	1.00×10^{12}	0	9591.3
256	$C_{10}H_{22}$+CH_3→s-$C_{10}H_{21}$+CH_4	1.00×10^{12}	0	9591.3
257	$C_{10}H_{22}$+H→t-$C_{10}H_{21}$+H_2	4.50×10^{7}	2	4995.2
258	$C_{10}H_{22}$+H→s-$C_{10}H_{21}$+H_2	4.50×10^{7}	2	4995.2
259	$C_{10}H_{22}$+O→t-$C_{10}H_{21}$+OH	3.25×10^{13}	0	5210.3
260	$C_{10}H_{22}$+O→s-$C_{10}H_{21}$+OH	3.25×10^{13}	0	5210.3
261	s-$C_{10}H_{21}$→t-$C_{10}H_{21}$	2.00×10^{11}	0	18116.6
262	t-$C_{10}H_{21}$→s-$C_{10}H_{21}$	2.00×10^{11}	0	18116.6
263	s-$C_{10}H_{21}$+O_2→$C_{10}H_{21}O_2$	4.00×10^{12}	0	0
264	$C_{10}H_{21}O_2$→s-$C_{10}H_{21}$+O_2	3.75×10^{21}	-1.7	35659.7
265	t-$C_{10}H_{21}$+O_2→$C_{10}H_{21}O_2$	4.00×10^{12}	0	0
266	$C_{10}H_{21}O_2$→t-$C_{10}H_{21}$+O_2	3.75×10^{21}	-1.7	35659.7
267	$C_{10}H_{21}O_2$→$C_{10}H_{20}O_2H$	2.00×10^{11}	0	17017.2
268	C10H20O_2H→$C_{10}H_{21}O_2$	1.00×10^{11}	0	12500
269	$C_{10}H_{20}O_2H$=p-$C_{10}H_{20}$+HO_2	8.50×10^{12}	0	25621.4
270	p-$C_{10}H_{20}$=p-C_7H_{15}+C_3H_5	3.50×10^{16}	0	70936.9
271	$C_{10}H_{20}O_2H$+O_2=$O_2C_{10}H_{20}O_2H$	2.50×10^{11}	0	0
272	$O_2C_{10}H_{20}O_2H$=$OC_{10}H_{19}O_2H$+OH	3.50×10^{13}	0	24976.1
273	$OC_{10}H_{19}O_2H$→CH_2O+CO+3C_2H_4+C_2H_5+OH	7.00×10^{15}	0	41945.5
274	2C_3H_3→$A_1C_6H_6$	5.00×10^{11}	0	0

275	$C_3H_4+C_3H_3\rightarrow A_1C_6H_6+H$	2.00×10^{11}	0	2000.5
276	$A_1C_6H_6\rightarrow C_4H_4+C_2H_2$	1.00×10^{15}	0	107552.6
277	$A_1C_6H_6\rightarrow A_1C_6H_5+H$	4.41×10^{29}	-3.9	117088.9
278	$A_1C_6H_6+H=A_1C_6H_5+H_2$	7.90×10^{13}	0	9990.4
279	$A_1C_6H_6+OH=A_1C_6H_5+H_2O$	1.63×10^{08}	1.4	1457.9
280	$A_1C_6H_6+O=A_1C_6H_5+OH$	3.55×10^{01}	3.8	939.3
281	$A_1C_6H_6+O_2=A_1C_6H_5+HO_2$	6.30×10^{13}	0	60000
282	$A_1C_6H_6+O=C_6H_5O+H$	2.78×10^{13}	0	4909.2
283	$A_1C_6H_5+HO_2=C_6H_5O+OH$	5.00×10^{13}	0	999
284	$A_1C_6H_5+O_2\rightarrow C_6H_5O+O$	8.09×10^{11}	0	7468.9
285	$C_6H_5O+H=C_6H_5OH$	2.50×10^{14}	0	0
286	$C_6H_5OH+H=C_6H_5O+H_2$	1.15×10^{14}	0	12399.6
287	$C_6H_5OH+H=A_1C_6H_6+OH$	2.21×10^{13}	0	7906.3
288	$C_6H_5OH+OH=C_6H_5O+H_2O$	6.00×10^{12}	0	0
289	$C_6H_5OH+O=C_6H_5O+OH$	1.26×10^{13}	0	2899.1
290	$C_6H_5O=C_5H_5+CO$	2.51×10^{11}	0	43905.3
291	$C_5H_5+O=u\text{-}C_4H_5+CO$	1.00×10^{14}	0	0
292	$C_5H_5+O=C_5H_5O$	1.00×10^{13}	0	0
293	$C_5H_5+HO_2=C_5H_5O+OH$	3.00×10^{13}	0	0
294	$C_5H_5O=u\text{-}C_4H_5+CO$	2.51×10^{11}	0	43900.6
295	$A_1C_2H+H=A_1C_6H_5+C_2H_2$	1.00×10^{14}	0	0
296	$A_1C_2H+OH\rightarrow A_1C_6H_6+HCCO$	1.00×10^{13}	0	0
297	$A_1CH_3+OH=A_1CH_2O+H_2$	2.29×10^{12}	0	-358.5
298	$A_1CH_3+H=A_1C_6H_6+CH_3$	1.20×10^{13}	0	5121.9
299	$A_1CH_3=A_1C_6H_5+CH_3$	1.00×10^{16}	0	96904.9
300	$A_1CH_3+O=A_1CH_2O+H$	1.55×10^{13}	0	3974.7
301	$u\text{-}C_4H_5+C_3H_4=A_1CH_3+H$	2.00×10^{11}	0	3699.8
302	$u\text{-}C_4H_5+p\text{-}C_3H_4=A_1CH_3+H$	3.16×10^{11}	0	3699.8
303	$CH_2+H_2=H+CH_3$	5.00×10^{5}	2	7241.9
304	$CH_2+O=CO+H_2$	4.82×10^{13}	0	0
305	$CH_2+O\rightarrow CO+2H$	7.23×10^{12}	0	0

306	$CH_2+OH=CH_2O+H$	2.00×10^{13}	0	0
307	$2CH_2=C_2H_2+2H$	1.20×10^{14}	0	798.3
308	$CH_2+CH_3=C_2H_4+H$	4.22×10^{13}	0	0
309	$CH_2+O_2\rightarrow CO+OH+H$	1.30×10^{13}	0	1481.8
310	$CH_2+O_2\rightarrow CO_2+H_2$	1.20×10^{13}	0	1481.8
311	$CH_3+M\rightarrow CH_2+H+M$	1.02×10^{16}	0	90583.2
312	$OH+CH_3=CH_2+H_2O$	5.60×10^{7}	1.6	5425.4
313	$CH_4+CH_2=2CH_3$	1.30×10^{13}	0	9536.3
314	$2CH_2=C_2H_2+H_2$	1.20×10^{13}	0	798.3
315	$C_2H_2+O=CH_2+CO$	2.17×10^{6}	2.1	1570.3
316	$CH_2CO+M\rightarrow CH_2+CO+M$	1.00×10^{16}	0	59273.4
317	$C_2H_3+O=HCO+CH_2$	1.00×10^{13}	0	0
318	$CH_3CHO+CH_2=CH_3CO+CH_3$	2.50×10^{12}	0	3800.2
319	$C_2H_6+CH_2=C_2H_5+CH_3$	2.20×10^{13}	0	8675.9
320	$C_2H_2+CH_2=C_3H_3+H$	1.20×10^{13}	0	6596.6
321	$C_3H_3+CH_2=C_4H_4+H$	4.00×10^{13}	0	0
322	$C_2H+O_2=HCCO+O$	1.80×10^{13}	0	0
323	$C_2H_2+O_2\rightarrow C_2H+HO_2$	1.20×10^{13}	0	74450.3
324	$C_2H_2+H=C_2H+H_2$	6.62×10^{13}	0	27724.7
325	$C_2H_2+OH=C_2H+H_2O$	3.38×10^{7}	2	13986.6
326	$C_3H_3+O=CH_2O+C_2H$	2.00×10^{13}	0	0
327	$C_3H_3+CH_3\rightarrow C_2H_5+C_2H$	1.00×10^{13}	0	37464.2

(a) Rate constants are Written as $AT^n\exp(-E/RT)$

表 S2　正癸烷简化机理总包反应速率

Table S2　The global rates of reduced mechanism of *n*-decane

Reaction rates	Expressions
R_1	W_{271}-W_{273}
R_2	W_{269}-W_{270}-W_{240}-$W2_{41}$-W_{242}-W_{243}-W_{244}-W_{246}+W_{248}+W_{249}+W_{250}+W_{251}+W_{252}+W_{253}
R_3	W_{254}+W_{255}+W_{256}+W_{257}+W_{258}+W_{259}+W_{260}-W_{269}+W_{270}-W_{271}
R_4	-W_{247}-W_{248}-W_{249}-W_{250}-W_{251}-W_{252}-W_{253}-W_{254}-W_{255}-W_{256}-W_{257}-W_{258}-W_{259}-W_{260}
R_5	-W_{232}-W_{233}-W_{234}-W_{235}-W_{236}-W_{237}-W_{238}-W_{239}+W_{240}
R_6	-W_{231}+W_{246}+W_{247}
R_7	-W_{221}-W_{222}-W_{223}-W_{224}-W_{225}-W_{226}-W_{227}-W_{228}-W_{229}-W_{230}+W_{243}
R_8	-W_{216}-W_{217}-W_{218}-W_{219}-W_{220}+W_{241}
R_9	W_{188}+W_{192}+W_{194}-W_{195}-W_{196}-W_{197}-W_{198}-W_{199}-W_{200}-W_{201}-W_{202}-W_{203}-W_{204}-W_{205}-W_{206}-W_{207}-W_{208} -W_{209}+W_{210}+W_{212}+W_{213}+W_{224}+W_{227}+W_{230}+W_{242}+W_{246}
R_{10}	-W_{171}+W_{172}+W_{173}-W_{174}-W_{175}-W_{176}-W_{177}-W_{178}-W_{179}-W_{180}-W_{181}-W_{182}-W_{183}-W_{185}-W_{188}-W_{192}+W_{196}+W_{197}+W_{201}+W_{205}+W_{206}+W_{207}+W_{208}+W_{209}+W_{210}+W_{222}+W_{225}+W_{228}+W_{235}+W_{236}+ W_{237}+W_{238}+W_{239}
R_{11}	W_{138}-W_{139}-W_{140}-W_{141}-W_{142}-W_{143}-W_{144}-W_{145}+W_{146}-W_{147}+W_{148}-W_{149}+W_{150}-W_{151}+W_{152}-W_{153}+W_{154}-W_{155}+W_{156}-W_{157}+W_{158}-W_{159}+W_{160}
R_{12}	W_{118}-W_{123}-W_{124}+W_{126}+W_{127}+W_{128}+W_{182}-W_{193}-W_{194}-W_{210}-W_{215}+W_{216}+W_{217}+W_{218}+W_{219}+W_{220}+ W_{221}+W_{223}+W_{226}+W_{229}+W_{232}+W_{270}
R_{13}	-W_{114}-W_{115}-W_{116}-W_{117}-W_{118}-W_{119}+W_{123}+W_{124}+W_{180}+W_{274}-W_{276}-W_{291}-W_{294}+W_{302}
R_{14}	W_{110}-W_{111}-W_{112}-W_{113}+W_{114}+W_{115}+W_{116}+W_{117}+W_{121}+W_{122}-W_{173}+W_{174}-W_{274}-W_{276}-W_{291}-W_{294}+ W_{301}+W_{302}+W_{320}-W_{321}-W_{326}-W_{327}
R_{15}	-W_{85}-W_{86}-W_{87}-W_{88}-W_{89}-W_{90}-W_{91}-W_{92}-W_{93}+W_{183}+W_{198}+W_{202}-W_{318}
R_{16}	W_{79}+W_{87}+W_{89}
R_{17}	-W_{70}-W_{72}+W_{83}+W_{112}+W_{179}+W_{181}-W_{316}
R_{18}	-W_{65}-W_{66}-W_{67}+W_{68}+W_{69}-W_{110}+W_{296}+W_{323}+W_{324}+W_{325}+W_{326}+W_{327}
R_{19}	W_{57}-W_{58}-W_{59}-W_{60}-W_{61}-W_{62}-W_{63}+W_{64}+W_{157}-W_{158}+W_{159}-W_{160}
R_{20}	W_{36}+W_{84}-W_{104}-W_{105}-W_{106}-W_{107}-W_{108}-W_{109}+W_{191}+W_{203}+W_{209}+W_{238}-W_{319}

R_{21} $W_{35}-W_{99}+W_{100}-W_{101}-W_{102}-W_{103}+W_{104}+W_{105}+W_{106}+W_{107}+W_{108}+W_{109}+W_{130}+W_{131}-W_{138}+W_{181}-W_{191}-W_{192}+W_{195}+W_{199}+W_{202}-W_{209}-W_{212}-W_{213}+W_{216}+W_{231}+W_{232}+W_{234}+W_{238}+W_{241}+W_{244}+W_{247}+W_{273}+W_{319}+W_{327}$

R_{22} $W_{42}+W_{44}-W_{53}-W_{54}-W_{55}-W_{56}+W_{62}+W_{93}+W_{101}+W_{107}+W_{116}+W_{122}+W_{128}+W_{149}-W_{150}+W_{151}-W_{152}+W_{189}+W_{206}+W_{220}+W_{255}+W_{256}-W_{313}$

R_{23} $-W_{125}-W_{126}-W_{127}-W_{128}-W_{129}-W_{130}-W_{131}+W_{133}+W_{134}-W_{136}+W_{139}+W_{141}+W_{143}+W_{145}-W_{146}+W_{149}-W_{150}+W_{153}-W_{154}+W_{159}-W_{160}+W_{193}+W_{200}+W_{210}+W_{215}+W_{223}+W_{226}+W_{229}+W_{234}+W_{240}+W_{241}+W_{242}+W_{243}+2W_{244}-W_{248}-W_{270}$

R_{24} $W_{37}-W_{73}-W_{74}-W_{75}-W_{76}-W_{77}-W_{78}-W_{79}-W_{80}-W_{81}-W_{94}-W_{98}+W_{99}-W_{100}+W_{101}+W_{102}+W_{113}+W_{125}+W_{129}-W_{133}-W_{134}+W_{136}+W_{140}+W_{142}+W_{144}+W_{147}-W_{148}+W_{151}-W_{152}+W_{155}-W_{156}+W_{157}-W_{158}+2W_{171}-2W_{172}+W_{175}+W_{176}+W_{177}+W_{178}+W_{179}+W_{183}+2W_{185}+W_{192}+W_{195}+W_{198}+W_{204}-W_{212}-W_{213}+W_{217}+W_{218}+W_{219}+W_{220}+W_{221}+W_{222}+W_{224}+W_{225}+W_{227}+W_{228}+W_{230}+2W_{231}+W_{232}+3.00W_{233}+W_{234}+W_{235}+W_{236}+W_{237}+W_{238}+W_{239}+W_{242}+W_{244}+W_{247}+W_{248}+3.00W_{273}+W_{276}+W_{291}+W_{294}-W_{301}-W_{302}+W_{308}-W_{317}+W_{321}$

R_{25} $W_{30}-W_{31}-W_{32}-W_{33}-W_{34}+W_{38}+W_{39}+W_{43}+W_{45}+W_{46}+W_{47}+W_{49}+W_{58}+W_{60}+W_{61}+W_{62}+W_{63}-W_{64}+W_{72}+W_{78}+W_{103}+W_{129}+W_{131}+W_{162}+W_{163}-W_{169}+W_{175}+W_{176}+W_{177}+W_{178}+W_{180}+W_{182}+W_{200}+W_{204}+W_{273}+W_{276}+W_{291}+W_{294}-W_{301}-W_{302}+W_{306}+W_{321}+W_{326}$

R_{26} $-2W_{35}-2W_{36}-2W_{37}-W_{38}-W_{39}-W_{42}-W_{43}-W_{44}-W_{45}-W_{46}-W_{47}-W_{49}+W_{53}+W_{54}+W_{55}+W_{56}-W_{57}+W_{59}-W_{62}+W_{70}+W_{77}-W_{83}-2W_{84}+W_{85}+W_{86}+W_{88}+W_{90}+W_{91}+W_{92}+W_{98}-W_{101}+W_{103}-W_{107}-W_{116}+W_{119}-W_{121}-2W_{122}+W_{125}-W_{128}-W_{133}-W_{134}+W_{136}-W_{138}+W_{140}+W_{142}+W_{144}+W_{147}-W_{148}-W_{149}+W_{150}+W_{155}-W_{156}-W_{159}+W_{160}-W_{173}+W_{174}-W_{189}-W_{194}+W_{199}+W_{203}+W_{204}-W_{206}-W_{220}+W_{221}+W_{233}+W_{235}+W_{236}+W_{237}+W_{238}+W_{239}+W_{242}+W_{243}+W_{248}-W_{255}-W_{256}+W_{301}+W_{303}-W_{308}-W_{311}W_{312}+2W_{313}+2W_{318}+W_{319}-W_{327}$

R_{27} $-W_{68}-W_{69}+W_{73}+W_{74}+W_{75}+W_{76}+W_{80}+W_{81}+W_{94}-W_{110}+W_{111}+W_{119}-W_{121}-W_{122}-W_{162}-W_{163}+W_{276}-W_{296}-W_{302}-W_{303}-W_{304}-W_{305}-W_{306}-W_{307}-W_{308}-W_{309}-W_{310}+W_{311}+W_{312}-W_{313}-W_{314}+W_{316}+W_{317}-W_{318}-W_{319}-2W_{320}-W_{321}-W_{323}-W_{324}-W_{325}$

R_{28} $W_{20}+W_{21}+W_{22}+W_{23}+W_{27}+W_{66}+W_{310}$

R_{29} $W_{11}-W_{12}-W_{13}-W_{14}-W_{15}-W_{16}+W_{56}+W_{63}-W_{64}+W_{91}+W_{108}+W_{145}-W_{146}+W_{147}-W_{148}+W_{208}+W_{237}+W_{253}+W_{254}$

R_{30}	W_5-W_6-W_7-W_8-W_9-W_{10}-2W_{11}+W_{13}+W_{14}+W_{15}-W_{21}+W_{29}+W_{34}+W_{39}+W_{40}-W_{42}-W_{45}-W_{46}-W_{48}-W_{49}-W_{50}-W_{51}-W_{56}+W_{58}+W_{59}+W_{60}+W_{61}+W_{62}+W_{80}+W_{81}-W_{91}+W_{92}+W_{102}-W_{108}+W_{109}+W_{124}+W_{134}+W_{137}-W_{145}+W_{146}-W_{147}+W_{148}+W_{153}-W_{154}+W_{155}-W_{156}-W_{157}+W_{158}-W_{159}+W_{160}-W_{184}-W_{185}-W_{186}-2W_{188}-W_{189}-W_{190}-W_{191}-W_{192}-W_{193}+W_{196}+W_{197}+W_{201}+W_{205}+W_{206}+2W_{207}+W_{209} W_{210}+W_{213}+W_{222}+W_{225}+W_{228}-W_{237}+W_{240}+W_{249}+W_{250}-W_{253}-W_{254}+W_{269}+W_{281}+W_{282}+W_{284}-W_{287}-W_{291}+W_{292}-2W_{294}+W_{323}
R_{31}	W_3+W_4+W_8+W_9+W_{12}+W_{15}+W_{18}+W_{28}+W_{32}+W_{55}+W_{61}+W_{73}+W_{74}+W_{75}+2W_{76}+W_{77}+W_{78}+W_{79}+W_{80}+W_{81}+W_{90}-W_{95}-W_{96}+W_{106}-W_{113}+W_{117}+W_{121}-W_{125}+W_{127}+W_{143}+W_{144}-2W_{171}+W_{172}-W_{175}-W_{176}-W_{183}-W_{185}+W_{190}-W_{195}+W_{205}-W_{215}+W_{219}-W_{224}-W_{227}+W_{228}+W_{229}+W_{236}+W_{251}+W_{252}-W_{276}+W_{279}+W_{288}-W_{291}-W_{294}+W_{301}+W_{302}+W_{312}+W_{317}-W_{321}+W_{325}
R_{32}	-W_2-W_3+W_7+W_{13}+W_{17}+W_{25}+W_{31}+W_{37}+W_{46}+W_{51}+W_{53}+W_{58}+W_{59}+W_{74}+W_{83}+W_{86}+W_{87}+W_{94}+W_{96}+W_{104}+W_{115}+W_{123}+W_{126}+W_{139}+W_{140}+W_{166}+W_{167}+W_{175}+W_{176}+W_{186}+W_{197}+W_{217}+W_{222}+W_{223}+W_{224}+W_{235}+W_{257}+W_{258}+W_{278}+W_{286}-W_{300}-W_{303}+W_{304}+W_{310}+W_{314}+W_{324}
R_{33}	W_1-W_2+W_4+W_9-W_{10}-W_{14}-2W_{19}-W22+W_{23}-W_{26}-W_{27}-W_{38}-W_{48}-W_{49}-W_{54}-W_{60}-W_{65}-W_{69}-W_{75}-W_{77}+W_{79}-W_{88}-W_{89}-W_{98}-W_{103}-W_{105}-W_{111}-W_{113}-W_{129}-W_{130}-W_{141}-W_{142}-W_{179}-W_{180}-W_{198}-W_{199}-W_{200}-W_{201}-W_{218}-W_{225}-W_{226}-W_{227}-W_{239}-W_{259}-W_{260}+W_{277}+W_{278}+W_{279}+W_{281}+W_{284}-W_{287}-W_{289}-2W_{291}-W_{292}-W_{294}-W_{296}-W_{298}-W_{300}+W_{301}+W_{302}-W_{303}-2W_{304}-2W_{305}-W_{306}-2W_{307}-W_{308}-W_{309}-W_{310}+W_{311}+W_{312}-W_{313}-2W_{314}+W_{316}-W_{318}-W_{319}-W_{320}-W_{321}+W_{323}+W_{324}+W_{325}+W_{327}
R_{34}	W_1+W_2-W_3-2W_4+2W_6-W_8+W_{10}+W_{12}+W_{14}-W_{15}+2W_{16}-W_{18}-W_{20}+W_{21}+W_{26}-W_{28}-W_{32}-W_{39}-2W_{40}+W_{43}+W_{45}+W_{46}+W_{47}+W_{48}+2W_{49}+W_{54}-W_{55}-W_{57}-W_{59}+W_{60}-W_{61}+W_{67}+W_{68}-W_{72}-W_{73}-W_{74}-2W_{76}-W_{77}-W_{78}-W_{79}-W_{80}-W_{81}+W_{88}+W_{89}-W_{90}+W_{95}+W_{96}+W_{105}-W_{106}+W_{113}-W_{117}-W_{121}+W_{125}-W_{127}-W_{131}+W_{141}+W_{142}-W_{143}-W_{144}+W_{157}-W_{158}+W_{159}-W_{160}+2W_{171}-W_{172}+W_{175}+W_{176}-W_{181}-W_{182}+W_{185}-W_{190}+W_{195}+W_{201}-W_{202}-W_{203}-W_{204}-W_{205}+W_{215}+W_{218}-W_{219}+W_{224}+W_{225}+W_{226}+2W_{227}-W_{228}-W_{229}-W_{236}+W_{239}-W_{251}-W_{252}+W_{259}+W_{260}+W_{271}+W_{273}+W_{276}-W_{277}-W_{278}-2W_{279}-W_{281}-2W_{282}-W_{284}+3.00W_{287}-W_{288}+W_{289}+3.00W_{291}-W_{292}+4.00W_{294}+W_{298}+W_{300}-2W_{301}-2W_{302}-W_{306}+W_{309}-W_{312}-W_{317}+W_{321}-W_{325}