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汽油替代燃料燃烧过程中多环芳烃生成的化学动力学模型

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Chemical Kinetic Model for Polycyclic Aromatic Hydrocarbon Formation during Gasoline Surrogate Fuel Combustion

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PAHs 子机理

Sub-mechanisms of PAHs

Reactions	Kinetic Parameters			Reference
	A	n	E	
1. C2H2+O=CH2+CO	5.00E+06	2	1900	This work
2. C2H3=C2H2+H	9.20E+40	-8.8	46200	This work
3. C2H4+H=C2H3+H2	1.32E+06	2.5	12240	15
4. C2H+H2=H+C2H2	4.90E+05	2.5	560	15
5. CH3+C2H=C3H3+H	2.41E+13	0	0	15
6. CH4+C2H=C2H2+CH3	1.81E+12	0	500	15
7. C2H2+C2H3=C4H4+H	2.00E+18	-1.7	10600	15
8. C2H2+C2H=C4H2+H	9.03E+13	0	0	15
9. 2C2H2=C4H2+H2	1.51E+13	0	21350	15
10. C4H2+H2=C4H4	4.00E+14	0	26800	15
11. C4H4+H=n-C4H3+H2	6.65E+05	2.5	12240	15
12. C2H2+C2H=n-C4H3	4.50E+37	-7.7	7100	15
13. n-C4H3+C2H2=C-C6H4+H	6.90E+46	-10	30100	7
14. C-C6H4+H=A1-	2.40E+60	-13.7	29500	7
15. n-C4H3+C2H2=A1-	9.60E+70	-17.8	31300	7
16. C3H3+C3H3=A1	2.00E+12	0	0	21
17. C5H5+CH3=A1+2H	1.00E+17	0	30000	This work
18. C3H3+C2H2=C5H5	2.40E+11	0	5030	14
19. C3H3+C2H3=C5H5+H	9.60E+40	-7.8	14410	14
20. A1-+H(+M)=A1(+M)	1.00E+14	0	0	7
21. A1-+C2H4=A1C2H3+H	2.51E+12	0	6190	7
22. A1+C2H3=A1C2H3+H	7.90E+11	0	6400	7
23. A1-+C2H3=A1C2H3	1.20E+27	-4.2	7235	7
24. A1-+C2H3=n-A1C2H2+H	9.40E+00	4.1	23234	7
25. A1C2H3+H=n-A1C2H2+H2	6.65E+06	2.5	12240	7
26. A1C2H3+OH=n-A1C2H2+H2O	3.10E+06	2	3430	7
27. n-A1C2H2+H=A1C2H+H2	1.50E+13	0	0	7
28. A1+C2H=A1C2H+H	5.00E+13	0	0	7
29. A1-+C2H2=n-A1C2H2	7.00E+38	-8	16400	7
30. A1C2H+H=n-A1C2H2	3.00E+43	-9.2	15272	7
31. n-A1C2H2+OH=A1C2H+H2O	2.50E+12	0	0	7
32. A1C2H+OH=A1C2H*+H2O	1.60E+08	1.4	1450	7
33. A1C2H+OH=>A1-+CH2CO	2.18E-04	4.5	-1000	7
34. A1C2H*+C2H2=A2-1	2.20E+62	-14.6	33100	7
35. n-A1C2H2+C2H2=A2+H	1.60E+16	-1.3	5400	7
36. A1-+C4H4=A2+H	3.30E+33	-5.7	25500	7

37. C5H5+C5H5=A2+2H	2.87E+13	0	4888.3	This work
38. C5H5+C5H5=A2+H2	2.87E+36	-6.3	22835	This work
39. A2+H=A2-1+H2	2.50E+14	0	16000	7
40. A2+OH=A2-1+H2O	1.60E+08	1.4	1450	7
41. A2-1+H(+M)=A2(+M)	1.00E+14	0	0	7
42. A2+OH=>A1C2H+CH2CO+H	1.30E+13	0	10600	7
43. A2R5-+H(+M)=A2R5(+M)	1.00E+14	0	0	7
44. A2-1+C2H2=A2R5+H	9.70E+30	-5.3	21600	7
45. A2+C2H=A2C2HA+H	5.00E+13	0	0	7
46. A2C2HA+H=A2R5+H	4.60E+37	-7	23100	7
47. A2R5+H=A2R5-+H2	2.50E+14	0	16000	7
48. A2R5+OH=A2R5-+H2O	1.60E+08	1.4	1450	7
49. A2R5-+C2H2=A3-4	2.00E+13	0	55000	7
50. A2C2HA+OH=>A2-1+CH2CO	2.18E-04	4.5	-1000	7
51. A2-1+C4H4=A3+H	3.30E+33	-5.7	25500	15
52. A2-1+C4H2=A3-4	3.30E+33	-5.7	12750	15
53. A1-+A1C2H=A3+H	1.10E+23	-2.9	15890	15
54. A1C2H*+A1=A3+H	1.10E+23	-2.9	15890	15
55. A3+H=A3-4+H2	2.50E+14	0	16000	7
56. A3+OH=A3-4+H2O	1.60E+08	1.4	1450	7
57. A3+OH=A2C2HA+CH2CO+H	6.50E+12	0	10600	7
58. A3-4+C2H2=A4+H	9.90E+24	-3.4	17800	This work
59. C4H2+A2R5=>A4	2.41E+02	2.2	-569	15
60. A2R5-+C4H2=>A4-	7.00E+37	-8	8200	15
61. A4+H=A4-+H2	2.50E+14	0	16000	7
62. A4+OH=A4-+H2O	1.60E+08	1.4	1450	7
63. A4-+H=A4	1.00E+14	0	0	7
64. A4+OH=A3-4+CH2CO	2.00E+13	0	21000	7
65. A4+O=A3-4+HCCO	2.20E+13	0	4530	7

A units: mol, cm, s; *E* units: cal/mol.

$$k_f = AT^n \exp(-E/RT)$$