Table S7. Optimized lumped reaction mechanism list for PP pyrolysis at 8 K/ps

Reaction ID	Reaction	lnA	Ea (kJ/mol)
1	2 [C_{41}~C_{200}] → [C_3~C_5] + [C_{200+}] + CH_4	38. 82	160. 09
2	[C_{11}~C_{20}] + [C_3~C_5] → [C_{21}~C_{40}]	36. 81	197. 30
3	[C_3~C_5] + [C_{200+}] → C_2H_4 + 2 [C_{41}~C_{200}] + CH_4	43. 94	238. 92
4	[C_{41}~C_{200}] + CH_4 → [C_3~C_5] + 2[C_{21}~C_{40}]	43. 91	251. 18
5	[C_{11}~C_{20}] → 4[C_3~C_5]	31. 45	126. 51
6	[C_{21}~C_{40}] → [C_{11}~C_{20}] + 3[C_3~C_5] + C_2H_4	29. 99	137. 21
7	[C_{11}~C_{20}] → 4[C_3~C_5] + C_2H_4	36. 40	269. 28
8	[C_6~C_{10}] + CH_4 → 3[C_3~C_5]	39. 92	182. 07
9	2 [C_3~C_5] → [C_6~C_{10}]	40. 48	247. 90
10	[C_{21}~C_{40}] → [C_{11}~C_{20}] + [C_3~C_5] + [C_6~C_{10}] + CH_4	28. 32	110. 58
11	[C_{11}~C_{20}] + CH_4 → 2[C_3~C_5] + [C_6~C_{10}]	54. 19	485. 24
12	2[C_6~C_{10}] → [C_{11}~C_{20}]	36. 20	114. 72
13	[C_6~C_{10}] → [C_3~C_5] + C_2H_6 + CH_4	42. 49	372. 29
14	[C_{21}~C_{40}] → [C_{11}~C_{20}] + [C_3~C_5] + H2	33. 87	207. 30
15	2C_2H_6 → [C_3~C_5]	39. 12	71. 20
16	[C_{11}~C_{20}] + [C_{21}~C_{40}] → [C_3~C_5] + [C_{41}~C_{200}] + [C_6~C_{10}]	40. 10	180. 74
17	[C_{11}~C_{20}] → 3 [C_3~C_5] + [C_6~C_{10}] + H_2	29. 24	124. 33
18	[C_{200+}] → [C_{11}~C_{20}] + [C_3~C_5] +2[C_{21}~C_{40}] + 4[C_{41}~C_{200}]	52. 05	509. 78
19	[C_{200+}] → [C_{11}~C_{20}] + [C_3~C_5] + [C_{21}~C_{40}] + 5[C_{41}~C_{200}]	34. 76	208. 60
20	[C_{41}~C_{200}] → [C_3~C_5] +2 [C_{21}~C_{40}] + [C_6~C_{10}]	39. 49	334. 26
21	[C_{41}~C_{200}] → 3 [C_3~C_5] + [C_{21}~C_{40}] + [C_6~C_{10}] + CH_4	35. 34	241. 06
22	[C_{21}~C_{40}] → [C_{11}~C_{20}] +3[C_3~C_5] + CH_4	31. 11	124. 39
23	[C_3~C_5] + CH_4 → C_2H_4 + C_2H_6 + H2	36. 15	239. 56
24	[C_3~C_5] + [C_{21}~C_{40}] → 2 [C_{11}~C_{20}]	39. 36	231. 71
25	[C_6~C_{10}] → [C_3~C_5] + 2 C_2H_6 +2 CH_4	25. 81	148. 70
26	[C_3~C_5] → C_2H_4 + 2CH_4 + H_2	29. 36	218. 12
27	2[C_6~C_{10}] → 2 [C_3~C_5] + 2 CH_4	38. 68	171. 22