Table S6. Optimized lumped reaction mechanism list for PP pyrolysis at 2 K/ps

Reaction ID	Reaction	lnA	Ea (kJ/mol)
1	$[C_{200+}] \rightarrow [C_{21}\sim C_{40}] + 3\,[C_{41}\sim C_{200}]$	42. 43	332. 06
2	$2\,[C_{11}\sim C_{20}] \rightarrow [C_{21}\sim C_{40}]$	40. 82	145. 52
3	$2\,[C_{21}\sim C_{40}] \rightarrow [C_{41}\sim C_{200}] + [C_6\sim C_{10}]$	41. 06	166. 09
4	$[C_{41}\sim C_{200}] + [C_6\sim C_{10}] \rightarrow 3\,[C_3\sim C_5] + 2\,[C_{21}\sim C_{40}]$	42. 82	200. 61
5	$[C_{21}\sim C_{40}] + CH_4 \rightarrow [C_{11}\sim C_{20}] + [C_3\sim C_5]$	47. 24	289. 42
6	$[C_{41}\sim C_{200}] + CH_4 \rightarrow 2\,[C_{21}\sim C_{40}] + [C_{21}\sim C_{40}]$	37. 53	125. 48
7	$[C_3\sim C_5] + [C_6\sim C_{10}] \rightarrow [C_{11}\sim C_{20}]$	34. 36	63. 35
8	$2\,CH_4 \rightarrow C_2H_6 + H_2$	39. 13	162. 94
9	$[C_3\sim C_5] + C_2H_6 \rightarrow [C_6\sim C_{10}]$	40. 63	138. 04
10	$[C_3\sim C_5] \rightarrow C_2H_4 + C2H_6$	32. 44	211. 58
11	$H_2 + C_2H_4 \rightarrow C_2H_6$	34. 94	222. 67
12	$C_2H_6 + [C_6\sim C_{10}] \rightarrow 2[C_3\sim C_5]$	38. 91	102. 62
13	$[C_6\sim C_{10}] \rightarrow [C_3\sim C_5] + C_2H_6 + H_2$	38. 70	252. 38
14	$C_2H_6 \rightarrow C_2H_4 + H2$	39. 39	259. 35
15	$[C_{11}\sim C_{20}] + [C_3\sim C_5] + C_2H_6 \rightarrow 2\,[C_6\sim C_{10}] + H2$	52. 04	263. 57
16	$[C_{11}\sim C_{20}] + C_2H_6 + H2 \rightarrow 2[C_3\sim C_5] + [C_6\sim C_{10}]$	51. 97	180. 92
17	$[C_{21}\sim C_{40}] \rightarrow 2\,[C_{11}\sim C_{20}] + [C_3\sim C_5] + [C_6\sim C_{10}]$	36. 72	239. 68
18	$[C_{11}\sim C_{20}] \rightarrow 4\,[C_3\sim C_5] + [C_6\sim C_{10}]$	34. 95	173. 67
19	$2\,[C_3\sim C_5] \rightarrow 2\,C_2H_6 + 2CH_4$	38. 67	214. 38