

Table S5. Optimized lumped reaction mechanism list for PP pyrolysis at 1 K/ps

Reaction ID	Reaction	lnA	Ea (kJ/mol)
1	$2\text{CH}_4 \rightarrow \text{C}_2\text{H}_6 + \text{H}_2$	34. 80	25. 52
2	$[\text{C}_{41}\sim\text{C}_{200}] \rightarrow [\text{C}_3\sim\text{C}_5] + 2[\text{C}_{21}\sim\text{C}_{40}]$	44. 96	376. 53
3	$[\text{C}_{21}\sim\text{C}_{40}] + \text{CH}_4 \rightarrow 2 [\text{C}_{11}\sim\text{C}_{20}] + [\text{C}_3\sim\text{C}_5]$	45. 96	246. 32
4	$[\text{C}_3\sim\text{C}_5] + \text{C}_2\text{H}_6 \rightarrow [\text{C}_6\sim\text{C}_{10}]$	42. 03	150. 03
5	$[\text{C}_{21}\sim\text{C}_{40}] + [\text{C}_6\sim\text{C}_{10}] \rightarrow 2[\text{C}_{11}\sim\text{C}_{20}]$	47. 64	266. 38
6	$[\text{C}_{11}\sim\text{C}_{20}] \rightarrow [\text{C}_3\sim\text{C}_5] + 2[\text{C}_6\sim\text{C}_{10}] + \text{CH}_4$	34. 43	215. 90
7	$[\text{C}_3\sim\text{C}_5] \rightarrow \text{C}_2\text{H}_6 + 2\text{CH}_4$	34. 65	207. 75
8	$2[\text{C}_3\sim\text{C}_5] + \text{H}_2 \rightarrow 2\text{C}_2\text{H}_6 + 2\text{CH}_4$	43. 67	169. 17
9	$4[\text{C}_3\sim\text{C}_5] + \text{C}_2\text{H}_6 \rightarrow 2[\text{C}_6\sim\text{C}_{10}] + 2\text{H}_2$	55. 04	261. 85
10	$2[\text{C}_{11}\sim\text{C}_{20}] + [\text{C}_3\sim\text{C}_5] + 2\text{C}_2\text{H}_6 \rightarrow [\text{C}_{21}\sim\text{C}_{40}]$	60. 99	243. 30
11	$[\text{C}_3\sim\text{C}_5] + \text{C}_2\text{H}_6 + 2[\text{C}_6\sim\text{C}_{10}] \rightarrow [\text{C}_{11}\sim\text{C}_{20}]$	58. 83	475. 93
12	$2[\text{C}_{11}\sim\text{C}_{20}] \rightarrow [\text{C}_{21}\sim\text{C}_{40}] + \text{CH}_4$	42. 27	147. 38
13	$[\text{C}_{200+}] \rightarrow [\text{C}_{11}\sim\text{C}_{20}] + 2[\text{C}_{41}\sim\text{C}_{200}] + \text{CH}_4$	41. 73	306. 22
14	$[\text{C}_3\sim\text{C}_5] \rightarrow \text{C}_2\text{H}_4 + 2\text{CH}_4$	24. 46	81. 46
15	$[\text{C}_{21}\sim\text{C}_{40}] \rightarrow 2[\text{C}_{11}\sim\text{C}_{20}] + 3[\text{C}_3\sim\text{C}_5]$	37. 75	217. 70
16	$\text{C}_2\text{H}_6 + [\text{C}_6\sim\text{C}_{10}] \rightarrow 2[\text{C}_3\sim\text{C}_5] + \text{CH}_4$	41. 11	99. 45
17	$\text{C}_2\text{H}_4 + [\text{C}_6\sim\text{C}_{10}] + \text{H}_2 \rightarrow 2[\text{C}_3\sim\text{C}_5] + \text{C}_2\text{H}_6$	43. 92	319. 44
18	$[\text{C}_6\sim\text{C}_{10}] \rightarrow 2\text{C}_2\text{H}_6 + 2\text{CH}_4 + \text{H}_2$	40. 19	266. 08