

Supporting Information

Thermal Stability Improvement of *exo*-Tetrahydrodicyclopentadiene

by 1,2,3,4-Tetrahydroquinoxaline: Mechanism and Kinetics

Sun Hee Park,^{||,†} Cheong Hoon Kwon,^{||,†} Joongyeon Kim,[†] Jeong Hwan Chun,[†] Wonkeun Chung,[†]

Byung-Hee Chun,[†] Jeong Sik Han,[‡] Byung Hun Jeong,[‡] Hogyu Han,^{*,§} and Sung Hyun Kim^{*,†}

[†]Department of Chemical & Biological Engineering, Korea University, Seoul 136-701, Korea

[‡]Agency for Defense Development, 111 Sunam-dong , Yuseong-gu, Daejeon 305-152, Korea

[§]Department of Chemistry, Korea University, Seoul 136-701, Korea

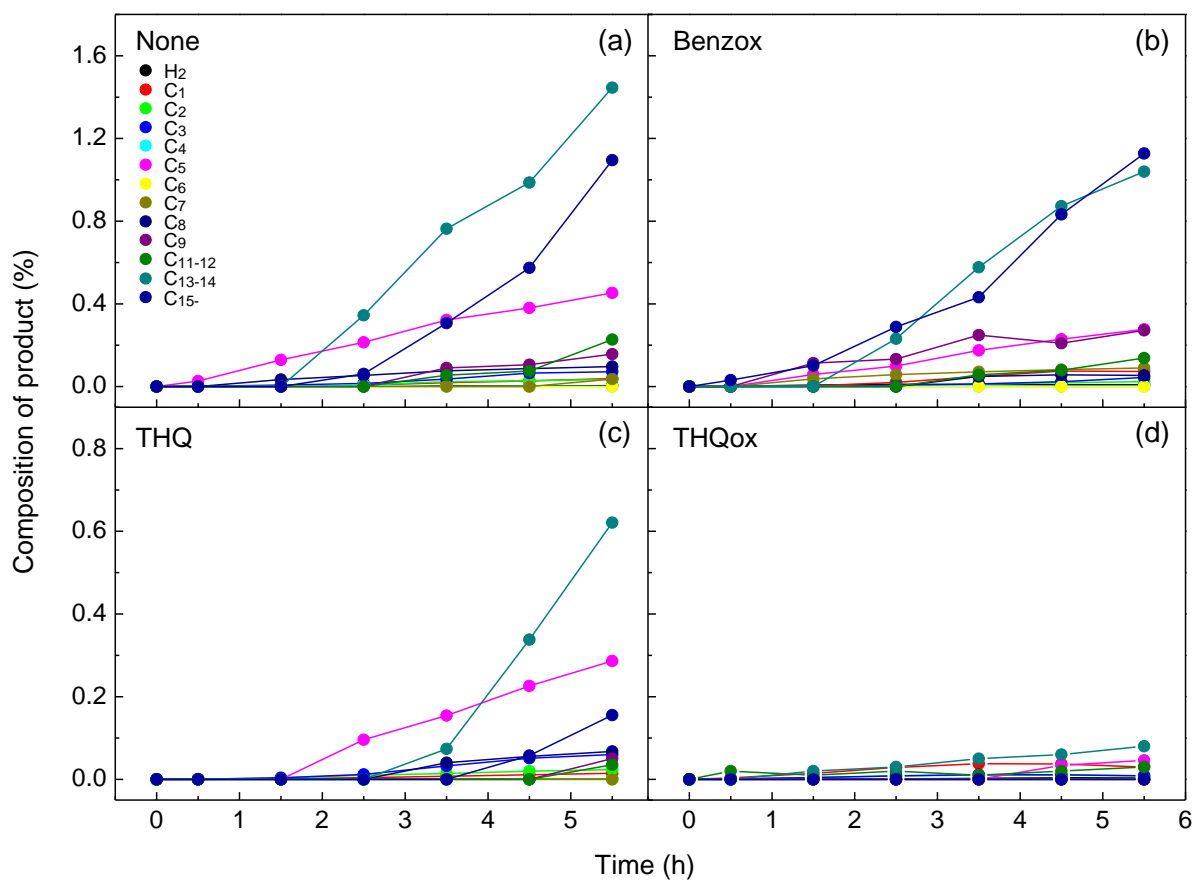


Figure S1. Compositions of products formed upon thermal decomposition of *exo*-THDCP in the absence and presence of H donors (0.5 wt %) at 395 °C. See also Figure 3. Note that Figure S1 shown here was obtained by redrawing Figure 3. They differ from each other in that the plot for C₁₀ is included (excluded) in Figure 3 (Figure S1). Note the different y-axis scale between Figures 3 and S1.

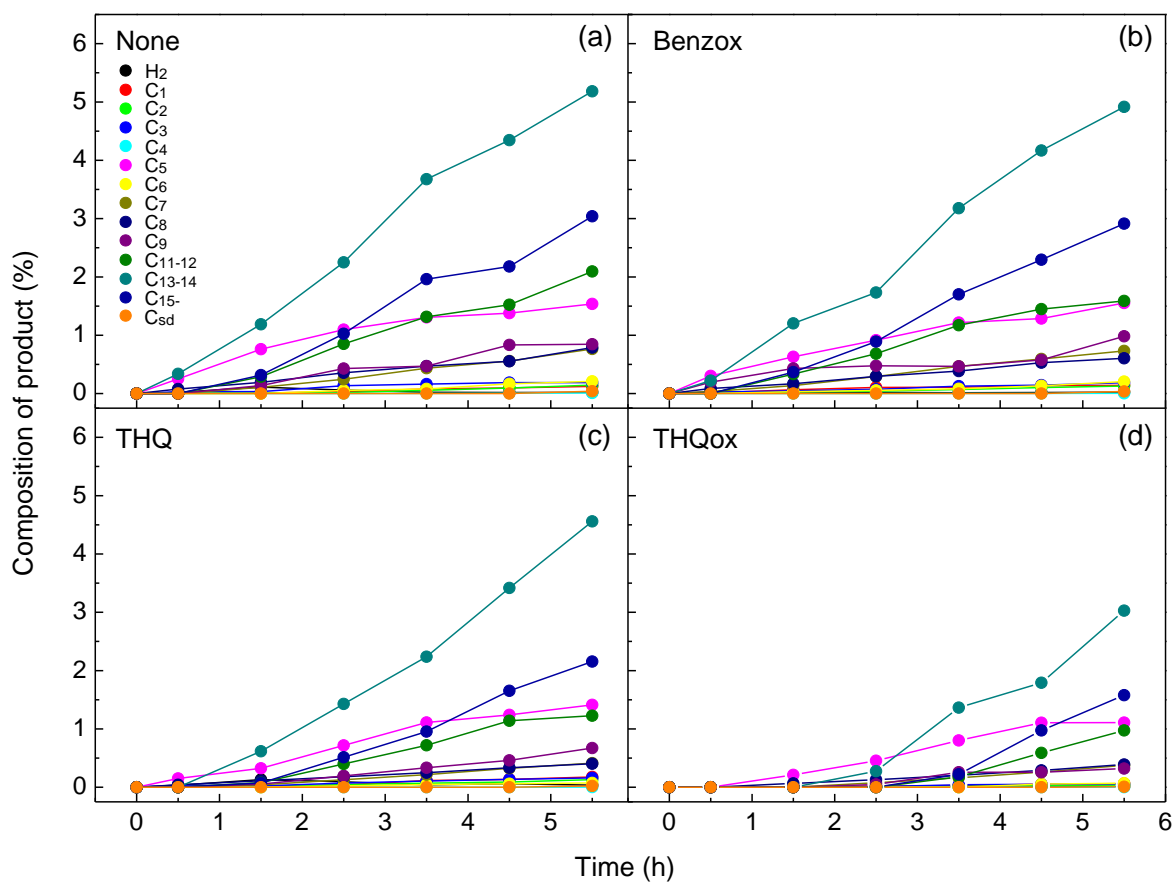


Figure S2. Compositions of products formed upon thermal decomposition of *exo*-THDCP in the absence and presence of H donors (0.5 wt %) at 415 °C. See also Figure 4. Note that Figure S2 shown here was obtained by redrawing Figure 4. They differ from each other in that the plot for C₁₀ is included (excluded) in Figure 4 (Figure S2). Note the different y-axis scale between Figures 4 and S2.

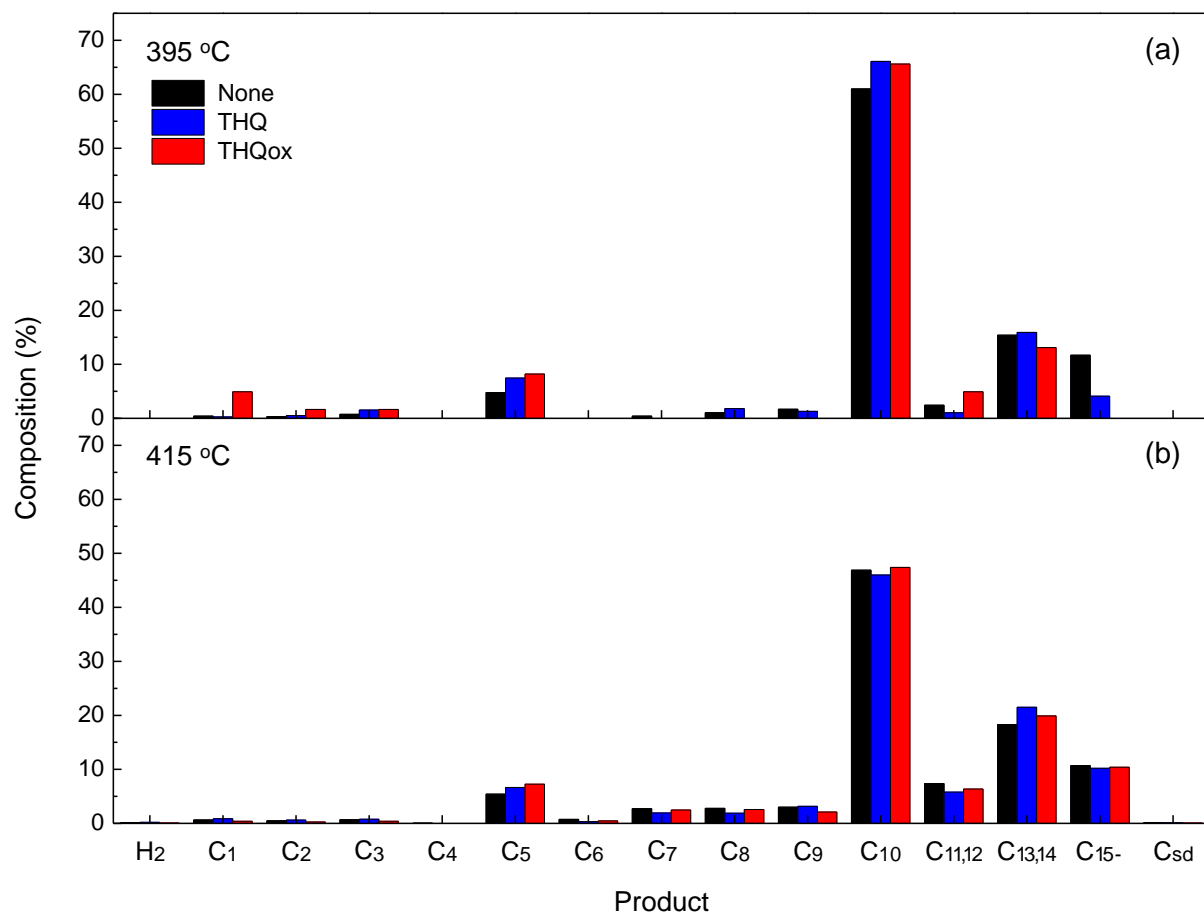


Figure S3. Comparison of product compositions obtained upon thermal decomposition of *exo*-THDCP in the absence and presence of THQ and THQox (0.5 wt %) at 395 and 415 °C for 5.5 h. See also Figures S1 and S2. Note that Figure S3 shown here was obtained by redrawing Figure 5. They differ from each other in the definition of product composition used, which is the ratio of C_n to all compounds (products) in Figure 5 (Figure S3). Note that the ratio of H_2 or C_n to all compounds (products) is obtained by including (excluding) observed *exo*-THDCP in the denominator for its calculation. See also Table S1.

Table S1. Comparison of Product Compositions Obtained upon Thermal Decomposition of *exo*-THDCP in the Absence and Presence of THQ and THQox (0.5 wt %) at 395 and 415 °C for 5.5 h^a

product	395 °C						415 °C					
	yield, Y (wt %)						yield, Y (wt %)					
	none	THQ	THQox	Δ_{THQ}	Δ_{THQox}	$\Delta_{\text{THQox-THQ}}$	none	THQ	THQox	Δ_{THQ}	Δ_{THQox}	$\Delta_{\text{THQox-THQ}}$
H ₂	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.19	0.07	0.05	-0.07	-0.12
C ₁₋₄	1.49	2.31	8.20	0.83	6.71	5.88	1.83	2.22	1.05	0.39	-0.78	-1.17
C ₅	4.78	7.46	8.20	2.68	3.42	0.74	5.43	6.65	7.27	1.22	1.84	0.62
C ₆₋₉	3.19	3.09	0.00	-0.10	-3.19	-3.09	9.24	7.31	7.60	-1.93	-1.64	0.29
C ₁₀	61.0	66.1	65.6	5.10	4.60	-0.50	46.9	46.0	47.4	-0.90	0.50	1.40
C ₁₁₋₁₄	17.8	17.0	18.0	-0.80	0.20	1.00	25.6	27.3	26.2	1.70	0.60	-1.10
C ₁₅₋	11.7	4.10	0.00	-7.60	-11.7	-4.10	10.7	10.2	10.4	-0.50	-0.30	0.20
C _{sd}	0.000	0.000	0.000	0.000	0.000	0.000	0.141	0.104	0.059	-0.037	-0.082	-0.045

^aSee also Figure S3. Note that Table S1 shown here differs from Table 1 in the definition of product composition (also referred to as yield) used, which is the ratio of C_n to all compounds (products) in Table 1 (Table S1). The ratio of H₂ or C_n to all compounds (products) is obtained by including (excluding) observed *exo*-THDCP in the denominator for its calculation. $\Delta_{\text{THQ}} = Y_{\text{THQ}} - Y_{\text{none}}$; $\Delta_{\text{THQox}} = Y_{\text{THQox}} - Y_{\text{none}}$; $\Delta_{\text{THQox-THQ}} = Y_{\text{THQox}} - Y_{\text{THQ}}$.