

Supplementary Information

Anisotropic Initial reaction Mechanism and Sensitivity Characterization of the Host-Guest Structure CL-20/H₂O₂ under Shock Loading

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Table S1 Bond order cutoff value for various atom pairs

	C	H	O	N
C	0.55	0.40	0.65	0.30
H	0.40	0.55	0.40	0.55
O	0.65	0.40	0.65	0.55
N	0.30	0.55	0.55	0.45

Table S2 Main reaction paths and relevant information of the CL-20/H₂O₂ system under the shock velocity of 7 km/s along a-axis in the first 10ps

Reaction_time/ps	Net flux ^a	Frequencies ^b	Reactions
3.0~9.93	5	25/-20	C ₁₂ H ₁₂ N ₂₄ O ₂₄ → C ₁₂ H ₁₂ N ₂₄ O ₂₄
2.65~9.98	7	76/-69	C ₆ H ₆ N ₁₂ O ₁₂ + C ₆ H ₆ N ₁₂ O ₁₂ → C ₁₂ H ₁₂ N ₂₄ O ₂₄
2.91~9.02	9	15/-6	C ₆ H ₆ N ₁₂ O ₁₂ + C ₆ H ₆ N ₁₂ O ₁₂ → C ₁₂ H ₁₂ N ₂₄ O ₂₄
5.2~8.85	7	9/-2	C ₆ H ₆ N ₁₂ O ₁₂ + C ₆ H ₆ N ₁₂ O ₁₂ → C ₁₂ H ₁₂ N ₂₄ O ₂₄
1.5~10.0	9	649/-640	C ₆ H ₆ N ₁₂ O ₁₂ → C ₆ H ₆ N ₁₂ O ₁₂
0.9~10.0	10	645/-635	C ₆ H ₆ N ₁₂ O ₁₂ → C ₆ H ₆ N ₁₂ O ₁₂
2.92~10.0	12	65/-53	C ₁₂ H ₁₂ N ₂₄ O ₂₄ → C ₆ H ₆ N ₁₂ O ₁₂ + C ₆ H ₆ N ₁₂ O ₁₂

^aThe reactions whose net fluxes below 5 times are excluded from the table.

^bThe frequencies of the forward and inverse reactions are separated with the “/” symbol.

Table S3 Main reaction paths and relevant information of the CL-20/H₂O₂ system under the shock velocity of 8 km/s along a-axis in the first 10ps

Reaction_time/ps	Net flux	Frequencies	Reactions
6.75~9.74	5	7/-2	C ₁₂ H ₁₃ N ₂₃ O ₂₂ → C ₁₂ H ₁₃ N ₂₃ O ₂₂
5.75~7.3	6	11/-5	C ₁₈ H ₁₈ N ₃₆ O ₃₃ → C ₁₈ H ₁₈ N ₃₆ O ₃₃
6.98~9.68	5	14/-9	C ₁₂ H ₁₃ N ₂₃ O ₂₂ → C ₁₂ H ₁₃ N ₂₃ O ₂₂
7.87~9.92	6	15/-9	C ₆ H ₆ N ₁₁ O ₁₁ → C ₆ H ₆ N ₁₁ O ₁₁
1.81~10.0	8	159/-151	H ₂ O ₂ + NO ₂ → HNO ₃ + HO
0.45~10.0	14	384/-370	HO + HO → H ₂ O ₂
2.9~9.96	6	81/-75	HO + C ₆ H ₇ N ₁₁ O ₁₁ → H ₂ O ₂ + C ₆ H ₆ N ₁₁ O ₁₀
4.63~9.86	5	9/-4	C ₁₂ H ₁₂ N ₂₄ O ₂₄ → C ₆ H ₆ N ₁₂ O ₁₂ + C ₆ H ₆ N ₁₂ O ₁₂
4.56~9.94	5	23/-18	C ₁₂ H ₁₂ N ₂₄ O ₂₄ → C ₁₂ H ₁₂ N ₂₄ O ₂₄

0.72~6.97	8	20/-12	$C_{12}H_{12}N_{24}O_{24} \rightarrow C_{12}H_{12}N_{23}O_{22} + NO_2$
0.87~9.99	6	119/-113	$C_{12}H_{12}N_{24}O_{24} \rightarrow C_6H_6N_{12}O_{12} + C_6H_6N_{12}O_{12}$
0.83~8.75	10	36/-26	$C_{12}H_{12}N_{23}O_{22} + NO_2 \rightarrow C_6H_6N_{12}O_{12} + C_6H_6N_{12}O_{12}$
6.93~9.85	7	13/-6	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
3.23~9.94	10	29/-19	$C_6H_6N_{12}O_{12} + C_6H_6N_{13}O_{14} \rightarrow C_{12}H_{12}N_{25}O_{26}$
2.44~8.75	5	94/-89	$C_6H_6N_{12}O_{12} + NO_2 \rightarrow C_6H_5N_{12}O_{12} + HNO_2$
1.57~9.96	9	34/-25	$C_6H_6N_{12}O_{12} + NO_2 \rightarrow C_6H_6N_{13}O_{14}$
1.0~10.0	5	78/-73	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.71~10.0	12	358/-346	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.7~9.99	6	101/-95	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.4~10.0	13	1090/-1077	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.44~10.0	5	329/-324	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
1.02~9.69	6	28/-22	$C_6H_6N_{11}O_{10} + NO_2 \rightarrow C_6H_6N_{12}O_{12}$
1.45~9.9	5	30/-25	$C_6H_6N_{11}O_{10} + NO_2 \rightarrow C_6H_6N_{12}O_{12}$
5.4~9.65	11	36/-25	$C_6H_6N_{11}O_{10} + N_2O_5 \rightarrow C_6H_6N_{13}O_{15}$
1.02~9.96	5	28/-23	$C_6H_7N_{12}O_{13} \rightarrow HO + C_6H_6N_{12}O_{12}$
2.65~9.82	6	15/-9	$C_6H_6N_{13}O_{14} \rightarrow C_6H_6N_{12}O_{11} + NO_3$
3.71~9.9	6	26/-20	$C_6H_6N_{13}O_{14} \rightarrow C_6H_6N_{13}O_{14}$
6.25~9.45	5	7/-2	$C_6H_6N_{13}O_{15} \rightarrow C_6H_6N_{11}O_{10} + N_2O_5$
0.5~9.95	5	52/-47	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.64~9.75	7	50/-43	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
1.84~9.72	7	15/-8	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.36~9.99	5	891/-886	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
2.34~7.41	6	7/-1	$C_{12}H_{12}N_{23}O_{22} \rightarrow C_{12}H_{12}N_{23}O_{22}$
0.77~8.58	5	16/-11	$C_{12}H_{12}N_{24}O_{24} \rightarrow C_{12}H_{12}N_{24}O_{24}$
4.68~8.64	7	23/-16	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{11}O_{10}$

Table S4 Main reaction paths and relevant information of the CL-20/H₂O₂ system under the shock velocity of 9 km/s along a-axis in the first 10ps

Reaction_time/ps	Net flux	Frequencies	Reactions
7.79~9.0	8	11/-3	$C_6H_6N_{14}O_{18} + NO_2 \rightarrow C_6H_6N_{13}O_{15} + N_2O_5$
9.22~9.99	5	5/0	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{11}O_{10}$
1.25~3.05	5	8/-3	$C_6H_6N_{12}O_{12} + C_6H_6N_{11}O_{11} \rightarrow C_{12}H_{12}N_{23}O_{23}$
2.87~4.28	5	8/-3	$C_6H_6N_{12}O_{11} + HO_2 \rightarrow C_6H_7N_{12}O_{13}$

0.6~7.2	6	28/-22	$C_6H_6N_{12}O_{11} \rightarrow C_6H_6N_{12}O_{11}$
0.96~9.02	5	17/-12	$C_6H_6N_{12}O_{11} \rightarrow C_6H_6N_{11}O_9 + NO_2$
1.26~5.53	5	16/-11	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{11}O_{10}$
6.13~9.91	5	42/-37	$C_6H_6N_{11}O_7 + HO \rightarrow C_6H_7N_{11}O_8$
6.02~6.75	5	9/-4	$C_6H_5N_{12}O_{10} + HNO_2 \rightarrow C_6H_6N_{12}O_{10} + NO_2$
5.68~7.34	6	8/-2	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
3.68~9.99	5	116/-111	$O_2 + NO_2 \rightarrow NO_4$
0.87~8.2	7	83/-76	$H_2O_2 + NO_2 \rightarrow HNO_3 + HO$
0.33~9.99	27	584/-557	$H_2O_2 \rightarrow HO + HO$
5.3~6.78	6	9/-3	$C_6H_7N_{12}O_{14} \rightarrow C_6H_7N_{11}O_{11} + NO_3$
6.47~8.09	6	13/-7	$C_6H_7N_{11}O_{12} \rightarrow C_6H_7N_{11}O_{12}$
4.42~5.87	5	9/-4	$C_6H_7N_{11}O_{12} + NO_2 \rightarrow C_6H_7N_{12}O_{14}$
1.0~9.99	15	194/-179	$HO + NO_2 \rightarrow HNO_3$
0.5~1.31	5	5/0	$C_{12}H_{12}N_{24}O_{24} \rightarrow C_{12}H_{12}N_{24}O_{24}$
3.05~4.2	6	9/-3	$C_{12}H_{12}N_{22}O_{20} \rightarrow C_{12}H_{12}N_{22}O_{20}$
0.39~3.33	10	32/-22	$C_6H_6N_{12}O_{12} + C_6H_6N_{12}O_{12} \rightarrow C_{12}H_{12}N_{24}O_{24}$
0.86~5.89	13	27/-14	$C_6H_6N_{12}O_{12} + NO_2 \rightarrow C_6H_6N_{13}O_{14}$
0.5~7.48	9	21/-12	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.37~9.91	23	214/-191	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.37~9.17	11	136/-125	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.3~9.86	33	417/-384	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.29~9.79	7	344/-337	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.31~9.88	14	198/-184	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
4.92~5.89	5	8/-3	$C_6H_6N_{11}O_{10} + NO_3 \rightarrow C_6H_6N_{12}O_{13}$
1.33~8.19	7	13/-6	$C_6H_6N_{11}O_{10} + NO_2 \rightarrow C_6H_6N_{12}O_{12}$
0.45~8.99	8	88/-80	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{11}O_{10}$
1.34~7.56	6	21/-15	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
5.28~5.77	6	6/0	$C_6H_6N_{11}O_{11} + NO_2 \rightarrow C_6H_6N_{11}O_{10} + NO_3$
6.02~9.67	5	12/-7	$C_6H_7N_{11}O_{12} \rightarrow C_6H_7N_{11}O_{12}$
4.01~4.69	5	8/-3	$C_{12}H_{12}N_{23}O_{23} \rightarrow C_{12}H_{12}N_{23}O_{23}$
0.56~7.55	5	57/-52	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{11}O_{10}$
2.18~9.97	16	115/-99	$NO_3 + NO_2 \rightarrow N_2O_5$
0.64~9.94	12	65/-53	$NO_2 + NO_2 \rightarrow N_2O_4$
0.44~3.81	5	22/-17	$C_6H_6N_{12}O_{13} \rightarrow C_6H_6N_{12}O_{11} + O_2$

3.02~4.35	5	9/-4	$C_{12}H_{12}N_{25}O_{27} \rightarrow C_6H_6N_{13}O_{14} + C_6H_6N_{12}O_{13}$
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Table S5 Main reaction paths and relevant information of the CL-20/H₂O₂ system under the shock velocity of 10 km/s along a-axis in the first 2.5ps

Reaction_time/ps	Net flux	Frequencies	Reactions
0.72~1.43	5	5/0	$C_6H_6N_{12}O_{11} \rightarrow C_6H_6N_{11}O_9 + NO_2$
0.74~2.5	10	56/-46	$O_2 + NO_2 \rightarrow NO_4$
0.33~2.35	12	28/-16	$H_2O_2 + NO_2 \rightarrow HNO_3 + HO$
0.27~2.5	22	187/-165	$H_2O_2 \rightarrow HO + HO$
0.42~2.44	9	30/-21	$HNO_3 \rightarrow HO + NO_2$
0.31~1.12	8	22/-14	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.33~0.99	7	16/-9	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$
0.28~0.51	5	6/-1	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.24~1.03	7	56/-49	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.23~1.05	18	52/-34	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
0.27~0.76	13	29/-16	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}$
1.49~2.49	7	16/-9	$NO_3 + NO_2 \rightarrow N_2O_5$
0.86~2.4	5	19/-14	$NO_5 \rightarrow NO_5$