

Mechanism of the impact-sensitivity reduction of energetic CL-20/TNT cocrystals: a nonequilibrium molecular dynamics study

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Supplementary Materials:

Figure S1: Change of pressure, density and temperature of CL-20 and TNT with time under different impact velocities; Table S1: Elementary reactions of CL-20/TNT decomposition at different impact velocities. Table S2: Elementary reactions of CL-20 decomposition at different impact velocities. Table S3: Elementary reactions of TNT decomposition at different impact velocities.

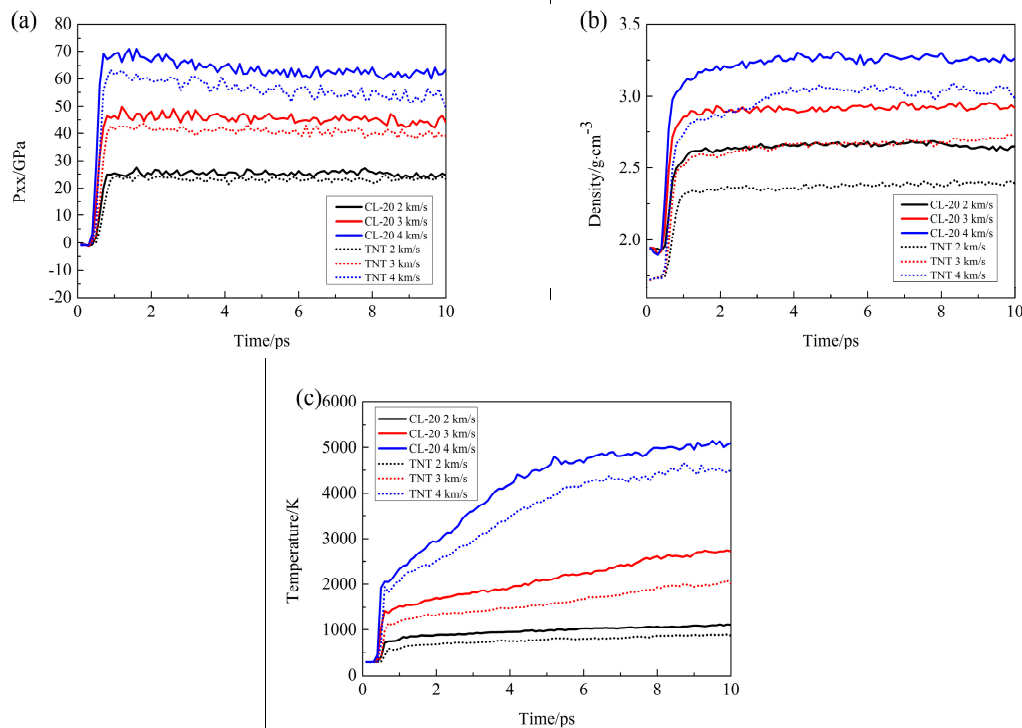


Figure S1. Change of pressure, density and temperature of CL-20 and TNT with time under different impact velocities.

Table S1. Elementary reactions of CL-20/TNT cocrystal decomposition at different impact velocities.

Impact velocities /km/s	Frequencies	Reaction time/ps	Elementary reactions	Illustration
2	4	1.0-6.0	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18}$	First occur
	2	1.9-7.1	$\text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_{19}\text{H}_{17}\text{N}_{27}\text{O}_{30}$	
	1	2.0-2.0	$\text{C}_{19}\text{H}_{17}\text{N}_{27}\text{O}_{30} \rightarrow \text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	2	2.7-5.9	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	3.0-3.0	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{NO}_2 + \text{C}_7\text{H}_5\text{N}_2\text{O}_4\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	

3	1	3.1-3.1	$\text{NO}_2 + \text{C}_7\text{H}_5\text{N}_2\text{O}_4 \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	Highest frequency
	4	1.0-6.0	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18}$	
	3	3.8-5.9	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	3	3.9-6.0	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	3	7.9-9.8	$\text{C}_7\text{H}_5\text{N}_5\text{O}_8 \rightarrow \text{N}_2 + \text{C}_7\text{H}_5\text{N}_3\text{O}_8$	
	3	7.8-8.7	$\text{N}_2 + \text{C}_7\text{H}_5\text{N}_3\text{O}_8 \rightarrow \text{C}_7\text{H}_5\text{N}_5\text{O}_8$	First occur
	2	0.5-0.8	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	0.6-0.6	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	1	0.6-0.6	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{38}\text{H}_{34}\text{N}_{54}\text{O}_{60}$	
	1	0.7-0.7	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	0.7-0.7	$\text{C}_{38}\text{H}_{34}\text{N}_{54}\text{O}_{60} \rightarrow \text{NO}_2 + \text{C}_{19}\text{H}_{17}\text{N}_{26}\text{O}_{28} + \text{C}_{19}\text{H}_{17}\text{N}_{27}\text{O}_{30}$	
	4	0.7-1.4	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_7\text{H}_5\text{N}_3\text{O}_6)$	
	2	0.8-0.8	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{X}(\text{C}_7\text{H}_5\text{N}_3\text{O}_6) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	4	4.1-8.5	$\text{NO}_2 \rightarrow \text{X}(\text{NO}_2) \rightarrow \text{NO}_2$	Highest frequency
	4	4.0-8.2	$\text{NO}_2 \rightarrow \text{NO}_2 \rightarrow \text{X}(\text{NO}_2)$	
	3	2.8-7.3	$\text{NO}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_4$	
	3	1.7-3.0	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}$	
	2	7.5-7.0	$\text{O} \rightarrow \text{X}(\text{N}_2\text{O}_3) + \text{N}_2 \rightarrow \text{N}_2\text{O} \rightarrow \text{X}(\text{N}_2\text{O}_3)$	
	2	6.4-7.2	$\text{NO}_2 \rightarrow \text{X}(\text{HO}) \rightarrow \text{NO}_2$	
	2	5.9-6.1	$\text{C}_7\text{H}_5\text{N}_6\text{O}_{11} \rightarrow \text{N}_2 + \text{C}_7\text{H}_5\text{N}_4\text{O}_{11}$	
	2	3.9-6.0	$\text{N}_2\text{O}_4 \rightarrow \text{NO}_2 + \text{NO}_2$	
	2	3.6-4.2	$\text{C}_{13}\text{H}_{11}\text{N}_{14}\text{O}_{17} \rightarrow \text{NO}_2 + \text{C}_{13}\text{H}_{11}\text{N}_{13}\text{O}_{15}$	
	2	2.3-2.9	$\text{C}_7\text{H}_5\text{N}_4\text{O}_8 \rightarrow \text{NO}_2 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6$	
	2	2.2-2.7	$\text{NO}_2 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_4\text{O}_8$	
	2	2.0-2.3	$\text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{13}\text{O}_{14}$	
4	2	1.8-2.6	$\text{C}_{13}\text{H}_{11}\text{N}_{14}\text{O}_{17} + \text{C}_6\text{H}_6\text{N}_{11}\text{O}_9 \rightarrow \text{C}_{19}\text{H}_{17}\text{N}_{25}\text{O}_{26}$	First occur
	2	1.6-2.4	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{X}(\text{NO}_2)$	
	2	1.3-1.5	$\text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18} \rightarrow \text{NO}_2 + \text{C}_{13}\text{H}_{11}\text{N}_{14}\text{O}_{16}$	
	2	0.5-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{13}\text{H}_{11}\text{N}_{15}\text{O}_{18}$	
	2	0.5-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}$	
	2	4.3-9.9	$\text{N}_2 \rightarrow \text{N}_2 \rightarrow \text{X}(\text{H})$	
	2	5.2-9.6	$\text{O} \rightarrow \text{X}(\text{H}_2) \rightarrow \text{O} \rightarrow \text{X}(\text{H})$	Highest frequency
	2	5.2-9.9	$\text{HO} \rightarrow \text{X}(\text{H}) \rightarrow \text{HO}$	
	2	6.1-9.4	$\text{N}_2 \rightarrow \text{X}(\text{H}) \rightarrow \text{N}_2$	
	28	4.5-9.9	$\text{N}_2 \rightarrow \text{X}(\text{H}) \rightarrow \text{N}_2$	
	21	4.3-9.9	$\text{N}_2 \rightarrow \text{N}_2 \rightarrow \text{X}(\text{H})$	
	11	5.2-9.6	$\text{O} \rightarrow \text{X}(\text{H}_2) \rightarrow \text{O} \rightarrow \text{X}(\text{H})$	
	10	5.1-8.7	$\text{O} \rightarrow \text{X}(\text{H}_2) \rightarrow \text{O} \rightarrow \text{X}(\text{H}_2)$	
	10	2.8-9.3	$\text{O} \rightarrow \text{X}(\text{H}) \rightarrow \text{O} \rightarrow \text{X}(\text{H}_2)$	
	9	5.7-9.7	$\text{N} \rightarrow \text{X}(\text{HN}) \rightarrow \text{N} \rightarrow \text{X}(\text{N})$	
	9	4.4-8.2	$\text{HO} \rightarrow \text{HO} \rightarrow \text{X}(\text{H})$	
	8	7.7-9.8	$\text{H} \rightarrow \text{X}(\text{N}_2) \rightarrow \text{H} \rightarrow \text{X}(\text{HO})$	
	8	5.2-9.9	$\text{HO} \rightarrow \text{X}(\text{H}) \rightarrow \text{HO}$	
	8	3.8-9.7	$\text{N}_2 \rightarrow \text{N}_2 \rightarrow \text{X}(\text{HO})$	
	7	5.7-9	$\text{H} \rightarrow \text{X}(\text{HO}) \rightarrow \text{H} \rightarrow \text{X}(\text{HO})$	
	6	7.8-9.9	$\text{H} \rightarrow \text{X}(\text{HO}) \rightarrow \text{H} \rightarrow \text{X}(\text{N}_2)$	
	6	5.8-7.4	$\text{N}_2 \rightarrow \text{X}(\text{H}_2) \rightarrow \text{N}_2 \rightarrow \text{X}(\text{H})$	

Table S2. Elementary reactions of CL-20 decomposition at different impact velocities.

Impact velocities	Frequencies	Reaction time/ps	Elementary reactions	Illustration
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/km/s				
2	9	0.3-4.1	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	First occur
	2	0.5-0.7	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}$	
	1	0.5-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	0.6-0.6	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24})$	
	1	0.6-0.6	$\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	5	0.7-8.2	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}$	
	13	2.7-9.5	$\text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10} \rightarrow \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	Highest frequency
	12	3.4-9.1	$\text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}$	
	9	0.3-4.1	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	6	0.8-4.2	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	5	0.7-8.2	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{11}\text{O}_{10}$	
	3	5.1-6.4	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{24}\text{H}_{24}\text{N}_{47}\text{O}_{45})$	
	3	5.0-6.3	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{24}\text{H}_{24}\text{N}_{47}\text{O}_{45}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	3	2.2-2.9	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{42}\text{H}_{42}\text{N}_{83}\text{O}_{82})$	
3	6	0.3-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	First occur
	4	0.4-0.7	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	1	0.4-0.4	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}$	
	1	0.5-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	0.5-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	1	0.5-0.5	$\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24} \rightarrow \text{NO}_2 + \text{C}_{12}\text{H}_{12}\text{N}_{23}\text{O}_{22}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	
	6	0.3-0.5	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12})$	Highest frequency
	4	7.5-9.7	$\text{O}_2 + \text{N}_2 \rightarrow \text{N}_2\text{O}_2$	
	4	0.4-0.7	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$	
	3	7.6-8.1	$\text{N}_2\text{O}_2 \rightarrow \text{O}_2 + \text{N}_2$	
	2	8.0-9.3	$\text{NO-X}(\text{HO}_2) \rightarrow \text{NO-X}(\text{O}_2)$	
	2	6.9-9.9	$\text{N}_2 \rightarrow \text{N}_2\text{-X}(\text{HO})$	
	2	6.3-8.2	$\text{NO} \rightarrow \text{NO-X}(\text{H})$	
	2	6.3-7.2	$\text{NO}_4\text{-X}(\text{HN}_2\text{O}_3) \rightarrow \text{NO}_4\text{-X}(\text{NO})$	
	2	6.3-6.7	$\text{NO}_2\text{-X}(\text{NO}_3) \rightarrow \text{NO}_2$	
	2	5.9-8.7	$\text{NO-X}(\text{O}) \rightarrow \text{NO-X}(\text{HNO}_4)$	
	2	5.0-9.7	$\text{NO}_2 \rightarrow \text{NO}_2\text{-X}(\text{H})$	
	2	4.2-4.6	$\text{NO}_2 + \text{NO}_3\text{-X}(\text{H}) \rightarrow \text{N}_2\text{O}_5\text{-X}(\text{H})$	
	2	3.7-5.0	$\text{O-X}(\text{N}_2\text{O}_4) \rightarrow \text{O-X}(\text{NO}_2)$	
	2	2.5-2.8	$\text{NO}_2 \rightarrow \text{NO}_2\text{-X}(\text{N}_2\text{O}_5)$	
	2	1.8-3.4	$\text{NO}_2 \rightarrow \text{NO}_2\text{-X}(\text{NO}_3)$	
4	1	0.2-0.2	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{18}\text{H}_{18}\text{N}_{32}\text{O}_{28})$	First occur
	1	0.2-0.2	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}\text{-X}(\text{C}_{198}\text{H}_{198}\text{N}_{380}\text{O}_{353})$	
	1	0.3-0.3	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} \rightarrow \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{O})$	
	1	0.3-0.3	$\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{24}\text{-X}(\text{C}_{198}\text{H}_{198}\text{N}_{380}\text{O}_{353}) + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{C}_{18}\text{H}_{18}\text{N}_{32}\text{O}_{28}) \rightarrow \text{NO}_2 + \text{NO}_2 + \text{C}_{12}\text{H}_{12}\text{N}_{23}\text{O}_{23}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) + \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{23}\text{-X}(\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{22}) + \text{C}_{30}\text{H}_{30}\text{N}_{59}\text{O}_{58}\text{-X}(\text{C}_{242}\text{H}_{240}\text{N}_{453}\text{O}_{441})$	
	1	0.4-0.4	$\text{C}_{12}\text{H}_{12}\text{N}_{23}\text{O}_{23}\text{-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}) + \text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{23}\text{-X}(\text{C}_{12}\text{H}_{12}\text{N}_{24}\text{O}_{22}) + \text{C}_{30}\text{H}_{30}\text{N}_{59}\text{O}_{58}\text{-X}(\text{C}_{242}\text{H}_{240}\text{N}_{453}\text{O}_{441}) + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12} + \text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}\text{-X}(\text{O}) \rightarrow \text{O-X}(\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{11}) + \text{NO}_2 + \text{NO}_2 + \text{NO}_2 + \text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{10}\text{O}_8 + \text{C}_{66}\text{H}_{66}\text{N}_{128}\text{O}_{123}\text{-X}(\text{C}_{347}\text{H}_{342}\text{N}_{645}\text{O}_{611})$	Highest frequency
	1	0.5-0.5	$\text{NO}_2 + \text{C}_6\text{H}_6\text{N}_{10}\text{O}_8 \rightarrow \text{NO}_3\text{-X}(\text{H}) + \text{C}_6\text{H}_6\text{N}_{10}\text{O}_7$	
	40	4.2-9.9	$\text{N}_2 \rightarrow \text{N}_2\text{-X}(\text{H})$	
	26	4.1-9.8	$\text{N}_2\text{-X}(\text{H}) \rightarrow \text{N}_2$	

22	3.0-9.4	$\text{N}_2\text{-X(HO)} \rightarrow \text{N}_2$
16	2.8-9.9	$\text{N}_2 \rightarrow \text{N}_2\text{-X(HO)}$
15	3.4-9.0	$\text{O-X(H)} \rightarrow \text{O-X(H}_2\text{)}$
10	3.8-9.5	$\text{O-X(H}_2\text{)} \rightarrow \text{O-X(H)}$
9	3.9-9.9	$\text{O-X(H}_2\text{)} \rightarrow \text{O-X(H}_2\text{)}$
8	3.9-8.6	$\text{N}_2\text{-X(H)} \rightarrow \text{N}_2\text{-X(H}_2\text{)}$
8	3.5-9.1	$\text{H-X(HO)} \rightarrow \text{H-X(HO)}$
8	1.7-9.5	$\text{N}_2 \rightarrow \text{N}_2\text{-X(N}_2\text{)}$
7	5.7-9.7	$\text{N}_2\text{-X(H}_2\text{)} \rightarrow \text{N}_2$
7	4.7-9.9	$\text{N-X(HN)} \rightarrow \text{N-X(N)}$

Table S3. Elementary reactions of TNT decomposition at different impact velocities.

Impact velocities /km/s	Frequencies	Reaction time/ps	Elementary reactions	Illustration
2	4	2.2-6.6	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	First occur
	3	4.4-6.3	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}$	
	2	4.5-4.8	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)} \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6$	
	1	5.3-5.3	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_{21}\text{H}_{15}\text{N}_9\text{O}_{18}\text{)}$	
	4	2.2-6.6	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	Highest frequency
	3	4.4-6.3	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}$	
	2	4.5-4.8	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)} \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6$	
3	8	0.4-1.2	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	First occur
	3	0.5-0.9	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)} \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6$	
	1	0.5-0.5	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}$	
	1	0.6-0.6	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{)}$	
	1	0.6-0.6	$\text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{21}\text{H}_{15}\text{N}_9\text{O}_{18}$	
	1	0.7-0.7	$\text{C}_{21}\text{H}_{15}\text{N}_9\text{O}_{18} \rightarrow \text{C}_{21}\text{H}_{15}\text{N}_9\text{O}_{18}\text{-X(C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{)}$	
	1	0.9-0.9	$\text{C}_{21}\text{H}_{15}\text{N}_9\text{O}_{18}\text{-X(O)} + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{28}\text{H}_{20}\text{N}_{12}\text{O}_{24}\text{X(O)}$	
	8	0.4-1.2	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	Highest frequency
4	3	0.5-0.9	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)} \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6$	Highest frequency
	1	0.3-0.3	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}$	First occur
	3	0.3-0.4	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	
	1	0.4-0.4	$\text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12} \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{-X(C}_{347}\text{H}_{238}\text{N}_{144}\text{O}_{293}\text{)}$	
	1	0.4-0.4	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)} \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{-X(C}_7\text{H}_5\text{N}_3\text{O}_6\text{)}$	
	1	0.4-0.4	$\text{C}_7\text{H}_5\text{N}_3\text{O}_6 + \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{-X(C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{)}$	
	1	0.5-0.5	$\text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{-X(C}_{347}\text{H}_{238}\text{N}_{144}\text{O}_{293}\text{)} \rightarrow \text{C}_{14}\text{H}_{10}\text{N}_6\text{O}_{12}\text{-X(C}_{385}\text{H}_{266}\text{N}_{158}\text{O}_{313}\text{)}$	
	5	6.7-9.2	$\text{N-X(N)} \rightarrow \text{N-X(HN)}$	Highest frequency
	5	3.4-7.9	$\text{O-X(H}_2\text{)} \rightarrow \text{O-X(H)}$	
	3	8.3-9.7	$\text{O-X(H}_2\text{)} \rightarrow \text{O-X(H}_2\text{)}$	
	3	8.0-9.7	$\text{N-X(H}_3\text{)} \rightarrow \text{N-X(H}_2\text{)}$	
	3	5.9-8.8	$\text{N}_2 \rightarrow \text{N}_2\text{-X(H)}$	
	3	5.8-9.5	$\text{N-X(HN)} \rightarrow \text{N-X(H}_2\text{N)}$	
	3	5.8-8.1	$\text{N-X(H}_4\text{)} \rightarrow \text{N-X(H}_3\text{)}$	