Mechanism of the reduced shock sensitivity of CL-20/MTNP co-crystals from reactive molecular dynamics simulations

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Supplementary Materials:

The earliest and most frequent elementary reactions occurring in CL-20/MTNP, CL-20, and MTNP crystals at an impact velocity of 3 km/s (Table S1) and 4 km/s (Table S2).

Table S1 Earliest and most frequent elementary reactions in CL-20/MTNP, CL-20, and MTNP crystals at an impact velocity of 3 km/s

Crystals	Frequencies	Reaction time(ps)	Elementary reactions	Illustration
CL-20/MTNP	3	0.2-0.2	$C_4H_3N_5O_6 \rightarrow \mathbf{C_4H_3N_5O_6\text{-}M(C_6H_6N_{12}O_{12})}$	First occur
	6	0.3-0.3	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}\text{-}M(C_{10}H_9N_{17}O_{18})$	
	2	0.3-0.3	$C_4H_3N_5O_6\text{-}M(C_6H_6N_{12}O_{12})+C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_{10}H_9N_{17}O_{18}\text{-}M(C_6H_6N_{12}O_{12})}$	
	1	0.3-0.3	$C_4H_3N_5O_6+C_6H_6N_{12}O_{12}\text{-}M(C_{10}H_9N_{17}O_{18}) \rightarrow C_{10}H_9N_{17}O_{18}\text{-}M(C_{34}H_{30}N_{56}O_{60})$	
	1	0.3-0.3	$C_4H_3N_5O_6+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}\text{-}M(C_{10}H_9N_{17}O_{18}) \rightarrow \mathbf{C_{16}H_{15}N_{29}O_{30}\text{-}M(C_{20}H_{18}N_{33}O_{33})}$	
	1	0.4-0.4	$C_{10}H_9N_{17}O_{18}\text{-}M(C_6H_6N_{12}O_{12}) \rightarrow C_{10}H_9N_{17}O_{18}\text{-}M(C_{14}H_{12}N_{22}O_{24})$	
	3	0.4-0.4	$C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_6H_6N_{12}O_{12}\text{-}M(C_4H_3N_5O_6)}$	
	1	0.4-0.4	$C_{16}H_{15}N_{29}O_{30}\text{-}M(C_{20}H_{18}N_{33}O_{33}) \rightarrow C_{10}H_9N_{17}O_{18}+C_6H_6N_{12}O_{12}$	
	6	0.4-1.6	$\mathbf{C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{12}O_{12}\text{-}M(C_{10}H_9N_{17}O_{18})}$	Highest frequency
	6	1.4-6.3	$\mathbf{NO_2+NO_2 \rightarrow N_2O_4}$	
	4	5.0-7.6	$\mathbf{N_2O_5 \rightarrow NO_2+NO_3}$	
	3	0.9-2.3	$C_6H_6N_{12}O_{12}\text{-}M(C_{10}H_9N_{17}O_{18}) \rightarrow C_6H_6N_{12}O_{12}$	
	3	0.8-1.4	$C_6H_6N_{12}O_{12}\text{-}M(C_4H_3N_5O_6) \rightarrow C_6H_6N_{12}O_{12}$	
	3	0.6-1.3	$C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_6H_6N_{12}O_{12}\text{-}M(C_4H_3N_5O_6)}$	
	3	0.3-1.2	$C_4H_3N_5O_6 \rightarrow \mathbf{C_4H_3N_5O_6\text{-}M(C_6H_6N_{12}O_{12})}$	
	3	1.9-5.0	$\mathbf{N_2O_4 \rightarrow NO_2+NO_2}$	
CL-20	1	0.2-0.2	$C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_6H_6N_{12}O_{12}\text{-}M(C_6H_6N_{12}O_{12})}$	First occur
	1	0.3-0.3	$C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_{12}H_{12}N_{24}O_{24}}\text{-}M(C_{48}H_{49}N_{96}O_{91})$	
	1	0.3-0.3	$C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12} \rightarrow \mathbf{C_{18}H_{18}N_{36}O_{36}}\text{-}M(C_{30}H_{29}N_{59}O_{62})$	

	1	0.3-0.3	$C_6H_6N_{12}O_{12}$+$C_6H_6N_{12}O_{12}$+$C_6H_6N_{12}O_{12}$+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)→$C_{24}H_{24}N_{48}O_{48}$-M($C_{24}H_{23}N_{43}O_{43}$)	
	1	0.4-0.4	$C_{24}H_{24}N_{48}O_{48}$-M($C_{24}H_{23}N_{43}O_{43}$)→$C_{18}H_{18}N_{36}O_{36}$-M($C_{36}H_{35}N_{66}O_{64}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)	
	1	0.4-0.4	$C_{18}H_{18}N_{36}O_{36}$-M($C_{30}H_{29}N_{59}O_{62}$)→$C_{12}H_{12}N_{24}O_{24}$-M($C_{42}H_{40}N_{81}O_{79}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)	
	1	0.4-0.4	$C_{18}H_{18}N_{36}O_{36}$-M($C_{30}H_{29}N_{56}O_{56}$)→**$C_{12}H_{12}N_{24}O_{24}$-M($C_{54}H_{53}N_{101}O_{98}$)**+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)	
	1	0.4-0.4	$C_{12}H_{12}N_{24}O_{24}$-M($C_{48}H_{49}N_{96}O_{91}$)→$C_6H_6N_{12}O_{12}$-M($C_{12}H_{12}N_{24}O_{24}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)	
	4	5.8-8.1	**NO_2-M(NO_3)+N_2**→N_3O_2-M(NO_3)	
	3	5.9-8.2	N_3O_2-M(NO_3)→NO_2-M(NO_3)+N_2	
	2	8.1-9.2	HO→HO-M(NO_2)	
	2	7.5-8.1	**N-M(HN_2O)**→N-M(N_2)	
	2	7.4-7.6	N-M(N_2)→N-M(HN_2O)	
	2	7.3-7.6	**NO_2-M(O)**+N_2→N_3O_2-M(O)	Highest frequency
	2	6.2-8.6	HO→HO-M(N_2)	
	2	5.8-6.1	**O-M(O)+NO**→NO_2-M(O)	
	2	5.7-5.9	NO_2-M(O)→O-M(O)+NO	
	2	1.6-2.2	**NO_2-M(NO_2)**→NO_2-M(N_2O_4)	
	2	1.6-1.9	NO_2→NO_2-M(NO_2)	
	2	1.5-2.1	**NO_2-M(N_2O_4)**→NO_2-M(NO_2)	
MTNP	6	0.3-0.5	$C_4H_3N_5O_6$→**$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)**	First occur
	2	0.4-0.6	$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)→$C_4H_3N_5O_6$	
	1	0.4	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)→**$C_8H_6N_{10}O_{12}$-M($C_8H_6N_{10}O_{12}$)**	
	1	0.4	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)→$C_8H_6N_{10}O_{12}$-M($C_4H_3N_5O_6$)	
	1	0.4	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$→$C_8H_6N_{10}O_{12}$-M(**$C_{55}H_{37}N_{62}O_{74}$**)	
	1	0.4	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$→$C_8H_6N_{10}O_{12}$	
	6	0.3-0.5	$C_4H_3N_5O_6$→**$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)**	Highest frequency
	3	4.4-5.5	NO_2→NO_2-M($C_4H_3N_5O_6$)	
	2	0.9-1.1	$C_7H_3N_{10}O_{12}$→$C_3N_5O_7$+$C_4H_3N_5O_5$	
	2	7.1-9.0	**NO_2→NO_2-M(NO_2)**	
	2	0.4-0.6	$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)→$C_4H_3N_5O_6$	

Table S2 Earliest and most frequent elementary reactions in CL-20/MTNP, CL-20, and MTNP crystals at an impact velocity of 4 km/s

Crystals	Frequencies	Reaction time(ps)	Elementary reactions	Illustration
CL-20/MTNP	1	0.2-0.2	$C_4H_3N_5O_6+C_4H_3N_5O_6+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}$→**$C_{32}H_{30}N_{58}O_{60}$-M($C_{142}H_{130}N_{242}O_{251}$)**	First occur
	1	0.3-0.3	$C_{32}H_{30}N_{58}O_{60}$-M($C_{142}H_{130}N_{242}O_{251}$)+$C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}$→$C_{12}H_{12}N_{24}O_{24}$-M($C_{10}H_9N_{17}O_{18}$)+$C_{12}H_{12}N_{24}O_{24}$-M($C_{14}H_{12}N_{22}O_{23}$)+$C_{16}H_{15}N_{29}O_{30}$-M($C_{117}H_{107}N_{193}O_{191}$)+$C_{16}H_{15}N_{29}O_{30}$-M($C_6H_6N_{12}O_{11}$)	
	1	0.4-0.4	$C_{16}H_{15}N_{29}O_{30}$-M($C_6H_6N_{12}O_{11}$)→NO_2+$C_{10}H_9N_{16}O_{17}$-M($C_{10}H_9N_{17}O_{20}$)+$C_6H_6N_{12}O_{11}$	
	1	0.4-0.4	$C_{16}H_{15}N_{29}O_{30}$-M($C_{117}H_{107}N_{193}O_{191}$)→O-M($C_4H_3N_5O_6$)+$CH_3N_2O$+$C_{15}H_{12}N_{27}O_{28}$-M($C_{137}H_{121}N_{224}O_{218}$)	
	1	0.4-0.4	$C_{12}H_{12}N_{24}O_{24}$-M($C_{10}H_9N_{17}O_{18}$)+$C_{12}H_{12}N_{24}O_{24}$-M($C_{14}H_{12}N_{22}O_{23}$)+$C_4H_3N_5O_6$→**O**-M($C_{20}H_{18}N_{34}O_{35}$)+**$2O_2$**+**NO_2**+$C_{16}H_{15}N_{28}O_{25}$-M($C_4H_3N_5O_6$)+**$C_6H_6N_{12}O_{11}$**+$C_6H_6N_{12}O_{11}$-M($C_4H_3N_5O_6$)	
	13	4.3-9.8	**N_2-M(H)**→N_2	Highest frequency
	13	4.2-9.2	N_2→N_2-M(H)	
	11	5.1-9.8	N_2→N_2-M(HO)	
	11	5.0-9.7	**N-M(N)**→N-M(HN)	
	10	3.1-9.9	N_2-M(HO)→N_2	
	8	5.1-9.4	**O-M(H_2)**→O-M(H_2)	
	8	4.0-9.8	O-M(H_2)→O-M(H)	
CL-20	1	0.2-0.2	$C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}$→**$C_{12}H_{12}N_{24}O_{24}$**	First occur
	7	0.2-0.3	$C_6H_6N_{12}O_{12}$→$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)	
	1	0.3-0.3	$C_6H_6N_{12}O_{12}$→**$C_6H_6N_{12}O_{12}$-M($C_{12}H_{12}N_{24}O_{24}$)**	
	1	0.3-0.3	$C_{12}H_{12}N_{24}O_{24}$+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)→O-M(O)+**NO_2**+**$C_{30}H_{30}N_{59}O_{57}$($C_6H_6N_{12}O_{12}$+$C_6H_6N_{12}O_{12}$+$C_{18}H_{18}N_{35}O_{33}$)**-M($C_{176}H_{174}N_{330}O_{308}$)	
	1	0.4-0.4	$C_6H_6N_{12}O_{12}$→**NO_2**+$C_6H_6N_{11}O_{10}$	
	1	0.4-0.4	$C_{30}H_{30}N_{59}O_{57}$(**$C_6H_6N_{12}O_{12}$+$C_6H_6N_{12}O_{12}$+$C_{18}H_{18}N_{35}O_{33}$**)-M($C_{176}H_{174}N_{330}O_{308}$)+$C_6H_6N_{12}O_{12}+C_6H_6N_{12}O_{12}$-M($C_{12}H_{12}N_{24}O_{24}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)+$C_6H_6N_{12}O_{12}$-M($C_6H_6N_{12}O_{12}$)→**$4NO_2$**+$C_{18}H_{18}N_{33}O_{30}$-M($C_{12}H_{12}N_{25}O_{25}$)+$C_{48}H_{48}N_{94}O_{91}$-M($C_{252}H_{242}N_{478}O_{449}$)	
	1	0.4-0.4	O-M(O)→O-M($C_6H_8N_{11}O_9$)	
	19	2.1-9.9	N_2→**N_2-M(H)**	Highest frequency
	18	2.2-9.1	N_2-M(H)→N_2	
	14	3-9.9	N-M(N)→N-M(HN)	
	13	2.8-9.7	**N_2-M(HO)**→N_2	
	11	2.7-9.6	N_2→N_2-M(HO)	

	11	2.7-9.5	**N-M(HN)**→N-M(N)	
	10	2.7-9.4	O-M(H_2)→O-M(H)	
MTNP	3	0.2-0.3	$C_4H_3N_5O_6$→**$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)**	First occur
	1	0.2-0.2	$C_4H_3N_5O_6$→$C_4H_3N_5O_6$-M($C_7H_4N_9O_{10}$)	
	1	0.2-0.2	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$→$C_8H_6N_{10}O_{12}$-M($C_7H_5N_8O_9$)	
	1	0.2-0.2	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$→$C_8H_6N_{10}O_{12}$-M($C_{65}H_{43}N_{75}O_{97}$)	
	1	0.3-0.3	$C_4H_3N_5O_6$-M($C_7H_4N_9O_{10}$)→$C_4H_3N_5O_6$	
	1	0.3-0.3	$C_4H_3N_5O_6$+$C_4H_3N_5O_6$+$C_4H_3N_5O_6$+$C_4H_3N_5O_6$+$C_4H_3N_5O_6$+$C_4H_3N_5O_6$+$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)+$C_4H_3N_5O_6$-M($C_4H_3N_5O_6$)+$C_8H_6N_{10}O_{12}$-M($C_{65}H_{43}N_{75}O_{97}$)+$C_8H_6N_{10}O_{12}$-M($C_7H_5N_8O_9$)→$C_{16}H_{12}N_{20}O_{24}$-M($C_{23}H_{16}N_{27}O_{30}$)+$C_{36}H_{27}N_{45}O_{54}$-M($C_{104}H_{78}N_{125}O_{155}$)	
	1	0.4-0.4	$C_6H_6N_{12}O_{12}$→$C_6H_6N_{12}O_{12}$-M($C_4H_3N_5O_6$)	
	13	3.7-9.7	**N-M(HN)**→N-M(N)	Highest frequency
	11	3.6-9.7	N-M(N)→N-M(HN)	
	10	2.1-9.1	**N_2-M(H)**→N_2	
	8	2.3-8.6	**O-M(H_2)**→O-M(H)	
	8	2.4-9.7	N_2→N_2-M(H)	
	6	3.6-9.9	N_2-M(HO)→N_2	
	6	4.0-8.8	O-M(H)→O-M(H_2)	