Multi-aspect Simulation insight on Thermolysis Mechanism and Interaction of NTO/HMX Based Plastic Bonded Explosives: New conception of mixed explosive model

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Supporting information

Table S1 Lattice parameters of NTO and HMX

	NTO	HMX
Empirical formula	$C_2H_2O_3N_4$	$C_4H_8O_8N_8$
a(Å)	9.326	6.540
b(Å)	5.450	11.050
c(Å)	9.040	8.700
α(°)	90.00	90.00
β(°)	101.474	124.30
γ(°)	90.00	90.00
V(Å^3)	450.291	519.387
Density (g·cm^{-3})	1.919	1.894

Table S2 Topological parameters of NTO/HMX mixture

Interaction	$H(r)$	$\rho(r)$	$\nabla^2\rho(r)$
H291…O130	0.000953	0.00625	0.0238
H289…O130	0.000680	0.00227	0.0100
H116…O271	-0.000589	0.0554	0.2000
H289…O102	0.00102	0.00683	0.0257
H264…O96	0.00112	0.0208	0.0745
H248…O96	0.000766	0.00284	0.0112
H94…O255	0.00155	0.0498	0.203
H83…O242	-0.000186	0.0512	0.183
H236…O58	0.000919	0.00309	0.0134
H50…O185	-0.00309	0.0634	0.216
H180…O36	0.000970	0.0180	0.0641
H135…O8	0.00112	0.0234	0.0850
H6…O143	-0.00209	0.0604	0.214

Note: All topological parameters are in a.u.

Table S3 Primary reactions of NTO/HMX system

Temperature/K	Reaction time/ps	Frequencies	Reactions
2500	0.10-1.29	41	$C_4H_8O_8N_8 \rightarrow C_4H_8O_6N_7+NO_2$
	0.05-3.15	23	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_2H_3O_3N_4+C_2HO_3N_4$
	0.23-2.61	15	$C_4H_8O_4N_6 \rightarrow C_4H_8O_2N_5+NO_2$
	0.27-9.97	12	$HNO_2 \rightarrow OH+NO$
	0.70-8.75	8	$C_2H_2O_3N_4+NO_2 \rightarrow C_2HO_3N_4+HNO_2$
	0.25-1.85	6	$C_4H_9O_6N_7 \rightarrow C_4H_8O_4N_6+HNO_2$
	0.66-9.72	6	$C_2H_2O_3N_4+OH \rightarrow C_2HO_3N_4+H_2O$
	1.41-4.97	5	$C_2HO_3N_4+OH \rightarrow C_2O_3N_4+H_2O$
	0.23-0.55	3	$C_2H_2O_3N_4+C_4H_8O_6N_7 \rightarrow C_2HO_3N_4+C_4H_9O_6N_7$
	0.40-1.70	2	$C_4H_9O_8N_8 \rightarrow C_4H_8O_6N_7+HNO_2$
2750	0.09-0.82	33	$C_4H_8O_8N_8 \rightarrow C_4H_8O_6N_7+NO_2$
	0.60-9.99	29	$HNO_2 \rightarrow OH+NO$
	0.14-1.11	23	$C_4H_8O_6N_7 \rightarrow C_4H_8O_4N_6+NO_2$
	0.05-1.12	21	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_2H_3O_3N_4+C_2HO_3N_4$
	0.18-1.69	15	$C_4H_8O_4N_6 \rightarrow C_4H_8O_2N_5+NO_2$
	0.47-4.89	6	$C_2H_2O_3N_4+NO_2 \rightarrow C_2HO_3N_4+HNO_2$
	0.31-1.66	5	$C_2H_2O_3N_4+OH \rightarrow C_2HO_3N_4+H_2O$
	0.12-0.22	4	$C_2H_2O_3N_4+C_4H_8O_8N_8 \rightarrow C_2HO_3N_4+C_4H_9O_8N_8$
	2.27-3.88	4	$C_2HON_3+NO_2 \rightarrow C_2ON_3+HNO_2$
	0.37-0.66	2	$C_4H_9O_6N_7 \rightarrow C_4H_8O_4N_6+HNO_2$
3000	0.25-9.98	79	$HNO_2 \rightarrow OH+NO$
	0.09-0.35	34	$C_4H_8O_8N_8 \rightarrow C_4H_8O_6N_7+NO_2$
	0.05-0.84	17	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_2H_3O_3N_4+C_2HO_3N_4$
	0.40-9.63	16	$H+NO_2 \rightarrow HNO_2$
	0.56-9.60	13	$HN_2+NO_2 \rightarrow HNO_2+N_2$
	0.07-3.23	11	$C_2H_2O_3N_4 \rightarrow C_2HO_3N_4+H$
	0.29-0.70	8	$C_2H_2O_3N_4+NO_2 \rightarrow C_2HO_3N_4+HNO_2$
	0.04-1.56	5	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_4H_4O_6N_8$
	0.32-8.37	3	$C_2H_2O_3N_4+OH \rightarrow C_2HO_3N_4+H_2O$
	0.12-0.18	2	$C_2H_2O_3N_4+C_4H_8O_8N_8 \rightarrow C_2HO_3N_4+C_4H_9O_8N_8$
3250	0.25-10.00	70	$HNO_2 \rightarrow OH+NO$
	0.09-0.48	33	$C_4H_8O_8N_8 \rightarrow C_4H_8O_6N_7+NO_2$
	0.12-0.81	24	$C_4H_8O_6N_7 \rightarrow C_4H_8O_4N_6+NO_2$
	0.05-1.05	19	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_2H_3O_3N_4+C_2HO_3N_4$
	0.43-9.57	19	$H+NO_2 \rightarrow HNO_2$
	0.07-3.15	11	$C_2H_2O_3N_4 \rightarrow C_2HO_3N_4+H$
	0.04-0.76	9	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_4H_4O_6N_8$
	0.21-0.94	7	$C_2H_2O_3N_4+OH \rightarrow C_2HO_3N_4+H_2O$
	0.12-0.13	2	$C_2H_2O_3N_4+C_4H_8O_8N_8 \rightarrow C_2HO_3N_4+C_4H_9O_8N_8$
	0.19-1.25	2	$C_2H_2O_3N_4+NO_2 \rightarrow C_2HO_3N_4+HNO_2$

Table S3 (Continued)

Temperature/K	Reaction time/ps	Frequencies	Reactions

3500	0.20-9.99	64	$HNO_2 \rightarrow OH+NO$
	0.09-0.21	37	$C_4H_8O_8N_8 \rightarrow C_4H_8O_6N_7+NO_2$
	0.12-0.48	22	$C_4H_8O_6N_7 \rightarrow C_4H_8O_4N_6+NO_2$
	0.05-0.55	18	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_2H_3O_3N_4+C_2HO_3N_4$
	0.04-0.51	13	$C_2H_2O_3N_4+C_2H_2O_3N_4 \rightarrow C_4H_4O_6N_8$
	2.12-7.13	8	$CHON+NO_2 \rightarrow CON+HNO_2$
	0.36-3.08	7	$C_2H_2O_3N_4+OH \rightarrow C_2HO_3N_4+H_2O$
	0.18-1.40	6	$C_2H_2O_3N_4+NO_2 \rightarrow C_2HO_3N_4+HNO_2$
	0.18-0.31	3	$C_2H_2O_3N_4+C_4H_8O_4N_6 \rightarrow C_2HO_3N_4+C_4H_9O_4N_6$
	0.28-1.61	3	$C_2HO_3N_4+OH \rightarrow C_2O_3N_4+H_2O$

Table S4 Reaction between product molecules

Temperature	Reaction time/ps	Frequencies	Reactions
2500	0.40-106.90	35	$HNO_2 \rightarrow OH+NO$
	1.70-296.65	31	$CON_2 \rightarrow CO+N_2$
	3.30-165.55	23	$OH+HNO \rightarrow H_2O+NO$
	11.90-298.15	16	$H_2N+H_2O \rightarrow H_3N+OH$
	1.80-296.30	13	$CHON+OH \rightarrow CON+H_2O$
	1.95-124.85	11	$HN_2+NO_2 \rightarrow HNO_2+N_2$
	7.50-297.80	10	$CH_2O_2N \rightarrow CO_2+H_2N$
	7.95-271.45	7	$CHON+HN_2 \rightarrow CON+H_2+N_2$
	22.75-296.55	5	$CON+CON_3 \rightarrow C_2O_2N_2+N_2$
	9.25-290.15	5	$CON+H_2 \rightarrow CHON+H$
2750	0.60-125.25	51	$HNO_2 \rightarrow OH+NO$
	1.00-294.20	32	$CON_2 \rightarrow CO+N_2$
	1.80-274.65	27	$CN_3 \rightarrow CN+N_2$
	20.75-299.30	18	$H_2N_2 \rightarrow H_2+N_2$
	1.05-299.85	15	$HON_2 \rightarrow OH+N_2$
	3.20-75.25	13	$CHON+NO \rightarrow CON+HNO$
	3.70-283.95	12	$CON+HN_2 \rightarrow CHON+N_2$
	0.90-278.50	11	$CHON+OH \rightarrow CON+H_2O$
	2.65-54.85	11	$OH+HNO \rightarrow H_2O+NO$
	2.75-28.75	8	$CHON+NO_2 \rightarrow CON+HNO_2$
3000	0.25-75.10	56	$HNO_2 \rightarrow OH+NO$
	1.00-300.00	38	$HON_2 \rightarrow OH+N_2$
	7.25-299.70	25	$C_2O_4 \rightarrow CO_2+CO_2$
	4.15-299.00	24	$CHO_2N_2 \rightarrow CO_2+HN_2$
	1.05-24.90	12	$CHON+NO_2 \rightarrow CON+HNO_2$
	2.00-291.85	11	$CHON+H_2N \rightarrow CON+H_3N$
	0.60-60.95	10	$HN_2+NO_2 \rightarrow HNO_2+N_2$

Table S4 (Continued)

Temperatur	Reaction time/ps	Frequencies	Reactions

e			
3000	1.50-299.70	10	$CHO_2+N_2 \rightarrow CO_2+HN_2$
	2.20-39.35	8	$H_2O_2N \rightarrow H_2O+NO$
	90.95-295.95	8	$HN_2+HN_2 \rightarrow H_2+{}_2N_2$
3250	2.50-299.45	41	$CON_2 \rightarrow CO+N_2$
	7.40-299.70	40	$C_2O_4 \rightarrow CO_2+CO_2$
	0.50-202.80	37	$HNO_2 \rightarrow OH+NO$
	1.30-300.00	31	$CO_2N_2 \rightarrow CO_2+N_2$
	3.60-297.25	18	$CO+OH \rightarrow CO_2+H$
	1.00-299.25	16	$CHON_3 \rightarrow CHON+N_2$
	0.65-300.00	15	$HON_2 \rightarrow OH+N_2$
	5.60-298.70	14	$H_2N_2 \rightarrow H_2+N_2$
	2.95-290.65	14	$CON+HN_2 \rightarrow CHON+N_2$
	1.75-298.90	11	$CON+H_2O \rightarrow CHON+OH$
3500	1.10-300.00	61	$CO_2N_2 \rightarrow CO_2+N_2$
	0.80-300.00	56	$HON_2 \rightarrow OH+N_2$
	6.05-299.60	51	$H_2O+HN_2 \rightarrow H_2+OH+N_2$
	0.75-299.95	35	$H+OH \rightarrow H_2O$
	0.25-215.60	31	$HNO_2 \rightarrow OH+NO$
	3.95-299.40	22	$HN_2+OH \rightarrow H_2O+N_2$
	5.35-290.85	21	$HN_2+HON_2 \rightarrow H_2O+N_2+N_2$
	1.35-296.80	10	$OH+HNO \rightarrow H_2O+NO$
	0.70-7.35	9	$HNO_2+NO \rightarrow HNO+NO_2$
	1.10-300.00	6	$CON_2 \rightarrow CO+N_2$

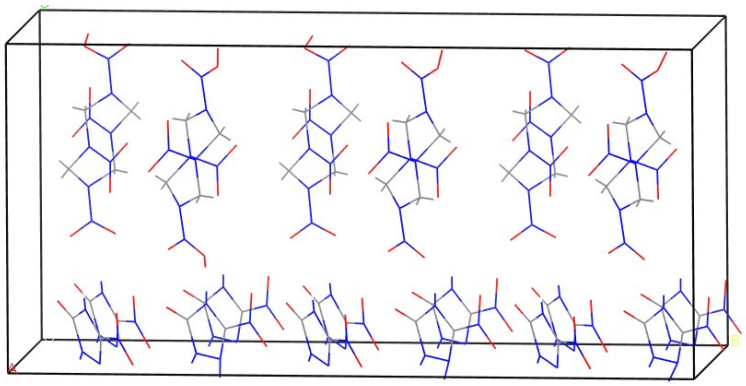

Fig. S1 The initial layer model of CP2K

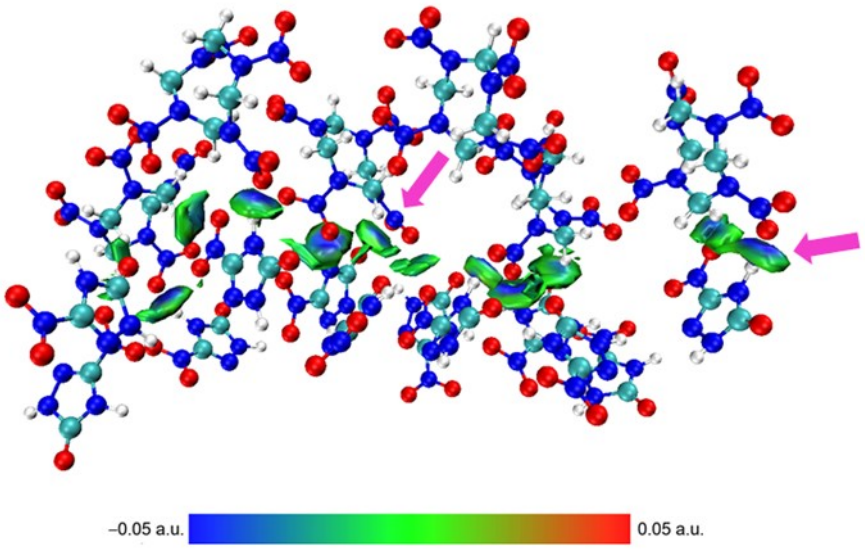

Fig. S2 IGMH analysis diagram of NTO/HMX mixture

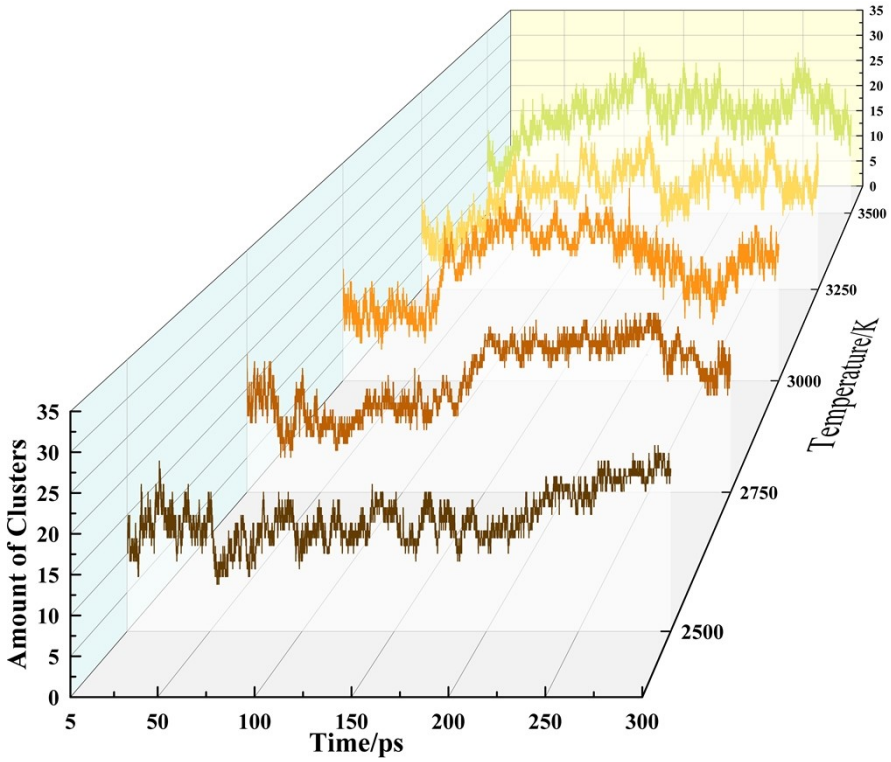

Fig. S3 Trends of the total amount of clusters at different temperatures

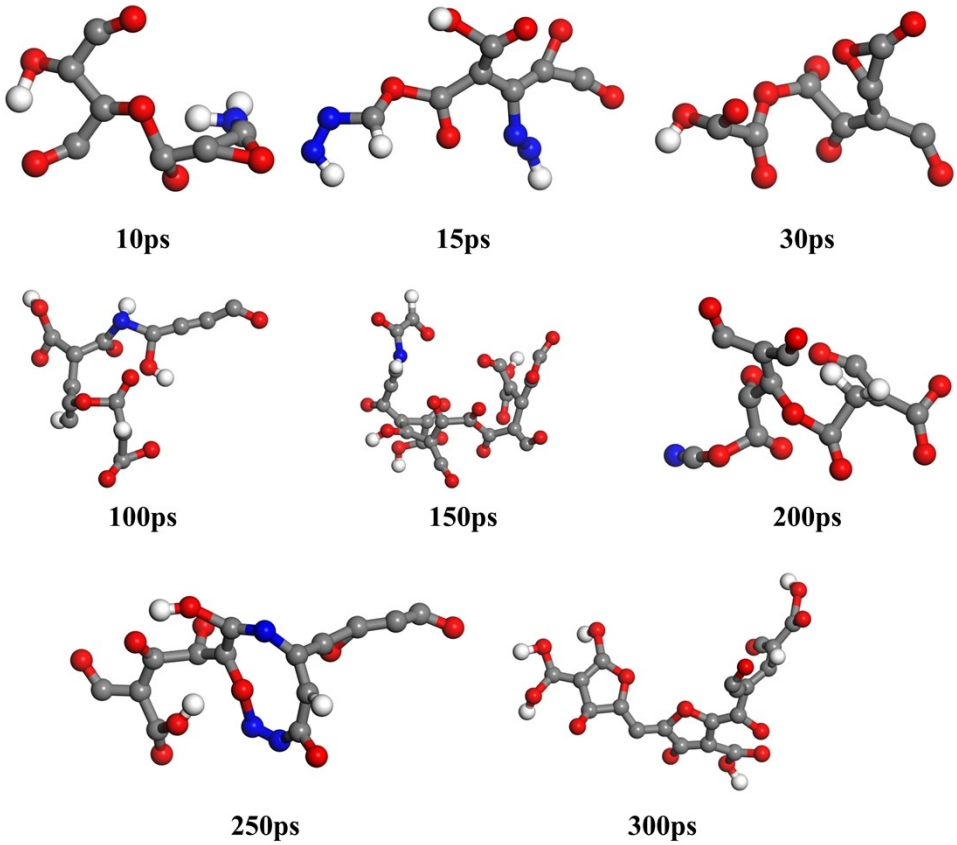

Fig. S4 Maximum cluster structure at different times at 3500 K