

Supplementary Information

**Reactive molecular dynamics study on localized high-temperature region
formation and thermal decompositions of defect-contained β -HMX crystals:
Influence of different types and concentrations of liquid inclusion defects**

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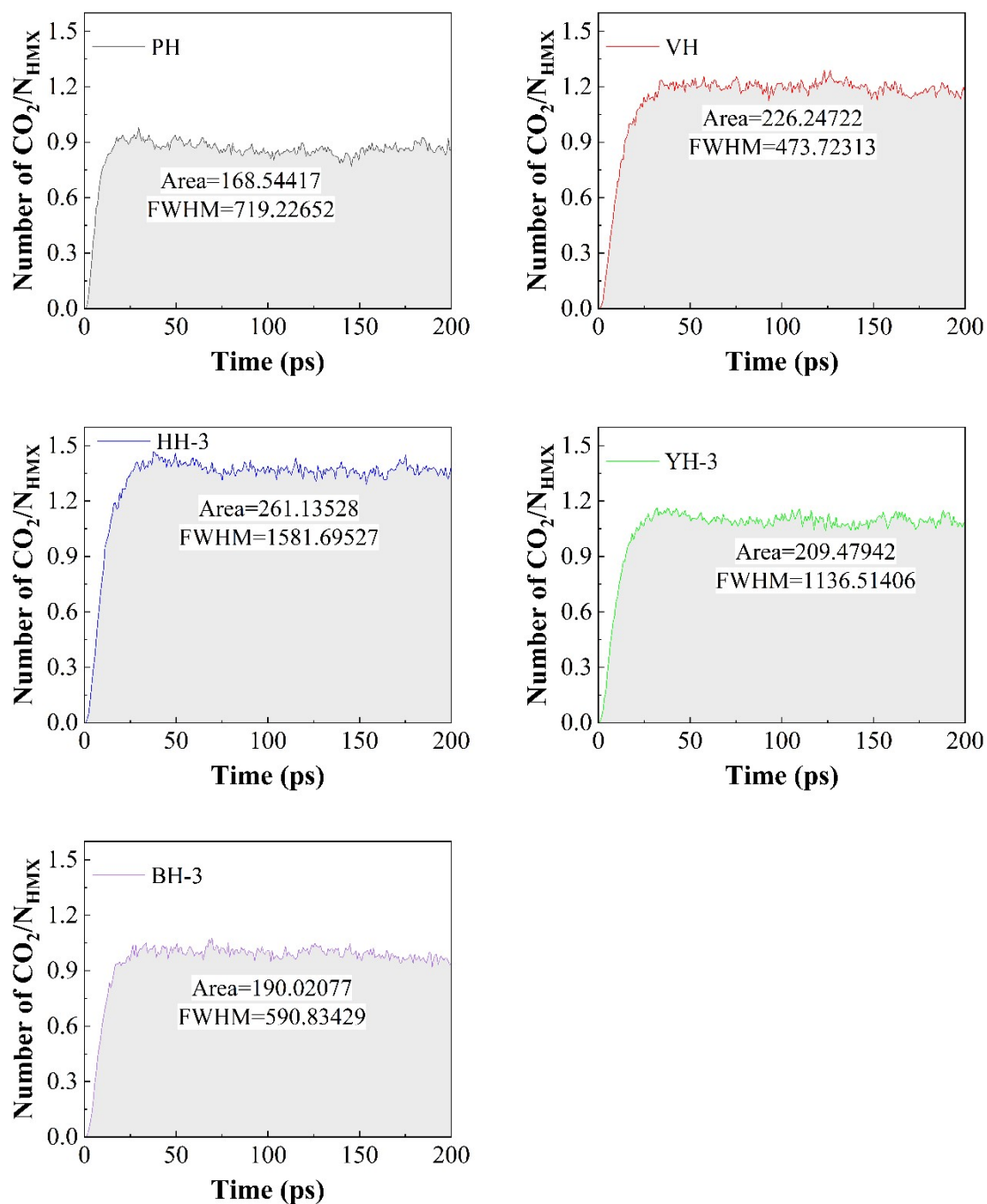


Fig.S1 The integral value of the amount of CO_2 for PH, VH, HH-3, YH-3 and BH-3.

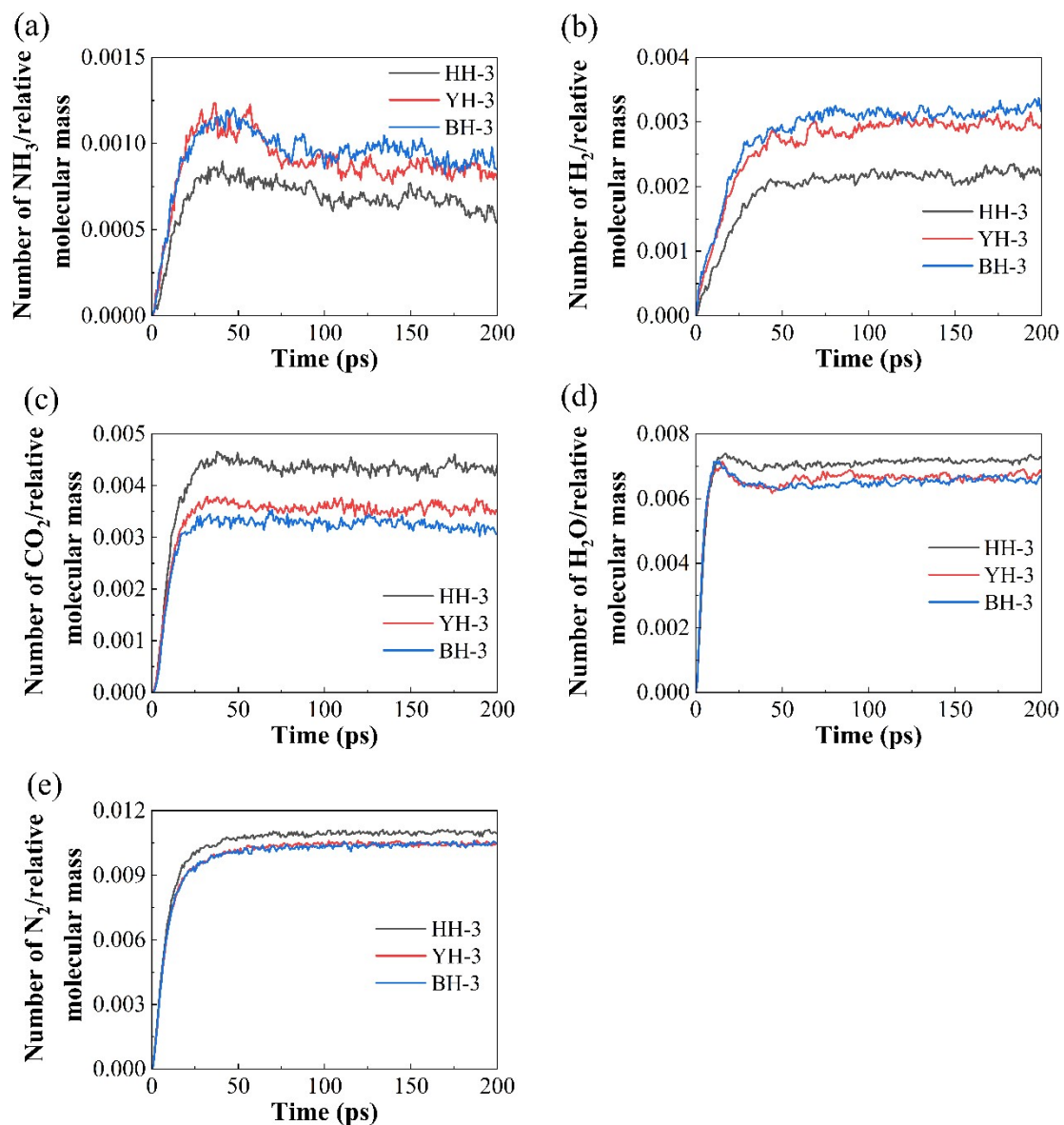


Fig. S2 The variation of the number of products after normalization of molecular mass over time.

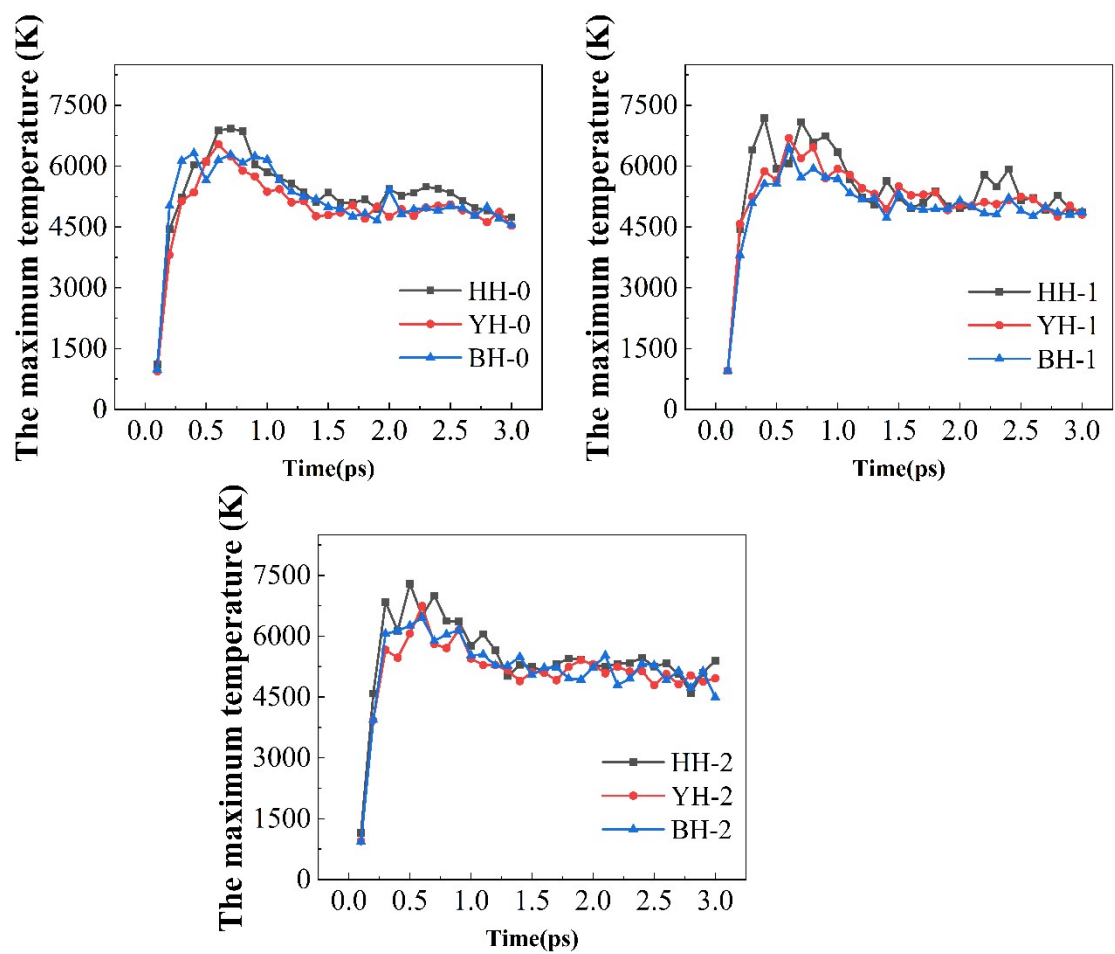


Fig. S3 Evolution of the maximum temperatures for the other systems over time.

Table S1 The lattice parameters for all the model before and after relaxation.

Model	a (Å)	b (Å)	c (Å)	ρ /(g•cm ⁻³)	V (Å ³)
PH (expt)	65.4000	66.3000	69.6000	1.8937	249305.7221
PH	64.8578	65.7504	69.0230	1.9415	243156.8567
VH (expt)	65.4000	66.3000	69.6000	1.5958	249305.7221
VH	64.9518	65.8457	69.1231	1.6291	244215.5685
HH-0 (expt)	65.4000	66.3000	69.6000	1.6126	249305.7221
HH-0	64.9337	65.8273	69.1038	1.6476	244011.5728
HH-1 (expt)	65.4000	66.3000	69.6000	1.6294	249305.7221
HH-1	64.9812	65.8755	69.1543	1.6611	244547.1498
HH-2 (expt)	65.4000	66.3000	69.6000	1.6630	249305.7221
HH-2	64.9672	65.8613	69.1394	1.6964	244389.2107
HH-3 (expt)	65.4000	66.3000	69.6000	1.6965	249305.7221
HH-3	65.0184	65.9131	69.1939	1.7266	244967.1872
YH-0 (expt)	65.4000	66.3000	69.6000	1.6058	249305.7221
YH-0	64.9694	65.8635	69.1418	1.6379	244414.3586
YH-1 (expt)	65.4000	66.3000	69.6000	1.6158	249305.7221
YH-1	64.9338	65.8274	69.1039	1.6508	244012.6351
YH-2 (expt)	65.4000	66.3000	69.6000	1.6358	249305.7221
YH-2	64.907	65.8008	69.0759	1.6733	243716.3315
YH-3 (expt)	65.4000	66.3000	69.6000	1.6558	249305.7221
YH-3	64.9181	65.8115	69.0871	1.6929	243835.5467
BH-0 (expt)	65.4000	66.3000	69.6000	1.6035	249305.7221
BH-0	64.8807	65.7736	69.0474	1.6423	243415.0185
BH-1 (expt)	65.4000	66.3000	69.6000	1.6113	249305.7221
BH-1	64.8825	65.7754	69.0493	1.6501	243434.7928
BH-2 (expt)	65.4000	66.3000	69.6000	1.6267	249305.7221
BH-2	64.8699	65.76262	69.0358	1.6669	243292.5944
BH-3 (expt)	65.4000	66.3000	69.6000	1.6422	249305.7221
BH-3	64.8851	65.7780	69.0520	1.6816	243463.7598

Table S2 The reaction frequencies of the main reactions in all systems within the first 10 ps.

Primary reactions	Freq. (PH)	Freq.(VH)		
$C_4H_8N_8O_8 \rightarrow C_4H_8N_7O_6 + NO_2$	214	195		
$C_4H_8N_7O_6 \rightarrow C_4H_8N_6O_4 + NO_2$	38	39		
$C_4H_8N_8O_8 \rightarrow C_4H_7N_8O_8 + H$	10	9		
$C_4H_7N_8O_8 \rightarrow C_4H_7N_7O_6 + NO_2$	3	3		
$2C_4H_8N_8O_8 \rightarrow C_8H_{16}N_{16}O_{16}$	2	5		
$HNO_2 \rightarrow OH + NO$	1635	1791		
$HNO+OH \rightarrow H_2O + NO$	537	507		
Primary reactions	Freq. (HH-0)	Freq. (HH-1)	Freq. (HH-2)	Freq. (HH-3)
$C_4H_8N_8O_8 \rightarrow C_4H_8N_7O_6 + NO_2$	220	208	200	210
$C_4H_8N_7O_6 \rightarrow C_4H_8N_6O_4 + NO_2$	49	41	47	42
$C_4H_8N_8O_8 \rightarrow C_4H_7N_8O_8 + H$	10	9	8	5
$C_4H_7N_8O_8 \rightarrow C_4H_7N_7O_6 + NO_2$	2	2	1	3
$2C_4H_8N_8O_8 \rightarrow C_8H_{16}N_{16}O_{16}$	9	2	4	5
$HNO_2 \rightarrow OH + NO$	1926	1939	1993	2195
$HNO+OH \rightarrow H_2O + NO$	559	532	536	547
Primary reactions	Freq. (YH-0)	Freq. (YH-1)	Freq. (YH-2)	Freq. (YH-3)
$C_4H_8N_8O_8 \rightarrow C_4H_8N_7O_6 + NO_2$	205	217	227	242
$C_4H_8N_7O_6 \rightarrow C_4H_8N_6O_4 + NO_2$	49	37	38	41
$C_4H_8N_8O_8 \rightarrow C_4H_7N_8O_8 + H$	4	9	5	7
$C_4H_7N_8O_8 \rightarrow C_4H_7N_7O_6 + NO_2$	1	1	1	2
$2C_4H_8N_8O_8 \rightarrow C_8H_{16}N_{16}O_{16}$	2	2	4	1
$HNO_2 \rightarrow OH + NO$	1880	1833	1716	1694
$HNO+OH \rightarrow H_2O + NO$	216	505	433	469
Primary reactions	Freq. (BH-0)	Freq. (BH-1)	Freq. (BH-2)	Freq. (BH-3)
$C_4H_8N_8O_8 \rightarrow C_4H_8N_7O_6 + NO_2$	218	245	221	201
$C_4H_8N_7O_6 \rightarrow C_4H_8N_6O_4 + NO_2$	38	44	37	43
$C_4H_8N_8O_8 \rightarrow C_4H_7N_8O_8 + H$	7	5	3	7
$C_4H_7N_8O_8 \rightarrow C_4H_7N_7O_6 + NO_2$	2	3	2	5
$2C_4H_8N_8O_8 \rightarrow C_8H_{16}N_{16}O_{16}$	1	4	2	2
$HNO_2 \rightarrow OH + NO$	1808	1700	1743	1741
$HNO+OH \rightarrow H_2O + NO$	470	528	417	458