

# **Clusters Evolution at Early Stages of 1,3,5-Triamino-2,4,6-trinitrobenzene under Various Heating Conditions: A Molecular Reactive Force Field Study**

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## **Supporting Information**

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## S1. The detailed information of the supercells

Table s1. The detailed information of the supercells.

supercells	TATB		
enlargement times from unit cells	6×6×6		
Lattice Parameters	a	b	c
	54.06 Å	54.17 Å	40.87 Å
	$\alpha$	$\beta$	$\gamma$
	108.58°	119.97°	91.82°
Amounts of molecules	432		
Amounts of atoms	10368		

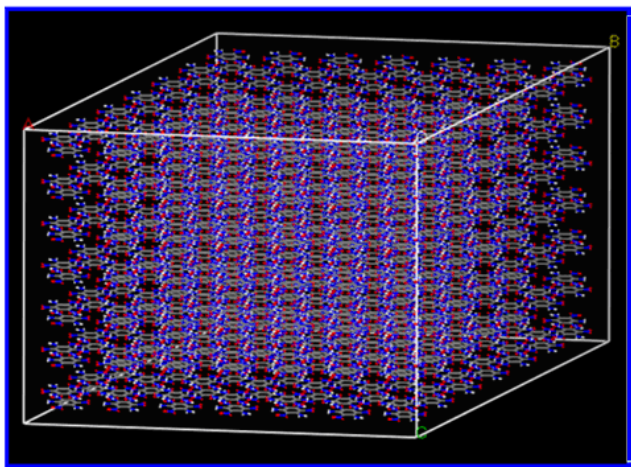


Fig. s1 Supercells of TATB. The carbon, hydrogen, oxygen and nitrogen atoms are indicated in grey, white, red and blue, respectively.

## S2. List of bond order minimum values used to determine molecules

Table s2. List of bond order minimum values used to determine molecules.

Atom type	Atom type	Bond order
C	N	0.3
C	C	0.55
C	O	0.65
C	H	0.4
O	O	0.65
N	O	0.4
O	H	0.4
H	H	0.55
H	N	0.55
N	N	0.55

### S3. The products of TATB heated under various conditions.

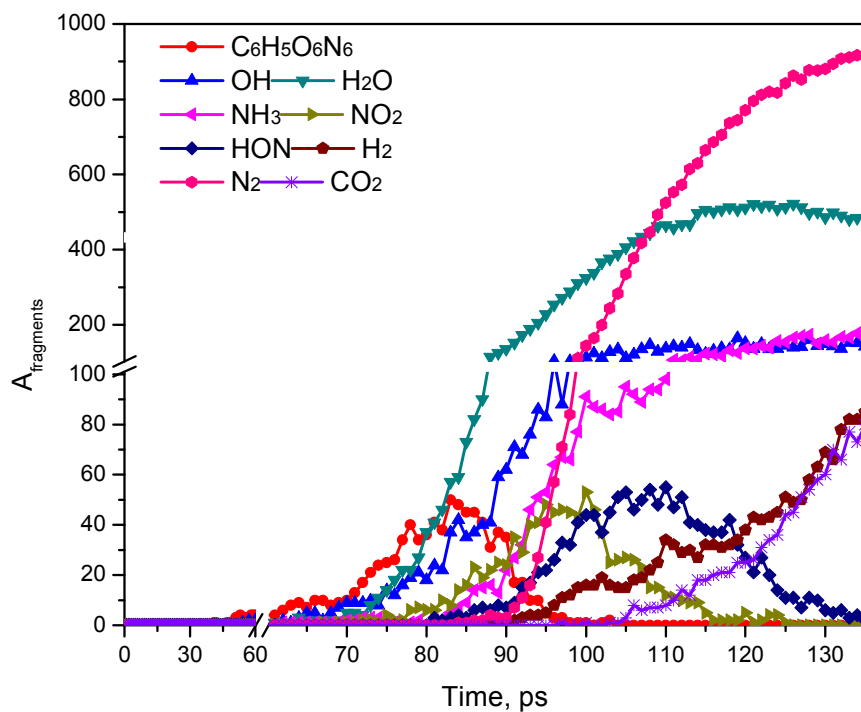


Fig. S2 The products of TATB programmed heated at a rate of 20 K/ps.

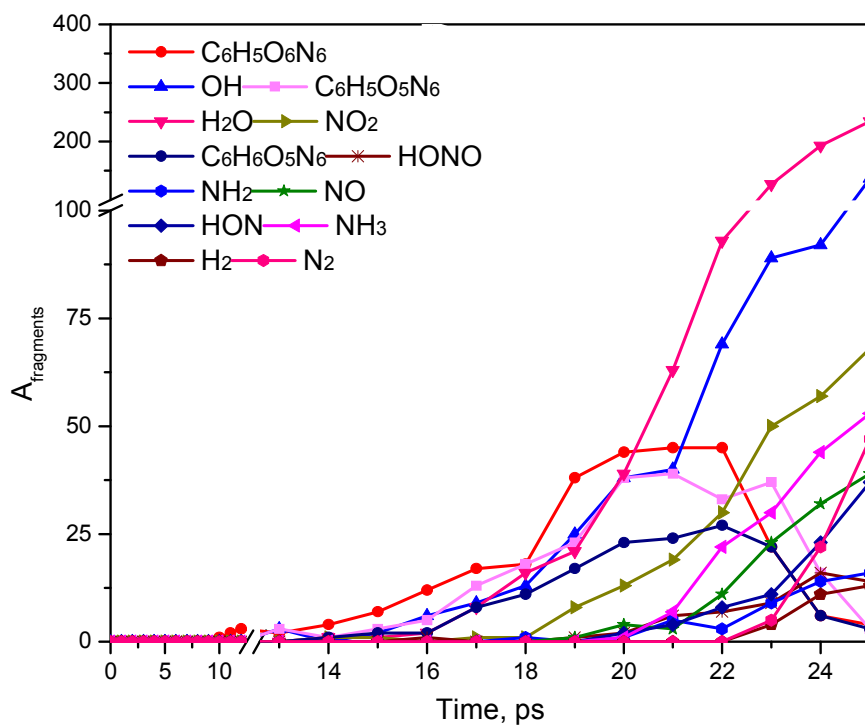


Fig. S3 The products of TATB programmed heated at a rate of 100 K/ps.

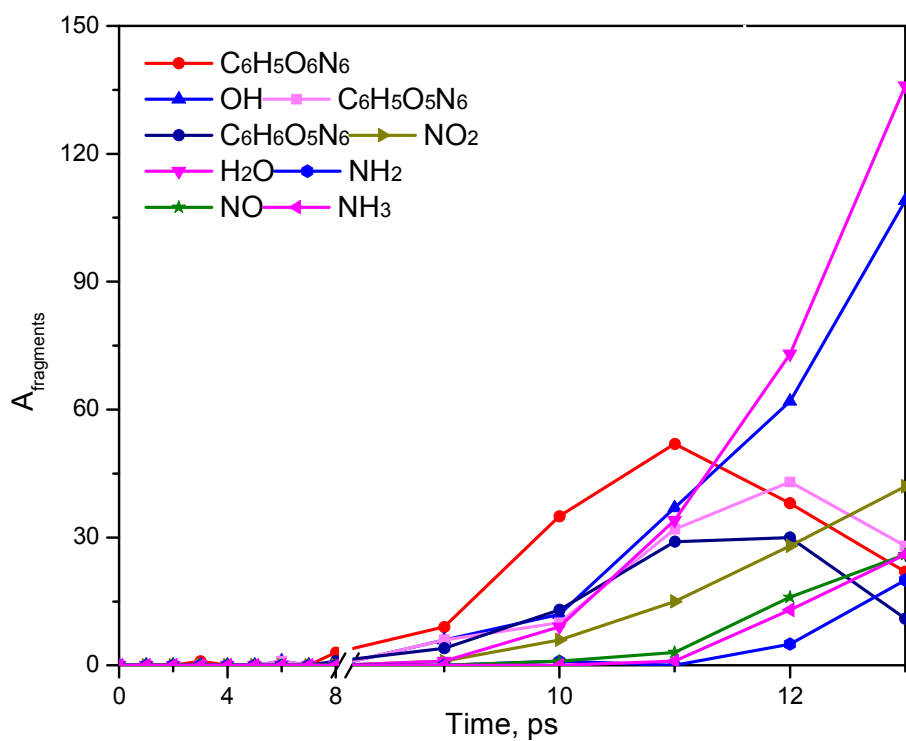


Fig. s4 The products of TATB programmed heated at a rate of 200 K/ps.

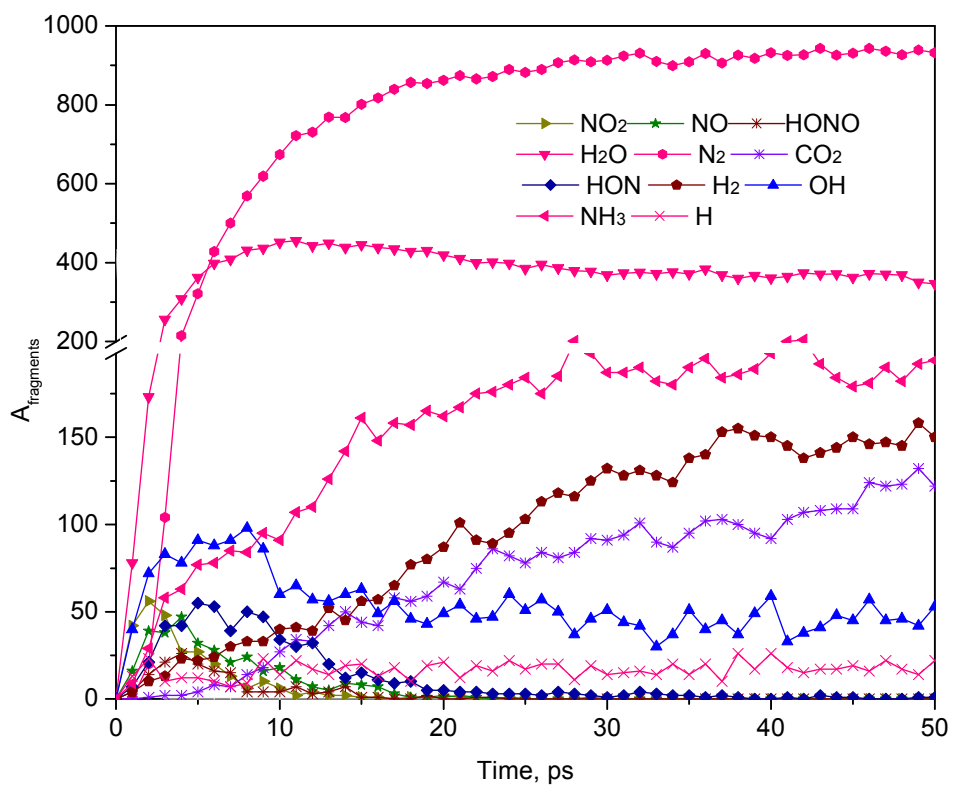


Fig. s5 The products of TATB heated at 3000 K.

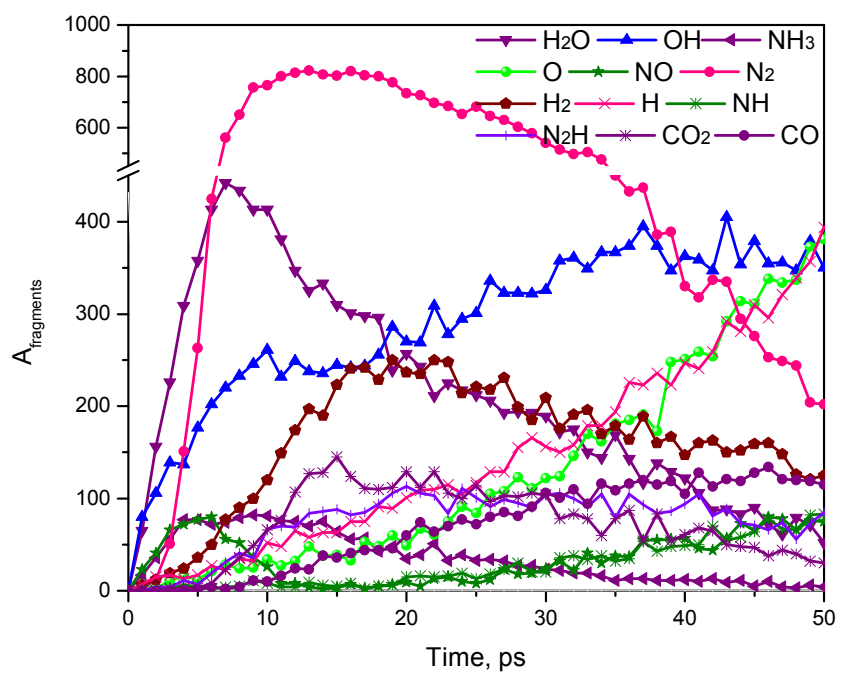


Fig. s6 The products of TATB adiabatic heated from 3000 K.

#### S4 Primary reactions under various heating conditions.

Table s3. Primary reactions and their frequencies under programmed heating with rate of 20 K/ps (time of statistics is 0~135ps with an interval of 1ps).

Frequency	Reactants	Products
31	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_6\text{N}_6 + \text{C}_6\text{H}_7\text{O}_6\text{N}_6$
28	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_5\text{N}_6 + \text{HO}$
14	$\text{C}_6\text{H}_7\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_6\text{O}_5\text{N}_6 + \text{HO}$
10	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{HO}$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_6\text{N}_6 + \text{H}_2\text{O}$
10	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_5\text{N}_6 + \text{C}_6\text{H}_5\text{O}_6\text{N}_6 + \text{H}_2\text{O}$
9	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_4\text{O}_5\text{N}_6 + \text{H}_2\text{O}$
9	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{HO}$	$\Rightarrow \text{C}_6\text{H}_7\text{O}_7\text{N}_6$
9	$\text{C}_6\text{H}_7\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_5\text{N}_6 + \text{H}_2\text{O}$
9	$\text{H}_2\text{N}_2$	$\Rightarrow \text{H}_2 + \text{N}_2$
8	$\text{H}_2\text{N} + \text{H}_2\text{O}$	$\Rightarrow \text{H}_3\text{N} + \text{HO}$
8	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_6\text{O}_5\text{N}_6 + \text{C}_6\text{H}_6\text{O}_7\text{N}_6$
8	$\text{HO} + \text{HO}$	$\Rightarrow \text{H}_2\text{O}_2$
6	$\text{H} + \text{HO}$	$\Rightarrow \text{H}_2\text{O}$
6	$\text{C}_6\text{H}_6\text{O}_6\text{N}_6 + \text{C}_6\text{H}_6\text{O}_6\text{N}_6$	$\Rightarrow \text{C}_6\text{H}_5\text{O}_6\text{N}_6 + \text{C}_6\text{H}_6\text{O}_5\text{N}_6 + \text{HO}$
5	$\text{HO}_3\text{N}$	$\Rightarrow \text{HO} + \text{NO}_2$

**Table s4.** Primary reactions and their frequencies under programmed heating with rate of 100 K/ps (time of statistics is 0~27 ps with an interval of 1 ps)

Frequency	Reactants	Products
28	$C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + HO$
17	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_7O_6N_6$
7	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + C_6H_5O_6N_6 + H_2O$
7	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_6O_5N_6 + C_6H_6O_7N_6$
6	$C_6H_6O_6N_6 + HO$	$\Rightarrow C_6H_5O_6N_6 + H_2O$
5	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + C_6H_7O_7N_6$
5	$C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + H$
5	$C_6H_7O_7N_6$	$\Rightarrow C_6H_6O_6N_6 + HO$
5	$C_6H_7O_6N_6$	$\Rightarrow C_6H_6O_5N_6 + HO$
4	$C_6H_6O_6N_6$	$\Rightarrow C_6H_6O_4N_5 + NO_2$
4	$C_6H_6O_6N_6$	$\Rightarrow C_6H_4O_5N_6 + H_2O$
4	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_{12}H_{12}O_{12}N_{12}$
4	$C_6H_6O_7N_6$	$\Rightarrow C_6H_6O_5N_5 + NO_2$
4	$C_6H_5O_5N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_6O_5N_6$
4	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_6O_5N_6 + HO$



**Table s5.** Primary reactions and their frequencies under programmed heating with rate of 200 K/ps (time of statistics is 0~13.5ps with an interval of 1ps)

Frequency	Reactants	Products
29	$C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + HO$
21	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_7O_6N_6$
9	$C_6H_6O_6N_6$	$\Rightarrow C_6H_6O_4N_5 + NO_2$
8	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + C_6H_5O_6N_6 + H_2O$
8	$C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + H$
8	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_6O_5N_6 + HO$
7	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_6O_5N_6 + C_6H_6O_7N_6$
5	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_{12}H_{12}O_{12}N_{12}$
3	$C_6H_7O_6N_6$	$\Rightarrow C_6H_5O_5N_6 + H_2O$
3	$C_6H_6O_6N_6 + C_6H_7O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_6O_5N_6 + H_2O$
3	$3C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_6N_6 + C_6H_6O_5N_6 + C_6H_7O_7N_6$
2	$C_6H_6O_6N_6 + HO$	$\Rightarrow C_6H_4O_7N_5 + NH_3$
2	$C_6H_5O_5N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_5O_4N_6 + C_6H_5O_6N_6 + HO$
2	$C_6H_6O_6N_6 + C_6H_6O_6N_6$	$\Rightarrow C_6H_6O_5N_5 + C_6H_6O_5N_6 + NO_2$
2	$C_6H_5O_6N_6 + H$	$\Rightarrow C_6H_5O_5N_6 + HO$

**Table s6.** Primary reactions and their frequencies under constant temperature heating (T=3000 K and the time of statistics is 0~5ps with an interval of 0.1ps)

Frequency	Reactants		Products
22	$C_6H_6O_6N_6$	=>	$C_6H_6O_4N_5+NO_2$
21	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_6H_5O_6N_6+C_6H_7O_6N_6$
18	$C_6H_6O_6N_6$	=>	$C_6H_5O_5N_6+HO$
15	$C_6H_6O_6N_6$	=>	$C_6H_5O_6N_6+H$
8	$C_6H_6O_6N_6$	=>	$C_6H_6O_5N_6+O$
6	$C_6H_6O_6N_6$	=>	$C_6H_4O_6N_5+H_2N$
6	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_6H_5O_5N_6+C_6H_5O_6N_6+H_2O$
5	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_{12}H_{12}O_{12}N_{12}$
5	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_6H_6O_5N_6+C_6H_6O_7N_6$
5	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_6H_5O_6N_6+C_6H_6O_5N_6+HO$
5	$C_6H_6O_6N_6+O$	=>	$C_6H_6O_7N_6$
5	$C_6H_6O_6N_6+HO$	=>	$C_6H_5O_6N_6+H_2O$
4	$C_6H_7O_6N_6$	=>	$C_6H_4O_6N_5+NH_3$
4	$C_6H_5O_6N_6$	=>	$C_6H_4O_5N_6+HO$
4	$C_6H_6O_6N_6+H$	=>	$C_6H_6O_5N_6+HO$

**Table s7.** Primary reactions and their frequencies under adiabatic heating with preheating at 3000 K for 0.5 ps (the time of statistics is 0~5ps with an interval of 0.1ps)

Frequency	Reactants		Products
33	$C_6H_6O_6N_6$	=>	$C_6H_5O_5N_6+HO$
16	$C_6H_6O_6N_6$	=>	$C_6H_6O_4N_5+NO_2$
13	$C_6H_6O_6N_6+HO$	=>	$C_6H_7O_7N_6$
11	$C_6H_7O_6N_6$	=>	$C_6H_6O_5N_6+HO$
11	$C_6H_6O_6N_6+C_6H_6O_6N_6$	=>	$C_6H_5O_6N_6+C_6H_7O_6N_6$
8	$C_6H_5O_5N_6$	=>	$C_6H_4O_4N_6+HO$
6	$C_6H_5O_6N_6+HO$	=>	$C_6H_4O_6N_6+H_2O$
6	$C_6H_5O_6N_6+C_6H_6O_6N_6$	=>	$C_{12}H_{11}O_{12}N_{12}$
6	$C_6H_6O_6N_6+H$	=>	$C_6H_7O_6N_6$
5	$C_6H_6O_7N_6$	=>	$C_6H_6O_5N_5+NO_2$
5	$C_6H_7O_6N_6$	=>	$C_6H_5O_5N_6+H_2O$
5	$C_6H_6O_5N_6$	=>	$C_6H_5O_4N_6+HO$
5	$C_6H_5O_5N_6$	=>	$C_6H_5O_3N_5+NO_2$
5	$C_6H_4O_4N_4$	=>	$C_6H_3O_3N_4+HO$
5	$O_2N$	=>	$O+NO$