Supplementary Information

Decomposition mechanism of 1,3,5-trinitro-2,4,6-trinitroaminobenzene under thermal and shock stimulus using ReaxFF molecular dynamics simulations

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To verify the adequacy of the applied potential, the dissociation energies (C-NO_2, N-NO_2) and average bond lengths were listed in Table S1 and S2. All data were calculated by ReaxFF force fields are excellently consistent with those by the DFT-B3LYP/6-311++G** method. The average bond length error does not exceed 10%. The BDE of three bond types are ranked as N-NO_2 > C-NO_2 >N-H under both ReaxFF and DFT simulation.

Table S1. The average bond lengths (*L*, Å) and relative error (*Er*, %) in TNTNB crystal

	N-C	N-H	N-O	N-N	C-C
$L_{ReaxFF-lg}$	1.49	1.11	1.28	1.55	1.44
L_{DFT}	1.44	1.01	1.22	1.43	1.41
Er (%)	3.33	9.81	5.75	8.29	2.48

Table. S2. The lattice parameters of TNTNB

	a (Å)	b (Å)	c (Å)	ρ (g/cm^3)
Exp [2]	10.825	7.075	17.673	1.995
ReaxFF	10.746	7.023	16.965	2.040
Er (%)	0.730	0.735	4.006	-2.256

Table S3. The total energies and bond dissociation energy (BDE in kcal/mol) [a]

Methods	Reaction [b]	E_{AB}	E_A	E_B	BDE
ReaxFF-lg	R1	-3230.20	-2964.76	-239.10	26.34
	R2	-3230.20	-2925.91	-239.04	65.25

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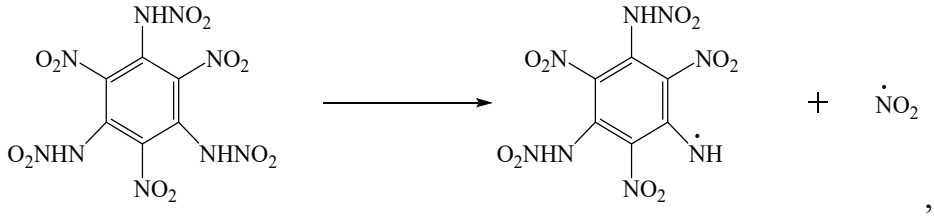
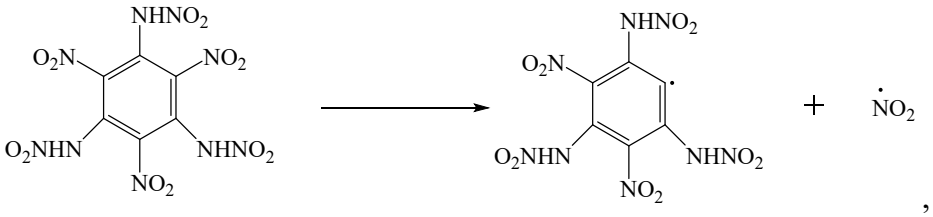
	R3	-3230.20	-3145.05	0.00	85.15
B3LYP	R1	-1020089.88	-891327.58	-128721.43	40.87
	R2	-1020089.88	-891307.84	-128719.45	62.57
	R3	-1020089.88	-1019657.99	-315.11	116.78

[a] BDE = $E_A + E_B - E_{AB}$,

[b] R1:  ,

R2:  ,

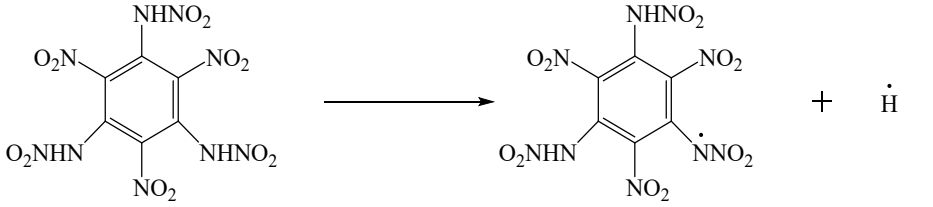
R3: 

Table S4. List of Bond Order Minimum Values Used to Determine Molecules

atom type	atom type	bond order
C	C	0.55
C	H	0.40
C	N	0.30
C	O	0.65
H	H	0.55
H	N	0.55
H	O	0.40
N	N	0.55
N	O	0.40
O	O	0.65

Table S5. Decomposition pathways (the five most frequency) of TNTNB in 10 ps under different shock velocities and temperatures

	Reactions	Frequency
7.0 km/s	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{24}N_{18}$	42
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	19

	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{22}N_{17} + NO_2$	13
	$C_{12}H_6O_{24}N_{18} + C_6H_3O_{12}N_9 \rightarrow C_{18}H_9O_{36}N_{27}$	12
	$C_{12}H_6O_{22}N_{17} + NO_2 \rightarrow C_{12}H_6O_{24}N_{18}$	11
7.5 km/s	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{24}N_{18}$	50
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	24
	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_6H_2O_{12}N_9 + C_6H_4O_{12}N_9$	15
	$C_{12}H_6O_{24}N_{18} + C_6H_3O_{12}N_9 \rightarrow C_{18}H_9O_{36}N_{27}$	12
	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{22}N_{17} + NO_2$	9
8.0 km/s	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{24}N_{18}$	60
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	49
	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{22}N_{17} + NO_2$	18
	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_6H_2O_{12}N_9 + C_6H_4O_{12}N_9$	11
	$C_6H_3O_{12}N_9 + NO_2 \rightarrow C_6H_3O_{14}N_{10}$	11
8.5 km/s	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{24}N_{18}$	57
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	41
	$C_6H_3O_{12}N_9 + C_6H_3O_{12}N_9 \rightarrow C_{12}H_6O_{22}N_{17} + NO_2$	14
	$C_{12}H_6O_{24}N_{18} + C_6H_3O_{12}N_9 \rightarrow C_{18}H_9O_{36}N_{27}$	14
	$C_6H_3O_{12}N_9 + NO_2 \rightarrow C_6H_3O_{14}N_{10}$	11
2500 K	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	338
	$C_6H_3O_8N_7 \rightarrow C_6H_3O_6N_6 + NO_2$	323
	$C_6H_3O_{10}N_8 \rightarrow C_6H_3O_8N_7 + NO_2$	248
	$C_6H_3O_6N_6 \rightarrow C_6H_3O_4N_5 + NO_2$	146
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_8N_7 + NO_2 + NO_2$	116
3000 K	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	288
	$C_6H_3O_8N_7 \rightarrow C_6H_3O_6N_6 + NO_2$	271
	$C_6H_3O_{10}N_8 \rightarrow C_6H_3O_8N_7 + NO_2$	183
	$C_6H_3O_6N_6 \rightarrow C_6H_3O_4N_5 + NO_2$	157
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_8N_7 + NO_2 + NO_2$	141
3500 K	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	225
	$C_6H_3O_8N_7 \rightarrow C_6H_3O_6N_6 + NO_2$	182
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_8N_7 + NO_2 + NO_2$	151
	$HNO_2 \rightarrow HO + NO$	120
	$C_6H_3O_{10}N_8 \rightarrow C_6H_3O_8N_7 + NO_2$	111
4000 K	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_{10}N_8 + NO_2$	193
	$HNO_2 \rightarrow HO + NO$	164
	$C_6H_3O_{12}N_9 \rightarrow C_6H_3O_8N_7 + NO_2 + NO_2$	137
	$C_6H_3O_8N_7 \rightarrow C_6H_3O_6N_6 + NO_2$	112
	$NO_2 \rightarrow O + NO$	89

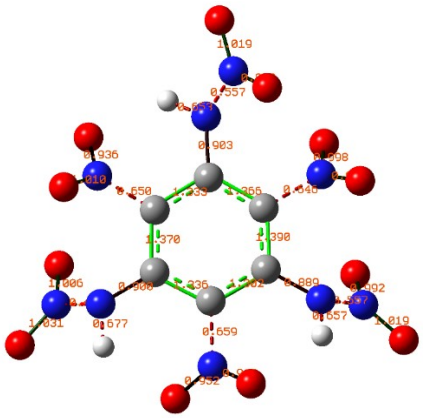


Figure S5. The Laplacian bond order of TNTNB

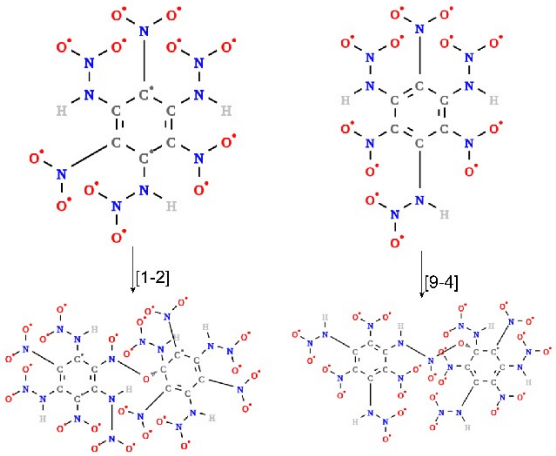


Figure S6. The shock decomposition pathways at 7.0 km/s within 1 ps (The reaction code names and their frequencies are listed in square brackets. Several reactions with a high frequency in this period are marked in blue.)

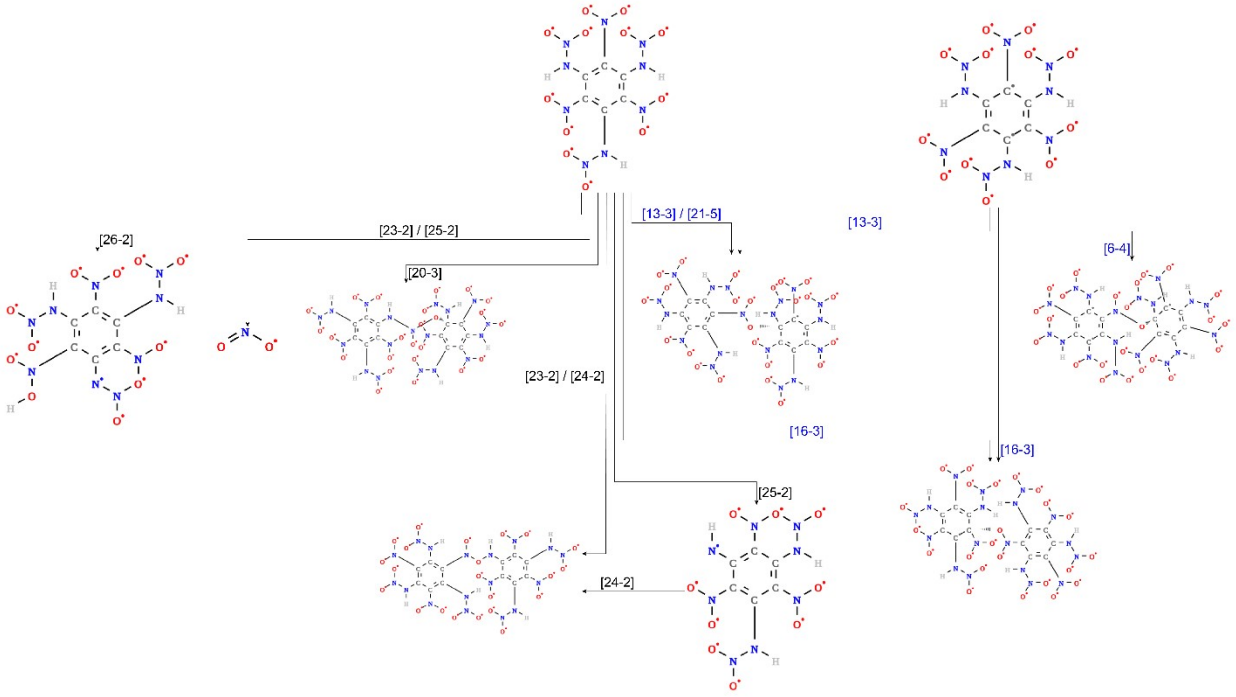


Figure S7. The shock decomposition pathways at 7.5 km/s within 1 ps (The reaction code names and their frequencies are listed in square brackets. Several reactions with a high frequency in this period are marked in blue.)

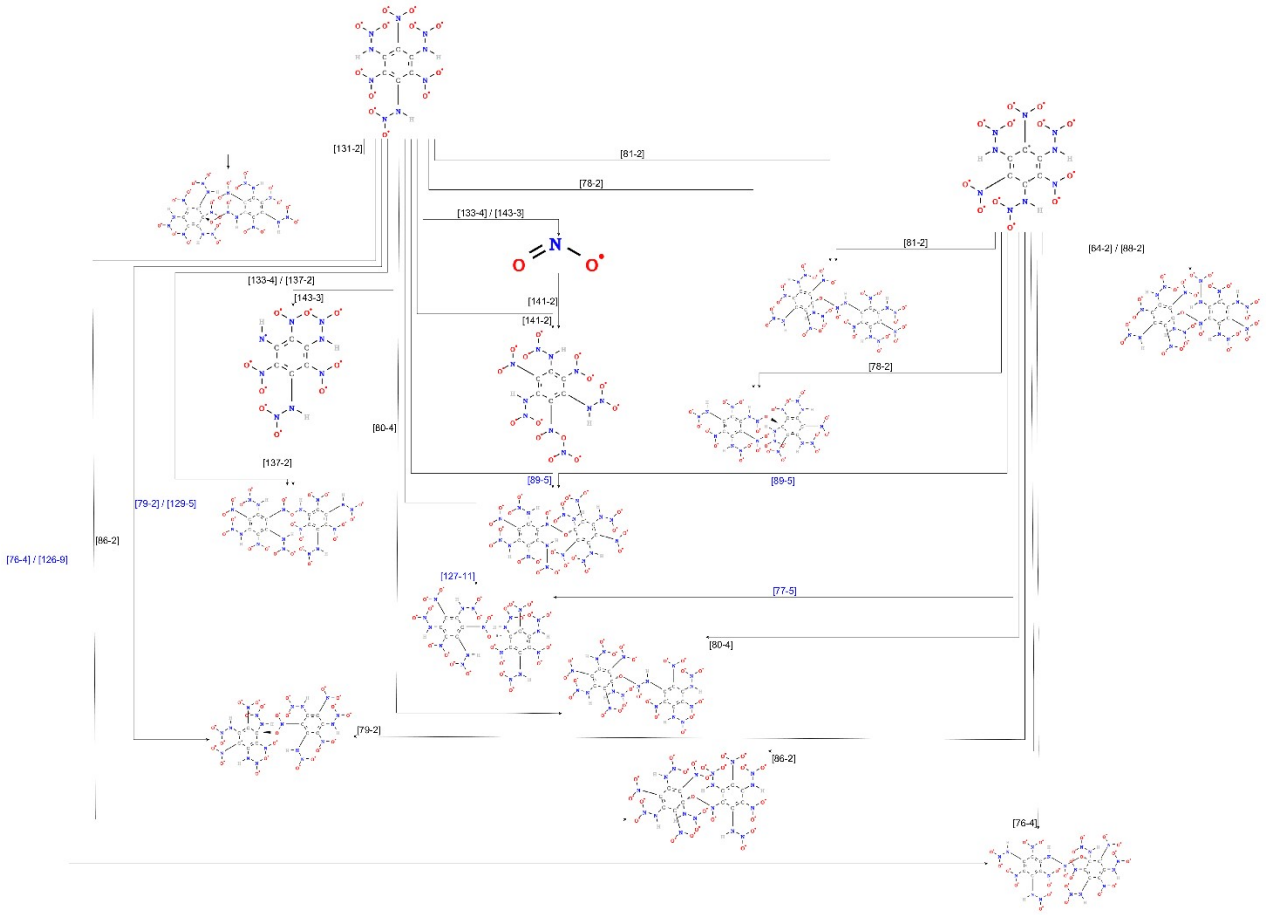


Figure S8. The shock decomposition pathways at 8.5 km/s within 1 ps (The reaction code names and their frequencies are listed in square brackets. Several reactions with a high frequency in this period are marked in blue.)