Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Ab Initio Neural Network MD Simulation of Thermal Decomposition of High Energy Material Cl-20/TNT

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1. More results from the MD simulations with NNPs.

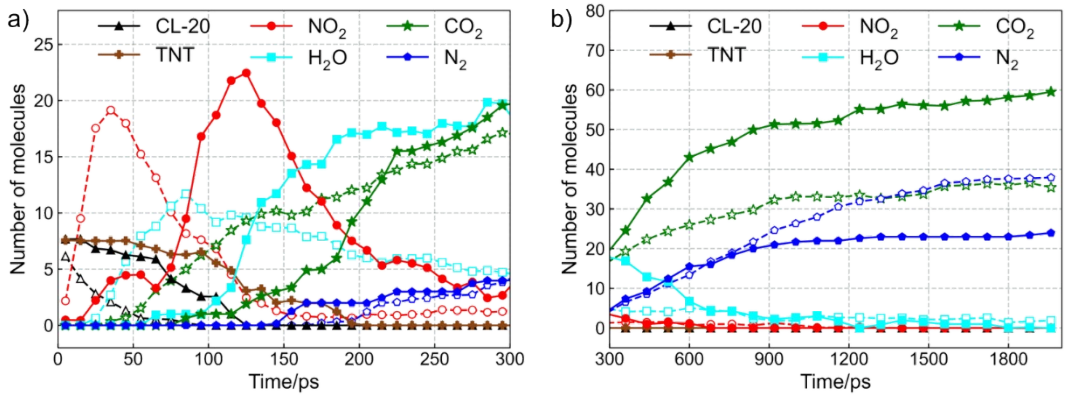

Figure S1. Evolution of the number of reactants and products during the MD simulations of pure CL-20 and CL-20/TNT systems at 1500 K. The dotted lines with hollow patterns represent the pure CL-20 system, and the solid lines with solid patterns represent the CL-20/TNT system. (a) for the first 300 ps. (b) from 300 ps to 2 ns.

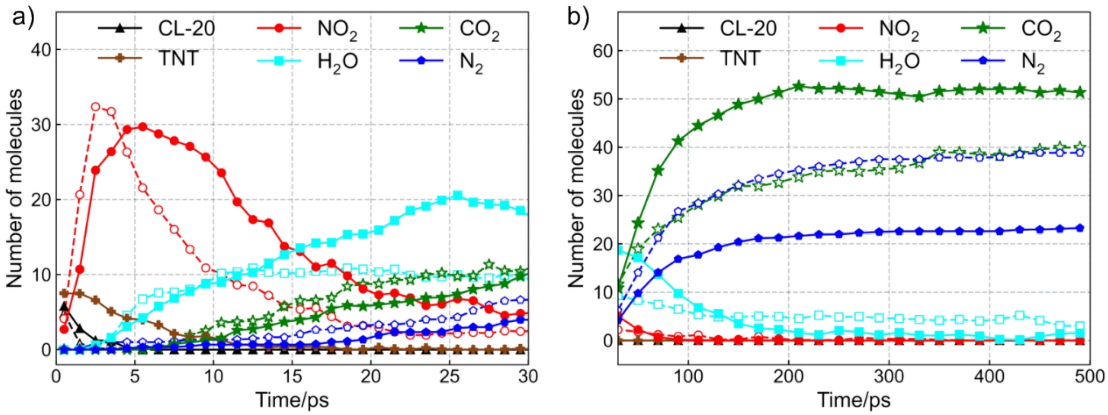

Figure S2. Evolution of the number of reactants and products during the MD simulations of pure CL-20 and CL-20/TNT systems at 2000 K. The dotted lines with hollow patterns represent the pure CL-20 system, and the solid lines with solid patterns represent the CL-20 /TNT system. (a) for the first 30 ps. (b) from 30 ps to 500 ps.

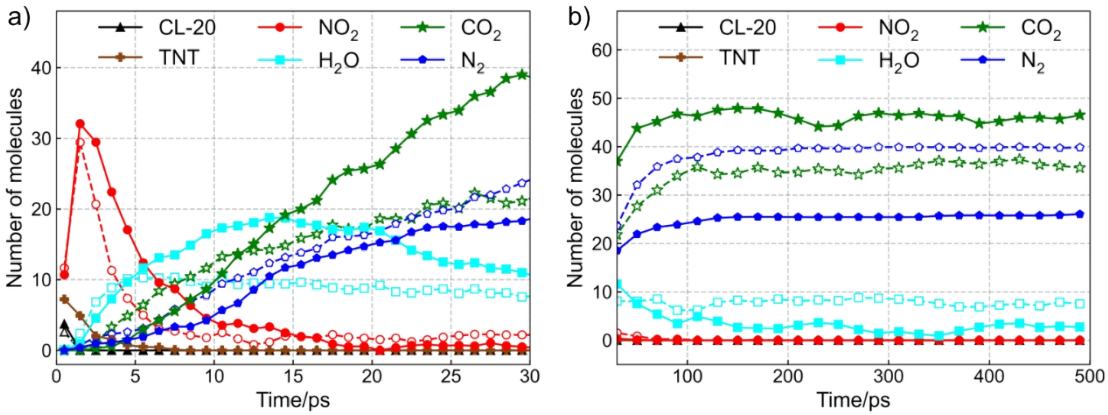

Figure S3. Evolution of the number of reactants and products during the MD simulations of pure CL-20 and CL-20/TNT systems at 2500 K. The dotted lines with hollow patterns represent the pure CL-20 system, and the solid lines with solid patterns represent the CL-20/TNT system. (a) for the first 30 ps. (b) from 30 ps to 500 ps.

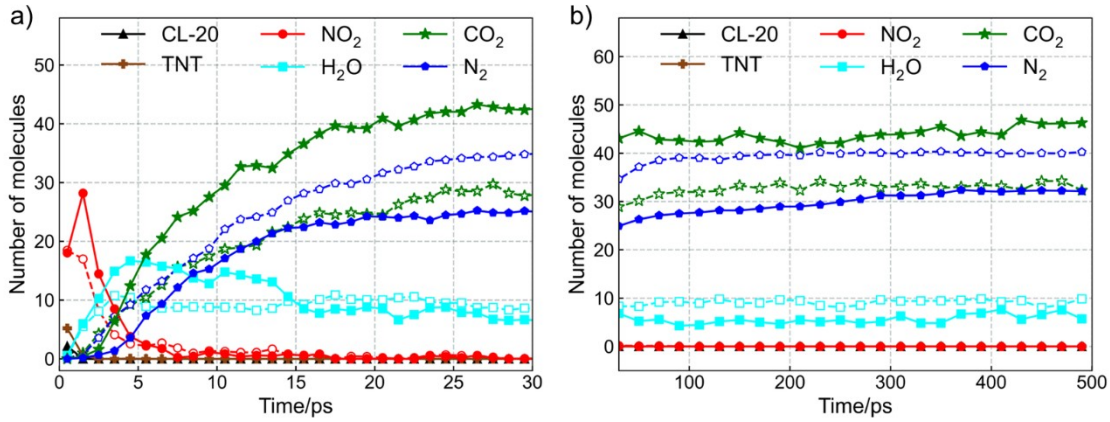

Figure S4. Evolution of the number of reactants and products during the MD simulations of pure CL-20 and CL-20/TNT systems at 3000 K. The dotted lines with hollow patterns represent the pure CL-20 system, and the solid lines with solid patterns represent the CL-20/TNT system. (a) for the first 30 ps. (b) from 30 ps to 500 ps.

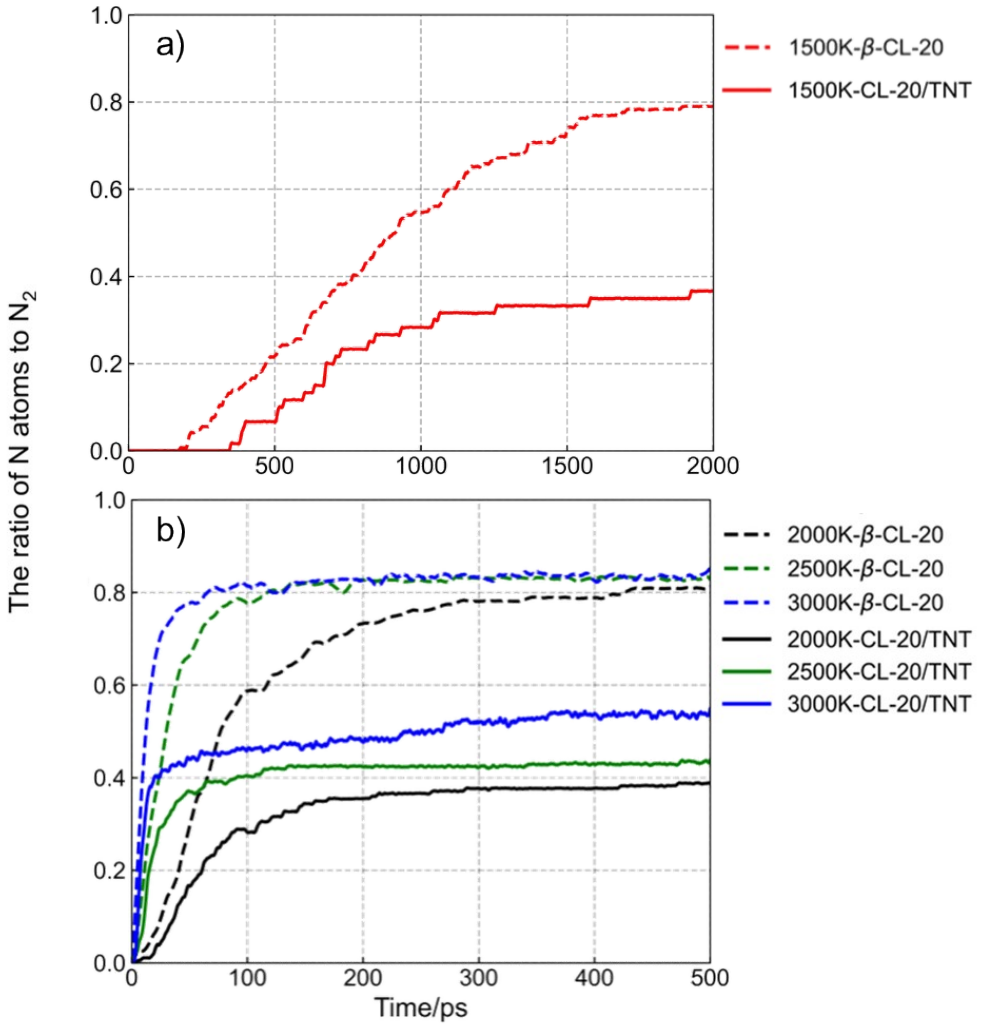

Figure S5. The conversion ratio of N atoms to N_2 molecules during the MD simulations of pure CL-20 and CL-20/TNT at (a)1500 K and (b)2000 K, 2500 K, and 3000 K.

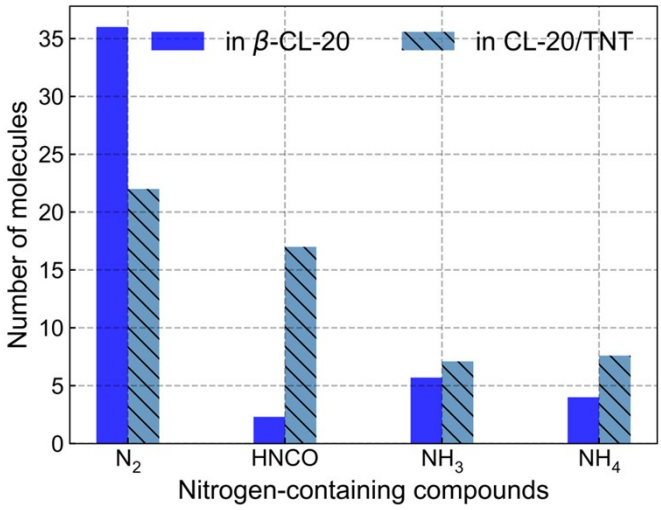

Figure S6. The production of main nitrogen-containing compounds in MD simulations of pure CL-20 and CL-20/TNT at 1500 K.

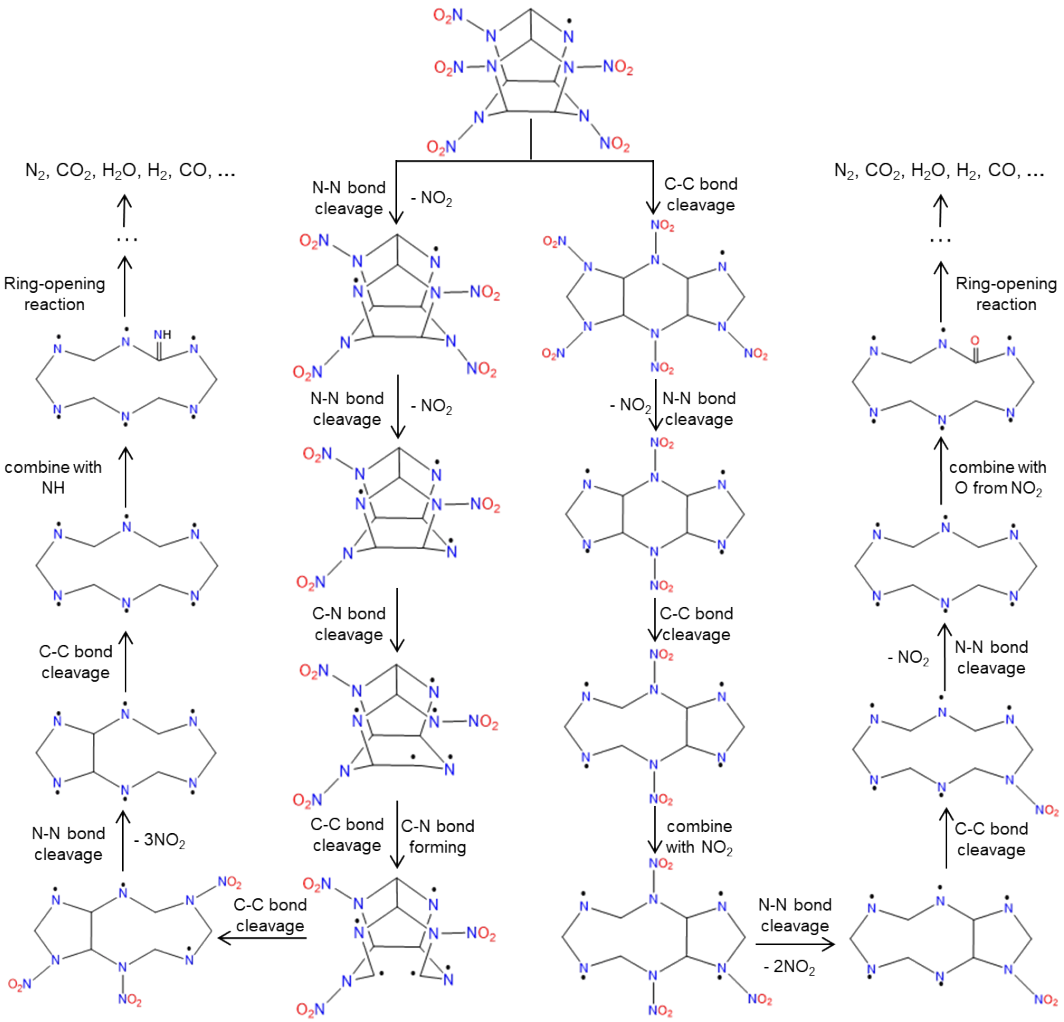

Figure S7. Continue from the most initial reaction of CL-20 cleavage to the next reaction paths in pure CL-20 system obtained in the heating simulations (1500 ~3000 K).

2. A sample input file for DFT calculation.

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PROJECT DPGEN
&END GLOBAL
&FORCE_EVAL
METHOD QS
STRESS_TENSOR ANALYTICAL
&DFT
BASIS_SET_FILE_NAME /home/test/soft/cp2k-8.1/data/BASIS_MOLOPT
POTENTIAL_FILE_NAME /home/test/soft/cp2k-8.1/data/GTH_POTENTIALS
CHARGE 0
UKS F
MULTIPLICITY 1
&MGRID
CUTOFF 400
REL_CUTOFF 50
NGRIDS 4
&END MGRID
&QS
EPS_DEFAULT 1.0E-12
&END QS
&SCF
SCF_GUESS ATOMIC
EPS_SCF 1.0E-6
MAX_SCF 200
&OT
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MINIMIZER DIIS

PRECONDITIONER FULL_SINGLE_INVERSE

&END OT

&OUTER_SCF

MAX_SCF 3

EPS_SCF 1e-06

&END OUTER_SCF

&END SCF

&XC

&XC_FUNCTIONAL PBE

&END XC_FUNCTIONAL

&VDW_POTENTIAL

POTENTIAL_TYPE PAIR_POTENTIAL

&PAIR_POTENTIAL

TYPE DFTD3

PARAMETER_FILE_NAME /home/test/soft/cp2k-8.1/data/dftd3.dat

REFERENCE_FUNCTIONAL PBE

&END PAIR_POTENTIAL

&END VDW_POTENTIAL

&END XC

&END DFT

&SUBSYS

&CELL

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B 0. 19.369 0.

C 0. 0. 24.69

&END CELL

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BASIS_SET DZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q6
&END KIND
&KIND N
BASIS_SET DZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q5
&END KIND
&KIND C
BASIS_SET DZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q4
&END KIND
&KIND H
BASIS_SET DZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q1
&END KIND
&END SUBSYS
&PRINT
&FORCES ON
&END FORCES
&END PRINT
&END FORCE_EVAL
```

3. A sample input file for MD simulation.

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neighbor        1.0 bin
box             tilt large
read_data       conf.lmp
change_box      all triclinic
mass            1 1.007940
mass            2 12.010700
mass            3 14.006700
mass            4 15.999400
pair_style      deepmd ../graph.000.pb ../graph.001.pb ../graph.002.pb ../graph.003.pb
  out_freq 100 out_file model_devi.out relative 1.0
pair_coeff
thermo_style    custom step temp pe ke etotal press vol lx ly lz xy xz yz
thermo          100
dump            1 all custom 100 traj/*.lammpstrj id type x y z
velocity        all create 3000 178100
fix             1 all nvt temp 3000 3000 100
timestep        0.000100
run             5000000
```