

## Electronic supplementary information

### Decomposition mechanism scenarios of CL-20 co-crystals revealed by ReaxFF molecular dynamics: similarities and differences

Chunxing Ren<sup>1,2</sup>, Han Liu<sup>1,2</sup>, Xiaoxia Li<sup>\*,1,2,3</sup>, Li Guo<sup>1,2,3</sup>

<sup>1</sup>State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, P. R. China

<sup>2</sup>University of Chinese Academy of Sciences, Beijing 100049, P. R. China

<sup>3</sup>Innovation Academy for Green Manufacture, Chinese Academy of Sciences, Beijing 100190, P. R. China

\*Email: xxia@ipe.ac.cn

#### S1. ReaxFF-lg force field parameters used in this work

39           ! Number of general parameters  
50.0000 !Overcoordination parameter  
9.4514 !Overcoordination parameter  
29.8953 !Valency angle conjugation parameter  
216.5421 !Triple bond stabilisation parameter  
12.2245 !Triple bond stabilisation parameter  
0.0000 !C2-correction  
1.0701 !Undercoordination parameter  
7.5000 !Triple bond stabilisation parameter  
11.9083 !Undercoordination parameter  
13.3822 !Undercoordination parameter  
-10.9834 !Triple bond stabilization energy  
0.0000 !Lower Taper-radius  
10.0000 !Upper Taper-radius  
2.8793 !Not used

33.8667 !Valency undercoordination  
 3.3976 !Valency angle/lone pair parameter  
 1.0563 !Valency angle  
 2.0384 !Valency angle parameter  
 6.1431 !Not used  
 6.9290 !Double bond/angle parameter  
 0.0283 !Double bond/angle parameter: overcoord  
 0.0570 !Double bond/angle parameter: overcoord  
 -2.4837 !Not used  
 5.8374 !Torsion/BO parameter  
 10.0000 !Torsion overcoordination  
 1.8820 !Torsion overcoordination  
 -1.2327 !Conjugation 0 (not used)  
 2.1861 !Conjugation  
 1.5591 !vdWaals shielding  
 0.0100 !Cutoff for bond order (\*100)  
 4.8414 !Valency angle conjugation parameter  
 3.5857 !Overcoordination parameter  
 38.6472 !Overcoordination parameter  
 2.1533 !Valency/lone pair parameter  
 0.5000 !Not used  
 1.0000 !Scale factor (d) in dispersion  
 5.0000 !Molecular energy (not used)  
 0.0000 !Molecular energy (not used)  
 6.9784 !Valency angle conjugation parameter

7 !Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#  
 alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.  
 cov.r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.  
 ov/un;val1;n.u.;val3,vval4

|   |          |          |          |         |          |         |         |         |
|---|----------|----------|----------|---------|----------|---------|---------|---------|
| C | 1.3742   | 4.0000   | 12.0000  | 1.9684  | 0.1723   | 0.8712  | 1.2385  | 4.0000  |
|   | 8.7696   | 100.0000 | 4.0000   | 31.0823 | 79.5548  | 5.7254  | 6.9235  | 0.0000  |
|   | 1.2104   | 0.0000   | 183.8108 | 5.7419  | 33.3951  | 11.9957 | 0.8563  | 0.0000  |
|   | -2.8983  | 4.7820   | 1.0564   | 4.0000  | 2.9663   | 1.6737  | 0.1421  | 14.0707 |
|   | 0.0001   | 1.9255   |          |         |          |         |         |         |
| H | 0.6867   | 1.0000   | 1.0080   | 1.3525  | 0.0616   | 0.8910  | -0.1000 | 1.0000  |
|   | 9.1506   | 100.0000 | 1.0000   | 0.0000  | 121.1250 | 3.8446  | 10.0839 | 1.0000  |
|   | -0.1000  | 0.0000   | 58.4369  | 3.8461  | 3.2540   | 1.0000  | 1.0698  | 0.0000  |
|   | -15.7683 | 2.1504   | 1.0338   | 1.0000  | 2.8793   | 1.2669  | 0.0139  | 12.4538 |
|   | 0.0001   | 1.4430   |          |         |          |         |         |         |
| O | 1.3142   | 2.0000   | 15.9990  | 1.9741  | 0.0880   | 0.8712  | 1.1139  | 6.0000  |
|   | 9.9926   | 100.0000 | 4.0000   | 29.5271 | 116.0768 | 8.5000  | 7.1412  | 2.0000  |
|   | 0.9909   | 14.7235  | 69.2921  | 9.1371  | 1.6258   | 0.1863  | 0.9745  | 0.0000  |
|   | -3.5965  | 2.5000   | 1.0493   | 4.0000  | 2.9225   | 1.7221  | 0.1670  | 13.9991 |
|   | 623.8417 | 1.7500   |          |         |          |         |         |         |

|    |          |          |          |         |          |        |         |         |
|----|----------|----------|----------|---------|----------|--------|---------|---------|
| N  | 1.2456   | 3.0000   | 14.0000  | 2.0437  | 0.1035   | 0.8712 | 1.1911  | 5.0000  |
|    | 9.8823   | 100.0000 | 4.0000   | 32.4758 | 100.0000 | 6.8453 | 6.8349  | 2.0000  |
|    | 1.0636   | 0.0276   | 127.9672 | 2.2169  | 2.8632   | 2.4419 | 0.9745  | 0.0000  |
|    | -4.0959  | 2.0047   | 1.0183   | 4.0000  | 2.8793   | 1.5967 | 0.1649  | 13.9888 |
|    | 1240.001 | 1.8300   |          |         |          |        |         |         |
| S  | 1.9647   | 2.0000   | 32.0600  | 2.0783  | 0.2176   | 1.0336 | 1.5386  | 6.0000  |
|    | 9.9676   | 5.0812   | 4.0000   | 35.1648 | 112.1416 | 6.5000 | 8.2545  | 2.0000  |
|    | 1.4703   | 9.4922   | 70.0338  | 8.5146  | 28.0801  | 8.5010 | 0.9745  | 0.0000  |
|    | -10.0773 | 2.7466   | 1.0338   | 6.2998  | 2.8793   | 1.8000 | 0.0000  | 14.0000 |
|    | 180.0000 | 2.0783   |          |         |          |        |         |         |
| Si | 2.0276   | 4.0000   | 28.0600  | 2.2042  | 0.1322   | 0.8218 | 1.5758  | 4.0000  |
|    | 11.9413  | 2.0618   | 4.0000   | 11.8211 | 136.4845 | 1.8038 | 7.3852  | 0.0000  |
|    | -1.0000  | 0.0000   | 126.5331 | 6.4918  | 8.5961   | 0.2368 | 0.8563  | 0.0000  |
|    | -3.8112  | 3.1873   | 1.0338   | 4.0000  | 2.5791   | 0.0000 | 0.0000  | 0.0000  |
|    | 180.0000 | 2.2042   |          |         |          |        |         |         |
| X  | -0.1000  | 2.0000   | 1.0080   | 2.0000  | 0.0000   | 1.0000 | -0.1000 | 6.0000  |
|    | 10.0000  | 2.5000   | 4.0000   | 0.0000  | 0.0000   | 8.5000 | 1.5000  | 0.0000  |
|    | -0.1000  | 0.0000   | -2.3700  | 8.7410  | 13.3640  | 0.6690 | 0.9745  | 0.0000  |
|    | -11.0000 | 2.7466   | 1.0338   | 4.0000  | 2.8793   | 0.0000 | 0.0000  | 0.0000  |
|    | 180.0000 | 2.0000   |          |         |          |        |         |         |

18 ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6

pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr

|   |   |          |          |          |         |         |        |         |        |
|---|---|----------|----------|----------|---------|---------|--------|---------|--------|
| 1 | 1 | 141.9346 | 113.4487 | 67.6027  | 0.1554  | -0.3045 | 1.0000 | 30.4515 | 0.4283 |
|   |   | 0.0801   | -0.2113  | 8.5395   | 1.0000  | -0.0933 | 6.6967 | 1.0000  | 0.0000 |
| 1 | 2 | 163.6889 | 0.0000   | 0.0000   | -0.4525 | 0.0000  | 1.0000 | 6.0000  | 0.5921 |
|   |   | 12.1053  | 1.0000   | 0.0000   | 1.0000  | -0.0097 | 8.6351 | 0.0000  | 0.0000 |
| 2 | 2 | 169.8421 | 0.0000   | 0.0000   | -0.3591 | 0.0000  | 1.0000 | 6.0000  | 0.7503 |
|   |   | 9.3119   | 1.0000   | 0.0000   | 1.0000  | -0.0169 | 5.9406 | 0.0000  | 0.0000 |
| 1 | 3 | 159.7219 | 116.8921 | 77.9315  | -0.4324 | -0.1742 | 1.0000 | 15.0019 | 0.5160 |
|   |   | 1.2934   | -0.3079  | 7.0252   | 1.0000  | -0.1543 | 4.5116 | 0.0000  | 0.0000 |
| 3 | 3 | 108.9631 | 158.3501 | 42.0558  | 0.1226  | -0.1324 | 1.0000 | 28.5716 | 0.2545 |
|   |   | 1.0000   | -0.2656  | 8.6489   | 1.0000  | -0.1000 | 6.8482 | 1.0000  | 0.0000 |
| 1 | 4 | 128.9104 | 171.2945 | 100.5836 | -0.1306 | -0.4948 | 1.0000 | 26.7458 | 0.4489 |
|   |   | 0.3746   | -0.3549  | 7.0000   | 1.0000  | -0.1248 | 4.9232 | 1.0000  | 0.0000 |
| 3 | 4 | 85.0402  | 118.8680 | 75.7263  | 0.7080  | -0.1062 | 1.0000 | 16.6913 | 0.2407 |
|   |   | 0.3535   | -0.1906  | 8.4054   | 1.0000  | -0.1154 | 5.6575 | 1.0000  | 0.0000 |
| 4 | 4 | 160.6599 | 73.3721  | 154.2849 | -0.7107 | -0.1462 | 1.0000 | 12.0000 | 0.6826 |
|   |   | 0.9330   | -0.1434  | 10.6712  | 1.0000  | -0.0890 | 4.6486 | 1.0000  | 0.0000 |
| 2 | 3 | 219.7016 | 0.0000   | 0.0000   | -0.6643 | 0.0000  | 1.0000 | 6.0000  | 0.9854 |
|   |   | 5.1146   | 1.0000   | 0.0000   | 1.0000  | -0.0532 | 5.1189 | 0.0000  | 0.0000 |
| 2 | 4 | 208.0443 | 0.0000   | 0.0000   | -0.3923 | 0.0000  | 1.0000 | 6.0000  | 0.3221 |
|   |   | 10.5505  | 1.0000   | 0.0000   | 1.0000  | -0.0690 | 6.2949 | 0.0000  | 0.0000 |
| 1 | 5 | 128.7959 | 56.4134  | 39.0716  | 0.0688  | -0.4463 | 1.0000 | 31.1766 | 0.4530 |
|   |   | 0.1955   | -0.3587  | 6.2148   | 1.0000  | -0.0770 | 6.6386 | 1.0000  | 0.0000 |

|    |                                                            |          |         |         |         |          |         |          |        |
|----|------------------------------------------------------------|----------|---------|---------|---------|----------|---------|----------|--------|
| 2  | 5                                                          | 128.6090 | 0.0000  | 0.0000  | -0.5555 | 0.0000   | 1.0000  | 6.0000   | 0.4721 |
|    |                                                            | 10.8735  | 1.0000  | 0.0000  | 1.0000  | -0.0242  | 9.1937  | 1.0000   | 0.0000 |
| 3  | 5                                                          | 0.0000   | 0.0000  | 0.0000  | 0.5563  | -0.4038  | 1.0000  | 49.5611  | 0.6000 |
|    |                                                            | 0.4259   | -0.4577 | 12.7569 | 1.0000  | -0.1100  | 7.1145  | 1.0000   | 0.0000 |
| 4  | 5                                                          | 0.0000   | 0.0000  | 0.0000  | 0.4438  | -0.2034  | 1.0000  | 40.3399  | 0.6000 |
|    |                                                            | 0.3296   | -0.3153 | 9.1227  | 1.0000  | -0.1805  | 5.6864  | 1.0000   | 0.0000 |
| 5  | 5                                                          | 96.1871  | 93.7006 | 68.6860 | 0.0955  | -0.4781  | 1.0000  | 17.8574  | 0.6000 |
|    |                                                            | 0.2723   | -0.2373 | 9.7875  | 1.0000  | -0.0950  | 6.4757  | 1.0000   | 0.0000 |
| 6  | 6                                                          | 109.1904 | 70.8314 | 30.0000 | 0.2765  | -0.3000  | 1.0000  | 16.0000  | 0.1583 |
|    |                                                            | 0.2804   | -0.1994 | 8.1117  | 1.0000  | -0.0675  | 8.2993  | 0.0000   | 0.0000 |
| 2  | 6                                                          | 137.1002 | 0.0000  | 0.0000  | -0.1902 | 0.0000   | 1.0000  | 6.0000   | 0.4256 |
|    |                                                            | 17.7186  | 1.0000  | 0.0000  | 1.0000  | -0.0377  | 6.4281  | 0.0000   | 0.0000 |
| 3  | 6                                                          | 191.1743 | 52.0733 | 43.3991 | -0.2584 | -0.3000  | 1.0000  | 36.0000  | 0.8764 |
|    |                                                            | 1.0248   | -0.3658 | 4.2151  | 1.0000  | -0.5004  | 4.2605  | 1.0000   | 0.0000 |
| 10 | ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2 |          |         |         |         |          |         |          |        |
| 1  | 2                                                          | 0.0464   | 1.8296  | 9.9214  | 1.0029  | -1.0000  | -1.0000 | 0.0000   |        |
| 2  | 3                                                          | 0.0403   | 1.6913  | 10.4801 | 0.8774  | -1.0000  | -1.0000 | 0.0000   |        |
| 2  | 4                                                          | 0.0524   | 1.7325  | 10.1306 | 0.9982  | -1.0000  | -1.0000 | 294.9500 |        |
| 1  | 3                                                          | 0.1028   | 1.9277  | 9.1521  | 1.3399  | 1.1104   | 1.1609  | 631.8500 |        |
| 1  | 4                                                          | 0.2070   | 1.7366  | 9.5916  | 1.2960  | 1.2008   | 1.1262  | 650.0000 |        |
| 3  | 4                                                          | 0.0491   | 1.7025  | 10.6101 | 1.3036  | 1.1276   | 1.0173  | 880.0000 |        |
| 2  | 6                                                          | 0.0470   | 1.6738  | 11.6877 | 1.1931  | -1.0000  | -1.0000 | 0.0000   |        |
| 3  | 6                                                          | 0.1263   | 1.8163  | 10.6833 | 1.6266  | 1.2052   | -1.0000 | 0.0000   |        |
| 1  | 5                                                          | 0.1408   | 1.8161  | 9.9393  | 1.7986  | 1.3021   | 1.4031  | 0.0000   |        |
| 2  | 5                                                          | 0.0895   | 1.6239  | 10.0104 | 1.4640  | -1.0000  | -1.0000 | 0.0000   |        |
| 62 | ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2          |          |         |         |         |          |         |          |        |
| 1  | 1                                                          | 1        | 74.0317 | 32.2712 | 0.9501  | 0.0000   | 0.1780  | 10.5736  | 1.0400 |
| 1  | 1                                                          | 2        | 70.6558 | 14.3658 | 5.3224  | 0.0000   | 0.0058  | 0.0000   | 1.0400 |
| 2  | 1                                                          | 2        | 76.7339 | 14.4217 | 3.3631  | 0.0000   | 0.0127  | 0.0000   | 1.0400 |
| 1  | 2                                                          | 2        | 0.0000  | 0.0000  | 6.0000  | 0.0000   | 0.0000  | 0.0000   | 1.0400 |
| 1  | 2                                                          | 1        | 0.0000  | 3.4110  | 7.7350  | 0.0000   | 0.0000  | 0.0000   | 1.0400 |
| 2  | 2                                                          | 2        | 0.0000  | 27.9213 | 5.8635  | 0.0000   | 0.0000  | 0.0000   | 1.0400 |
| 1  | 1                                                          | 3        | 65.1700 | 8.0170  | 7.5000  | 0.0000   | 0.2028  | 10.0000  | 1.0400 |
| 3  | 1                                                          | 3        | 71.7582 | 26.7070 | 6.0466  | 0.0000   | 0.2000  | 0.0000   | 1.8525 |
| 1  | 1                                                          | 4        | 65.4228 | 43.9870 | 1.5602  | 0.0000   | 0.2000  | 10.0000  | 1.8525 |
| 3  | 1                                                          | 4        | 73.7046 | 23.8131 | 3.9811  | 0.0000   | 0.2000  | 0.0000   | 1.8525 |
| 4  | 1                                                          | 4        | 65.6602 | 40.5852 | 1.8122  | 0.0000   | 0.2000  | 0.0000   | 1.8525 |
| 2  | 1                                                          | 3        | 56.4426 | 17.6020 | 5.3044  | 0.0000   | 0.9699  | 0.0000   | 1.1272 |
| 2  | 1                                                          | 4        | 71.0777 | 9.1462  | 3.4142  | 0.0000   | 0.9110  | 0.0000   | 1.0400 |
| 1  | 2                                                          | 4        | 0.0000  | 0.0019  | 6.3000  | 0.0000   | 0.0000  | 0.0000   | 1.0400 |
| 1  | 3                                                          | 1        | 72.1018 | 38.4720 | 1.3926  | 0.0000   | 0.4785  | 0.0000   | 1.2984 |
| 1  | 3                                                          | 3        | 89.9987 | 44.9806 | 0.5818  | 0.0000   | 0.7472  | 0.0000   | 1.2639 |
| 1  | 3                                                          | 4        | 70.3281 | 12.9371 | 7.5000  | 0.0000   | 0.7472  | 0.0000   | 1.2639 |
| 3  | 3                                                          | 3        | 84.2807 | 24.1938 | 2.1695  | -10.0000 | 0.7472  | 0.0000   | 1.2639 |

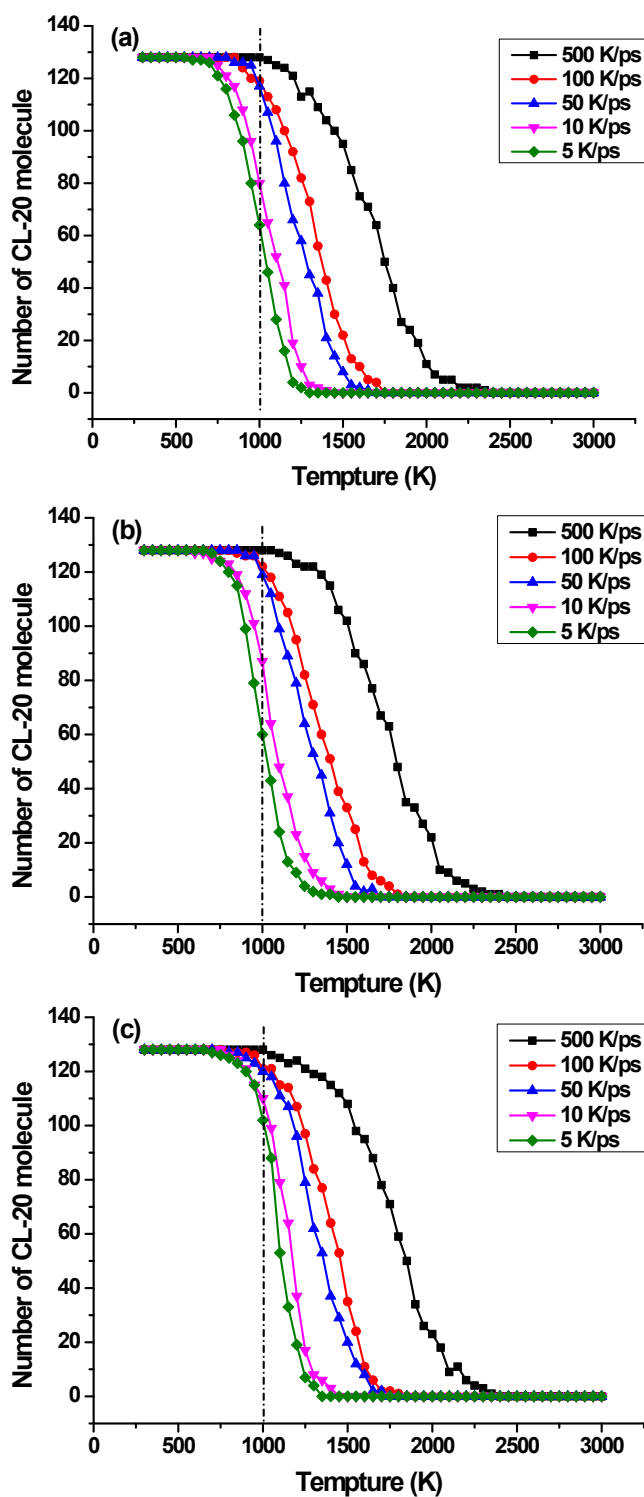
|   |   |   |         |         |        |          |         |         |        |
|---|---|---|---------|---------|--------|----------|---------|---------|--------|
| 3 | 3 | 4 | 84.2585 | 44.1039 | 0.9185 | 0.0000   | 0.7472  | 0.0000  | 1.2639 |
| 4 | 3 | 4 | 74.2312 | 25.7005 | 4.3943 | 0.0000   | 0.7472  | 0.0000  | 1.2639 |
| 1 | 3 | 2 | 89.0416 | 36.9460 | 0.4569 | 0.0000   | 2.7636  | 0.0000  | 2.0494 |
| 2 | 3 | 3 | 81.1709 | 4.2886  | 6.5904 | 0.0000   | 3.0000  | 0.0000  | 1.2618 |
| 2 | 3 | 4 | 75.9203 | 44.9675 | 0.8889 | 0.0000   | 3.0000  | 0.0000  | 1.2618 |
| 2 | 3 | 2 | 82.2020 | 12.7165 | 3.9296 | 0.0000   | 0.2765  | 0.0000  | 1.0470 |
| 1 | 4 | 1 | 68.3788 | 18.3716 | 1.8893 | 0.0000   | 2.4132  | 0.0000  | 1.3993 |
| 1 | 4 | 3 | 86.5585 | 37.6814 | 1.1611 | 0.0000   | 1.7325  | 0.0000  | 1.0440 |
| 1 | 4 | 4 | 74.4818 | 12.0954 | 7.5000 | 0.0000   | 1.7325  | 0.0000  | 1.0440 |
| 3 | 4 | 3 | 78.5850 | 44.3389 | 1.3239 | -26.2246 | 1.7325  | 40.0000 | 1.0440 |
| 3 | 4 | 4 | 77.6245 | 32.0866 | 1.8889 | -0.9193  | 1.7325  | 0.0000  | 1.0440 |
| 4 | 4 | 4 | 66.4718 | 15.9087 | 7.5000 | 0.0000   | 1.7325  | 0.0000  | 1.0440 |
| 1 | 4 | 2 | 90.0000 | 33.6636 | 1.1051 | 0.0000   | 0.2638  | 0.0000  | 1.1376 |
| 2 | 4 | 3 | 83.8493 | 44.9000 | 1.3580 | 0.0000   | 0.5355  | 0.0000  | 2.5279 |
| 2 | 4 | 4 | 78.7452 | 24.2010 | 3.7481 | 0.0000   | 0.5355  | 0.0000  | 2.5279 |
| 2 | 4 | 2 | 55.8679 | 14.2331 | 2.9225 | 0.0000   | 0.2000  | 0.0000  | 2.9932 |
| 1 | 2 | 3 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 1 | 2 | 4 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 1 | 2 | 5 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 3 | 2 | 3 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 3 | 2 | 4 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 4 | 2 | 4 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 2 | 2 | 3 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 2 | 2 | 4 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |
| 1 | 1 | 5 | 74.4180 | 33.4273 | 1.7018 | 0.1463   | 0.5000  | 0.0000  | 1.6178 |
| 1 | 5 | 1 | 79.7037 | 28.2036 | 1.7073 | 0.1463   | 0.5000  | 0.0000  | 1.6453 |
| 2 | 1 | 5 | 63.3289 | 29.4225 | 2.1326 | 0.0000   | 0.5000  | 0.0000  | 3.0000 |
| 1 | 5 | 2 | 85.9449 | 38.3109 | 1.2492 | 0.0000   | 0.5000  | 0.0000  | 1.1000 |
| 1 | 5 | 5 | 85.6645 | 40.0000 | 2.9274 | 0.1463   | 0.5000  | 0.0000  | 1.3830 |
| 2 | 5 | 2 | 83.8555 | 5.1317  | 0.4377 | 0.0000   | 0.5000  | 0.0000  | 3.0000 |
| 2 | 5 | 5 | 97.0064 | 32.1121 | 2.0242 | 0.0000   | 0.5000  | 0.0000  | 2.8568 |
| 6 | 6 | 6 | 69.3456 | 21.7361 | 1.4283 | 0.0000   | -0.2101 | 0.0000  | 1.3241 |
| 2 | 6 | 6 | 75.6168 | 21.5317 | 1.0435 | 0.0000   | 2.5179  | 0.0000  | 1.0400 |
| 2 | 6 | 2 | 78.3939 | 20.9772 | 0.8630 | 0.0000   | 2.8421  | 0.0000  | 1.0400 |
| 3 | 6 | 6 | 70.3016 | 15.4081 | 1.3267 | 0.0000   | 2.1459  | 0.0000  | 1.0400 |
| 2 | 6 | 3 | 73.8232 | 16.6592 | 3.7425 | 0.0000   | 0.8613  | 0.0000  | 1.0400 |
| 3 | 6 | 3 | 90.0344 | 7.7656  | 1.7264 | 0.0000   | 0.7689  | 0.0000  | 1.0400 |
| 6 | 3 | 6 | 22.1715 | 3.6615  | 0.3160 | 0.0000   | 4.1125  | 0.0000  | 1.0400 |
| 2 | 3 | 6 | 83.7634 | 5.6693  | 2.7780 | 0.0000   | 1.6982  | 0.0000  | 1.0400 |
| 3 | 3 | 6 | 73.4663 | 25.0761 | 0.9143 | 0.0000   | 2.2466  | 0.0000  | 1.0400 |
| 2 | 2 | 6 | 0.0000  | 47.1300 | 6.0000 | 0.0000   | 1.6371  | 0.0000  | 1.0400 |
| 6 | 2 | 6 | 0.0000  | 31.5209 | 6.0000 | 0.0000   | 1.6371  | 0.0000  | 1.0400 |
| 3 | 2 | 6 | 0.0000  | 31.0427 | 4.5625 | 0.0000   | 1.6371  | 0.0000  | 1.0400 |
| 2 | 2 | 5 | 0.0000  | 0.0019  | 6.0000 | 0.0000   | 0.0000  | 0.0000  | 1.0400 |

```

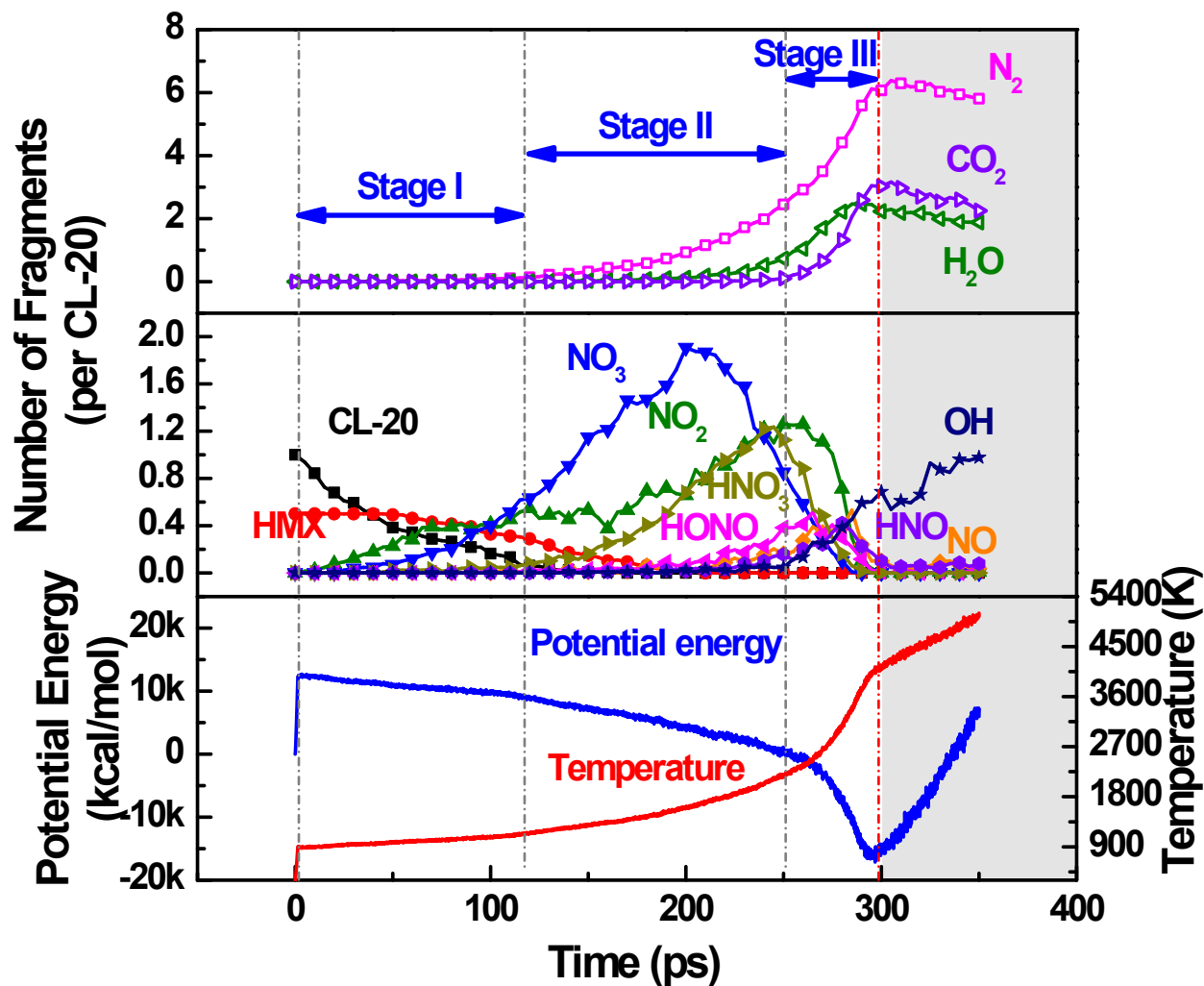
31      ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  1  1  1  0.0000  48.4194  0.3163 -8.6506 -1.7255  0.0000  0.0000
  1  1  1  2  0.0000  63.3484  0.2210 -8.8401 -1.8081  0.0000  0.0000
  2  1  1  2  0.0000  45.2741  0.4171 -6.9800 -1.2359  0.0000  0.0000
  0  1  2  0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
  0  2  2  0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
  0  1  3  0  1.7254  86.0769  0.3440 -4.2330 -2.0000  0.0000  0.0000
  0  2  3  0  0.0000  0.1000  0.0200 -2.5415  0.0000  0.0000  0.0000
  0  3  3  0  1.2314 116.5137  0.5599 -4.1412  0.0000  0.0000  0.0000
  0  1  4  0 -1.3258 149.8644  0.4790 -7.1541 -2.0000  0.0000  0.0000
  0  2  4  0  0.0000  0.1000  0.0200 -2.5415  0.0000  0.0000  0.0000
  0  3  4  0  1.3168  57.0732  0.2679 -4.1516 -2.0000  0.0000  0.0000
  0  4  4  0  2.0000  75.3685 -0.7852 -9.0000 -2.0000  0.0000  0.0000
  0  1  1  0  0.0930  18.6070 -1.3191 -9.0000 -1.0000  0.0000  0.0000
  4  1  4  4 -2.0000  20.6655 -1.5000 -9.0000 -2.0000  0.0000  0.0000
  0  1  5  0  4.0885  78.7058  0.1174 -2.1639  0.0000  0.0000  0.0000
  0  5  5  0 -0.0170 -56.0786  0.6132 -2.2092  0.0000  0.0000  0.0000
  0  2  5  0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
  0  6  6  0  0.0000  0.0000  0.1200 -2.4426  0.0000  0.0000  0.0000
  0  2  6  0  0.0000  0.0000  0.1200 -2.4847  0.0000  0.0000  0.0000
  0  3  6  0  0.0000  0.0000  0.1200 -2.4703  0.0000  0.0000  0.0000
  1  1  3  3  1.2707  21.6200  1.5000 -9.0000 -2.0000  0.0000  0.0000
  1  3  3  1 -1.8804  79.9255 -1.5000 -4.1940 -2.0000  0.0000  0.0000
  3  1  3  3 -2.0000  22.5092  1.5000 -8.9500 -2.0000  0.0000  0.0000
  1  4  4  3  0.1040  70.1152  0.5284 -3.5026 -2.0000  0.0000  0.0000
  1  1  3  4  1.2181 119.6186 -1.5000 -7.0635 -2.0000  0.0000  0.0000
  2  1  3  4 -2.0000 156.6604  1.1004 -7.3729 -2.0000  0.0000  0.0000
  1  3  4  3  2.0000  96.6281 -1.5000 -3.8076 -2.0000  0.0000  0.0000
  1  1  4  2 -2.0000 147.2445 -1.5000 -7.0142 -2.0000  0.0000  0.0000
  1  1  4  3 -2.0000  47.8326 -1.5000 -9.0000 -2.0000  0.0000  0.0000
  2  3  4  3 -0.2997 152.9040 -1.5000 -4.4564 -2.0000  0.0000  0.0000
  2  4  4  3  0.1040  70.1152  0.5284 -3.5026 -2.0000  0.0000  0.0000
9      ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
  3  2  3  2.1845 -2.3549  3.0582 19.1627
  3  2  4  1.6658 -3.8907  3.0582 19.1627
  4  2  3  1.8738 -3.5421  3.0582 19.1627
  4  2  4  1.8075 -4.1846  3.0582 19.1627
  3  2  5  2.6644 -3.0000  3.0000  3.0000
  4  2  5  4.0476 -3.0000  3.0000  3.0000
  5  2  3  2.1126 -4.5790  3.0000  3.0000
  5  2  4  2.2066 -5.7038  3.0000  3.0000
  5  2  5  1.9461 -4.0000  3.0000  3.0000

```

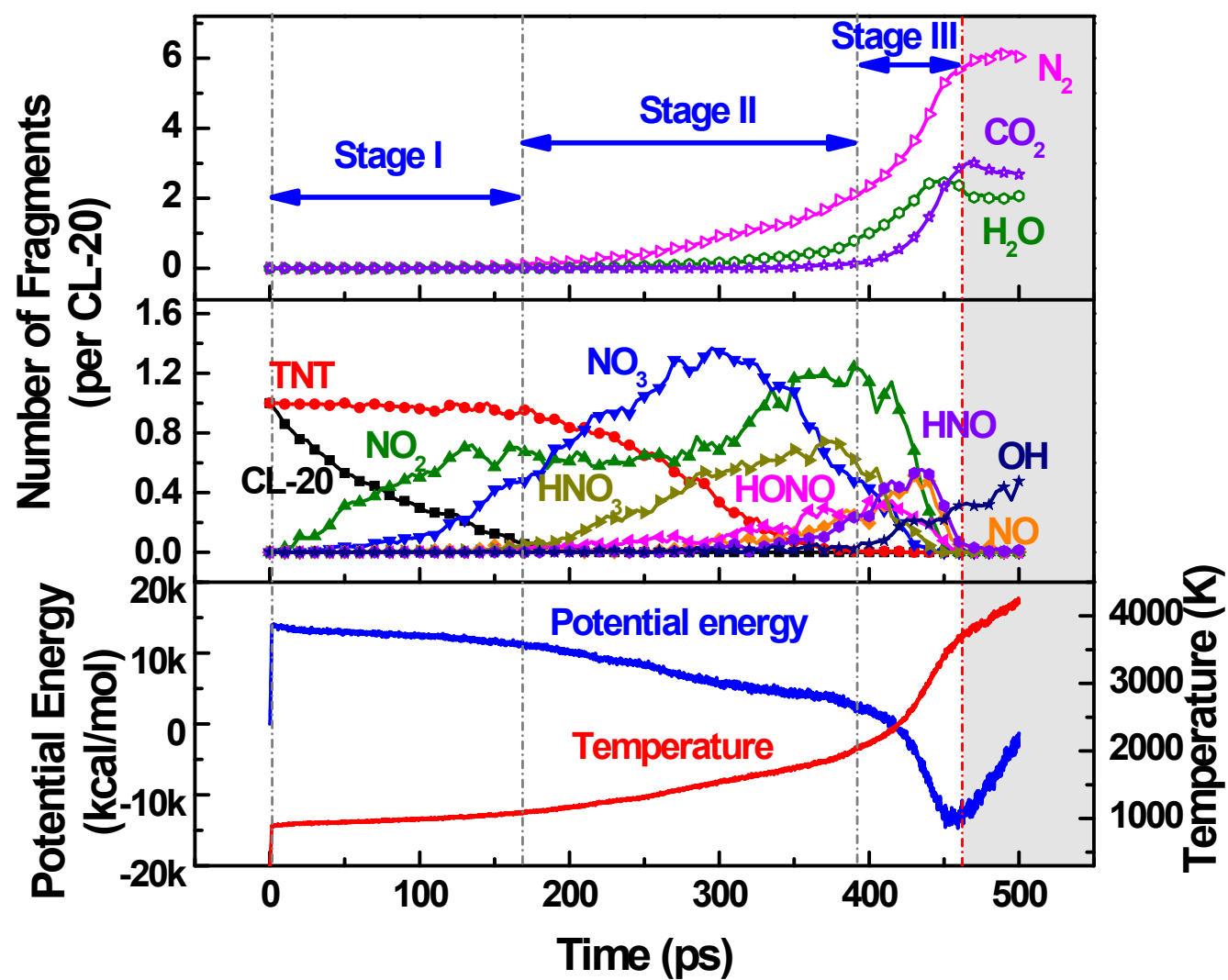
**S2. Evolutions of CL-20 molecules in thermolysis of (a)  $\beta$ -CL-20, (b) CL-20/HMX, and (c) CL-20/TNT with varied heating rates from 5 K/ps to 500 K/ps obtained by ReaxFF MD simulations in NVT ensemble.**



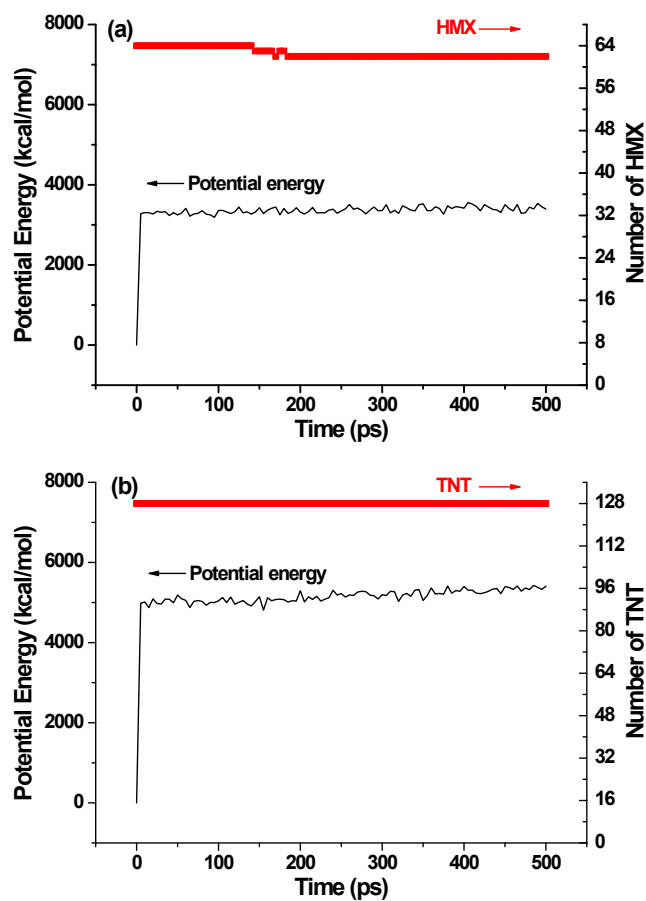
S3. Evolutions of temperature, relative potential energy, main intermediates and final products of CL-20/HMX thermolysis obtained by ReaxFF MD simulations in NVE ensemble.



S4. Evolutions of temperature, relative potential energy, main intermediates and final products of CL-20/TNT thermolysis obtained by ReaxFF MD simulations in NVE ensemble.



**S5. Evolutions of relative potential energy, HMX and TNT molecules in adiabatic thermolysis of pure HMX and TNT for 500 ps obtained in NVE ReaxFF MD simulations, (a) pure HMX and (b) TNT.**



**S6. Evolution of varied stable products in thermolysis of (a)  $\beta$ -CL-20, (b) CL-20/HMX, and (c) CL-20/TNT at 3000 K obtained by ReaxFF MD simulations in NVT ensemble.**

