Supplemental material

**Carbon Cluster Formation during Thermal Decomposition of HMX and TATB High Explosives from ReaxFF Reactive Molecular Dynamics Simulations**

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*Materials & Process Simulation Center, California Institute of Technology, Pasadena, CA 91125
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Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

The complete set of ReaxFF reactive force field parameters used in this paper organized in a form appropriate for input to the ReaxFF reactive dynamics program [Ref. 1].

**Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN)**

```plaintext
39       ! Number of general parameters
50.0000 !Overcoordination parameter
9.4514 !Overcoordination parameter
30.0000 !Valency angle conjugation parameter
216.4305 !Triple bond stabilisation parameter
12.4838 !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
-10.4637 !Triple bond stabilization energy
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
2.8793 !Not used
33.8667 !Valency undercoordination
3.5895 !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
```

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*
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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)
5.2216 !Valency angle conjugation parameter
3.4021 !Overcoordination parameter
38.5241 !Overcoordination parameter
2.1533 !Valency/lone pair parameter
0.5000 !Not used
20.0000 !Not used
5.0000 !Molecular energy (not used)
0.0000 !Molecular energy (not used)
6.5560 !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;nu.
cov r3;Elp;Heat inc.;nu.;nu.;nu.;nu.
ov/un;val1;nu.;val3,vval4

C    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712
    1.2385   4.0000
    9.4606   2.1346   4.0000  31.0823  79.5548   5.7254
    6.9235   0.0000
    1.2104   0.0000 183.7012   5.7419  33.3951  11.9957
    0.8563   0.0000
-2.8983   2.5000  1.0564   4.0000  2.9663   0.0000
0.0000   0.0000
H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910
    -0.1000   1.0000
    9.3858   5.0013   1.0000   0.0000 121.1250   3.8446
   10.0839   1.0000
   -0.1000   0.0000  58.4228   3.8461   3.2540   1.0000
    1.0698   0.0000
-15.7683   2.1504   1.0338   1.0000   2.8793   0.0000
0.0000   0.0000
O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712
    1.1139   6.0000
    10.2186   7.7719   4.0000  29.5271 116.0768   8.5000
    7.1412   2.0000
    0.9909  14.9473  69.2812   9.1371   1.6258   0.1863
    0.9745   0.0000
-3.5965   2.5000  1.0493   4.0000  2.9225   0.0000
0.0000   0.0000
N    1.2450   3.0000  14.0000  1.9951  0.1088   1.0512
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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  10.1311  1.0029 -1.0000 -1.0000
2  3   0.0375   1.7275  10.8037  0.8813 -1.0000 -1.0000
2  4   0.0509   1.7672  10.4261  0.9990 -1.0000 -1.0000
1  3   0.1036   1.8869   9.5668  1.3590  1.1099  1.1534
1  4   0.1971   1.7356  10.0734  1.2754  1.2113  1.1172
3  4   0.0535   1.6709  10.8180  1.2968  1.1416  1.0167
2  6   0.0470   1.6738  11.6877  1.1931 -1.0000 -1.0000
3  6   0.1263   1.8163  10.6833  1.6266  1.2052 -1.0000
1  5   0.1408   1.8161   9.9393  1.7986  1.3021  1.4031
2  5   0.0895   1.6239  10.0104  1.4640 -1.0000 -1.0000
62    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
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
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1  2   0.0000  0.0000  6.0000  0.0000  0.0000  0.0000
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1.0400
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1  1   4   65.8892  45.0000  1.6598  0.0000  0.2000  10.0000
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1.8525
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<p>| 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 |
| 0.0000 | 0.0000 |
| 1 | 1 | 1 | 2 | 0.0000 | 63.3484 | 0.2210 | -8.8401 | -1.8081 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 2 | 1 | 1 | 2 | 0.0000 | 45.2741 | 0.4171 | -6.9800 | -1.2359 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 1 | 2 | 0 | 0.0000 | 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 | 0.0000 |
| 0 | 1 | 3 | 0 | -0.0002 | 85.8794 | 0.3236 | -3.8134 | -2.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 2 | 3 | 0 | 0.0000 | 0.1000 | 0.0200 | -2.5415 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 3 | 3 | 0 | -0.9667 | 116.4743 | 0.0002 | -4.9422 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 1 | 4 | 0 | -0.0069 | 150.0000 | 0.4891 | -7.4921 | -2.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 2 | 4 | 0 | 0.0000 | 0.1000 | 0.0200 | -2.5415 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 3 | 4 | 0 | 1.6745 | 56.6301 | -0.0008 | -4.5064 | -2.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 4 | 4 | 0 | 1.1253 | 75.3447 | 0.0080 | -9.0000 | -2.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 1 | 1 | 0 | 0.0930 | 18.5962 | 0.0002 | -9.0000 | -1.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 4 | 4 | 4 | -2.0000 | 20.8732 | -1.5000 | -9.0000 | -2.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 1 | 5 | 0 | 4.0885 | 78.7058 | 0.1174 | -2.1639 | 0.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
| 0 | 5 | 5 | 0 | -0.0170 | -56.0786 | 0.6132 | -2.2092 | 0.0000 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 |
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| 4 2 4 1.6953 -4.0695 3.0000 3.0000 |
| 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 |