

Supplemental material

Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field

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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

Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN) added
Pt/N parameters

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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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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
8      ! 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;vall;n.u.;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
1.1911   5.0000

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	9.9303	7.8431	4.0000	32.4758	100.0000	6.7768	
6.8035	2.0000						
	1.0636	0.1045	128.0119	2.1604	2.9464	2.5181	
0.9745	0.0000						
	-4.0959	2.0047	1.0183	4.0000	2.8793	0.0000	
0.0000	0.0000						
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	0.0000	
0.0000	0.0000						
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						
Pt	1.9016	2.0000	195.0800	2.0278	0.2801	0.7409	-
1.0000	2.0000						
	12.5155	6.0083	2.0000	0.0000	0.0000	2.3622	
6.0000	0.0000						
	-1.0000	0.0000	143.1770	13.7107	6.9133	0.2609	
0.8563	0.0000						
	-6.9662	1.8780	1.0338	5.0000	2.5791	0.0000	
0.0000	0.0000						
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						
23	! 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	164.0476	117.4881	72.1261	-0.6031	-0.1795	1.0000
14.9755		0.5413					
		1.2626	-0.3063	7.0000	1.0000	-0.1588	4.5000
0.0000		0.0000					
3	3	110.4748	155.6441	40.0000	0.1150	-0.1054	1.0000
28.5221		0.2000					
		0.9590	-0.2635	8.5715	1.0000	-0.1007	6.8548
1.0000		0.0000					
1	4	130.7147	175.2276	97.2523	-0.0368	-0.4942	1.0000
26.7545		0.5133					
		0.3296	-0.3653	7.0000	1.0000	-0.1171	5.1025
1.0000		0.0000					
3	4	85.4950	114.0081	70.1453	0.5778	-0.1070	1.0000
16.6611		0.2339					
		0.3474	-0.1948	8.3762	1.0000	-0.1089	5.8148
1.0000		0.0000					
4	4	157.7518	67.1322	160.9732	-0.5869	-0.1824	1.0000
12.0000		0.7136					
		0.8204	-0.1657	10.6490	1.0000	-0.0967	4.5976
1.0000		0.0000					
2	3	224.3076	0.0000	0.0000	-0.6280	0.0000	1.0000
6.0000		1.0000					
		5.0050	1.0000	0.0000	1.0000	-0.0512	5.1982
0.0000		0.0000					
2	4	212.1772	0.0000	0.0000	-0.3585	0.0000	1.0000
6.0000		0.3316					
		10.4316	1.0000	0.0000	1.0000	-0.0658	6.4545
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					
1	7	139.5088	0.0000	0.0000	0.1815	-0.2000	1.0000
16.0000		0.4640					
		0.6661	-0.2000	15.0000	1.0000	-0.1421	5.3217
1.0000		0.0000					
2	7	169.4568	0.0000	0.0000	-0.2395	0.0000	0.0000
6.0000		0.3235					
		31.4287	1.0000	0.0000	1.0000	-0.0875	9.6458
0.0000		0.0000					
3	7	153.1449	0.0000	0.0000	-0.2518	-0.2000	1.0000
16.0000		0.1000					
		2.1627	-0.2000	15.0000	1.0000	-0.0854	6.3353
1.0000		0.0000					
4	7	168.0384	0.0000	0.0000	0.2993	-0.2000	1.0000
16.0000		0.4999					
		0.4102	-0.2000	15.0000	1.0000	-0.1523	5.0000
1.0000		0.0000					
7	7	109.6325	0.0000	0.0000	-0.1353	-0.2000	0.0000
16.0000		0.3122					
		0.2288	-0.2000	15.0000	1.0000	-0.1065	5.2199
0.0000		0.0000					
14		! 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	
1	7		0.1028	1.6085	13.9954	1.6948	-1.0000	-1.0000	
2	7		0.0290	1.7550	11.8053	1.5947	-1.0000	-1.0000	
3	7		0.1000	1.9704	11.2422	1.5030	-1.0000	-1.0000	
4	7		0.1240	2.0102	11.5503	1.5180	-1.0000	-1.0000	
73			! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2						
1.0400	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
1.8525	1	1	3	65.3104	6.3897	7.5000	0.0000	0.2000	10.0000
1.8525	3	1	3	71.9855	28.5708	6.4252	0.0000	0.2000	0.0000
1.8525	1	1	4	65.8892	45.0000	1.6598	0.0000	0.2000	10.0000
1.8525	3	1	4	73.1057	25.8227	4.2145	0.0000	0.2000	0.0000
1.8525	4	1	4	65.8759	40.9838	2.4369	0.0000	0.2000	0.0000
1.0400	2	1	3	56.3039	17.3681	5.3095	0.0000	0.9110	0.0000
1.0400	2	1	4	71.5505	11.1820	3.7129	0.0000	0.9110	0.0000
1.0400	1	2	4	0.0000	0.0019	6.3000	0.0000	0.0000	0.0000
1.2639	1	3	1	72.3642	37.8942	1.1566	0.0000	0.7472	0.0000
1.2639	1	3	3	90.0000	45.0000	0.5719	0.0000	0.7472	0.0000
1.2639	1	3	4	70.4313	14.4055	7.1593	0.0000	0.7472	0.0000
1.2639	3	3	3	83.8833	23.3345	2.3433	-10.0000	0.7472	0.0000

7	2	7	0.0000	10.2212	1.2355	0.0000	0.0968	0.0000
1.1000								
2	7	7	88.3592	8.1888	9.1917	0.0000	0.7886	0.0000
1.7277								
4	4	7	84.2429	31.9217	10.0000	0.0000	0.0223	0.0000
1.5344								
4	7	4	87.0000	35.6895	2.5642	0.0000	0.3767	0.0000
1.1220								
7	4	7	92.4683	15.3046	10.0000	0.0000	0.6567	0.0000
2.5208								
4	7	7	86.2048	35.0184	2.4808	0.0000	0.1176	0.0000
1.8035								
2	4	7	69.3018	20.4000	1.0200	0.0000	1.0200	0.0000
1.9600								
2	7	4	49.8181	12.1623	3.8229	0.5000	0.5092	0.0000
1.5000								
4	2	7	0.0000	25.0000	2.0000	0.0000	1.0000	0.0000
1.2500								

23 ! 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	-0.0002	85.8794	0.3236	-3.8134	-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	-0.9667	116.4743	0.0002	-4.9422	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	2	4	0	0.0000	0.1000	0.0200	-2.5415	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	4	4	0	1.1253	75.3447	0.0080	-9.0000	-2.0000
0.0000			0.0000					
0	1	1	0	0.0930	18.5962	0.0002	-9.0000	-1.0000
0.0000			0.0000					

4	1	4	4	-2.0000	20.8732	-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	-0.0002	21.5452	0.1727	-9.0000	-2.0000
0.0000		0.0000						
1	3	3	1	0.0002	79.3777	-1.5000	-5.2139	-2.0000
0.0000		0.0000						
3	1	3	3	-1.3476	22.4932	1.5000	-9.0000	-2.0000
0.0000		0.0000						
9		! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1						
3	2	3		2.0000	-5.0000	3.0000	3.0000	
3	2	4		1.7753	-5.0000	3.0000	3.0000	
4	2	3		1.3884	-5.0000	3.0000	3.0000	
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	