

ReaxFF Force Field Parameter File

Supporting information for the manuscript "A ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation" by Kimberly Chenoweth, Adri C.T. van Duin and William A. Goddard, III

Reactive MD-force field: c/h/o combustion force field November 2006

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39      ! Number of general parameters
50.0000 !p(boc1)
 9.5469 !p(boc2)
26.5405 !p(coa2)
 1.5105 !p(trip4)
 6.6630 !p(trip3)
 0.0000 !kc2
 1.0588 !p(ovun6)
 4.6000 !p(trip2)
12.1176 !p(ovun7)
13.3056 !p(ovun8)
-70.1292 !p(trip1)
 0.0000 !Lower Taper-radius (swa)
10.0000 !Upper Taper-radius (swb)
 0.0000 !not used
33.8667 !p(val7)
 6.0891 !p(lp1)
 1.0563 !p(val9)
 2.0384 !p(val10)
 6.1431 !not used
 6.9290 !p(pen2)
 0.3989 !p(pen3)
 3.9954 !p(pen4)
 0.0000 !not used
 5.7796 !p(tor2)
10.0000 !p(tor3)
 1.9487 !p(tor4)
 0.0000 !not used
 2.1645 !p(cot2)
 1.5591 !p(vdW1)
 0.1000 !Cutoff for bond order*100 (cutoff)
 2.1365 !p(coa4)
 0.6991 !p(ovun4)
50.0000 !p(ovun3)
 1.8512 !p(val8)
 0.0000 !not used
 0.0000 !not used
 0.0000 !not used
 0.0000 !not used
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2.6962 !p(coa3)
3 ! Nr of atoms; atomID;ro(sigma); Val;atom mass;Rvdw;Dij;gamma;ro
(pi);Val(e)
    alfa;gamma(w);Val(angle);p(ovun5);n.u.;chiEEM;etaEEM;n.u.
    ro(pipi);p(lp2);Heat increment;p(boc4);p(boc3);p
(boc5),n.u.;n.u.
    p(ovun2);p(val3);n.u.;Val(boc);p(val5);n.u.;n.u.;n.u.
C  1.3825  4.0000  12.0000  1.9133  0.1853  0.9000  1.1359  4.0000
   9.7602  2.1346  4.0000  33.2433  79.5548  5.8678  7.0000  0.0000
   1.2104  0.0000  199.0303  8.6991  34.7289  13.3894  0.8563  0.0000
  -2.8983  2.5000  1.0564  4.0000  2.9663  0.0000  0.0000  0.0000
H  0.7853  1.0000  1.0080  1.5904  0.0419  1.0206  -0.1000  1.0000
   9.3557  5.0518  1.0000  0.0000  121.1250  5.3200  7.4366  1.0000
  -0.1000  0.0000  62.4879  1.9771  3.3517  0.7571  1.0698  0.0000
 -15.7683  2.1488  1.0338  1.0000  2.8793  0.0000  0.0000  0.0000
O  1.2477  2.0000  15.9990  1.9236  0.0904  1.0503  1.0863  6.0000
  10.2127  7.7719  4.0000  36.9573  116.0768  8.5000  8.9989  2.0000
   0.9088  1.0003  60.8726  20.4140  3.3754  0.2702  0.9745  0.0000
  -3.6141  2.7025  1.0493  4.0000  2.9225  0.0000  0.0000  0.0000
6 ! Nr of bonds; at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(bo5);
13corr;n.u.;p(bo6),p(ovun1)
    p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)
1 1 156.5953 100.0397 80.0000 -0.8157 -0.4591 1.0000 37.7369
0.4235
   0.4527 -0.1000 9.2605 1.0000 -0.0750 6.8316 1.0000
0.0000
1 2 170.2316 0.0000 0.0000 -0.5931 0.0000 1.0000 6.0000
0.7140
   5.2267 1.0000 0.0000 1.0000 -0.0500 6.8315 0.0000
0.0000
2 2 156.0973 0.0000 0.0000 -0.1377 0.0000 1.0000 6.0000
0.8240
   2.9907 1.0000 0.0000 1.0000 -0.0593 4.8358 0.0000
0.0000
1 3 160.4802 105.1693 23.3059 -0.3873 -0.1613 1.0000 10.8851
1.0000
   0.5341 -0.3174 7.0303 1.0000 -0.1463 5.2913 0.0000
0.0000
3 3 60.1463 176.6202 51.1430 -0.2802 -0.1244 1.0000 29.6439
0.9114
   0.2441 -0.1239 7.6487 1.0000 -0.1302 6.2919 1.0000
0.0000
2 3 180.4373 0.0000 0.0000 -0.8074 0.0000 1.0000 6.0000
0.5514
   1.2490 1.0000 0.0000 1.0000 -0.0657 5.0451 0.0000
0.0000

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3      ! Nr of off-diagonal terms. at1;at2;Dij;RvdW;alfa;ro(sigma);ro
(pi);ro(pipi)
1 2  0.1219  1.4000  9.8442  1.1203 -1.0000 -1.0000
2 3  0.0344  1.6800 10.3247  0.9013 -1.0000 -1.0000
1 3  0.1131  1.8523  9.8442  1.2775  1.1342  1.0621
18     ! Nr of angles. at1;at2;at3;Thetao,o;p(val1);p(val2);p(coa1);p
(val7);p(pen1);p(val4)
1 1 1 67.2326 22.0695  1.6286  0.0000  1.7959 15.4141  1.8089
1 1 2 65.2527 14.3185  6.2977  0.0000  0.5645  0.0000  1.1530
2 1 2 70.0840 25.3540  3.4508  0.0000  0.0050  0.0000  3.0000
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 49.5561  7.3771  4.9568  0.0000  0.7533 15.9906  1.0010
3 1 3 77.1171 39.8746  2.5403 -24.3902  1.7740 -42.9758  2.1240
2 1 3 65.0000 14.2057  4.8649  0.0000  0.3504  0.0000  1.7185
1 3 1 74.3994 44.7500  0.7982  0.0000  3.0000  0.0000  1.0528
1 3 3 77.9854 36.6201  2.0201  0.0000  0.7434 67.0264  3.0000
3 3 3 80.7324 30.4554  0.9953  0.0000  1.6310 50.0000  1.0783
1 3 2 71.5018 21.7062  0.4735  0.0000  0.5186  0.0000  1.1793
2 3 3 84.9468 23.3540  1.5057  0.0000  2.6374  0.0000  1.3023
2 3 2 77.0645 10.4737  1.2895  0.0000  0.9924  0.0000  1.1043
1 2 3  0.0000 25.0000  3.0000  0.0000  1.0000  0.0000  1.0400
3 2 3  0.0000  0.0148  6.0000  0.0000  0.0000  0.0000  1.0400
2 2 3  0.0000  9.7025  6.0000  0.0000  0.0000  0.0000  1.0400
21     ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n.u;n.u.
1 1 1 1 -0.2500 11.5822  0.1879 -4.7057 -2.2047  0.0000  0.0000
1 1 1 2 -0.2500 31.2596  0.1709 -4.6391 -1.9002  0.0000  0.0000
2 1 1 2 -0.1770 30.0252  0.4340 -5.0019 -2.0697  0.0000  0.0000
1 1 1 3 -0.7098 22.2951  0.0060 -2.5000 -2.1688  0.0000  0.0000
2 1 1 3 -0.3568 22.6472  0.6045 -4.0088 -1.0000  0.0000  0.0000
3 1 1 3 -0.0528  6.8150  0.7498 -5.0913 -1.0000  0.0000  0.0000
1 1 3 1  2.0007 25.5641 -0.0608 -2.6456 -1.1766  0.0000  0.0000
1 1 3 2 -1.1953 42.1545 -1.0000 -8.0821 -1.0000  0.0000  0.0000
2 1 3 1 -0.9284 34.3952  0.7285 -2.5440 -2.4641  0.0000  0.0000
2 1 3 2 -2.5000 79.6980  1.0000 -3.5697 -2.7501  0.0000  0.0000
1 1 3 3 -0.0179  5.0603 -0.1894 -2.5000 -2.0399  0.0000  0.0000
2 1 3 3 -0.5583 80.0000  1.0000 -4.4000 -3.0000  0.0000  0.0000
3 1 3 1 -2.5000 76.0427 -0.0141 -3.7586 -2.9000  0.0000  0.0000
3 1 3 2  0.0345 78.9586 -0.6810 -4.1777 -3.0000  0.0000  0.0000
3 1 3 3 -2.5000 66.3525  0.3986 -3.0293 -3.0000  0.0000  0.0000
1 3 3 1  2.5000 -0.5332  1.0000 -3.5096 -2.9000  0.0000  0.0000
1 3 3 2 -2.5000  3.3219  0.7180 -5.2021 -2.9330  0.0000  0.0000
2 3 3 2  2.2500 -6.2288  1.0000 -2.6189 -1.0000  0.0000  0.0000
1 3 3 3  0.0531 -17.3983  1.0000 -2.5000 -2.1584  0.0000  0.0000
2 3 3 3  0.4723 -12.4144 -1.0000 -2.5000 -1.0000  0.0000  0.0000

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3	3	3	3	-2.5000	-25.0000	1.0000	-2.5000	-1.0000	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	2	3	0	0.0000	0.1000	0.0200	-2.5415	0.0000	0.0000	0.0000
0	1	1	0	0.0000	50.0000	0.3000	-4.0000	-2.0000	0.0000	0.0000
0	3	3	0	0.5511	25.4150	1.1330	-5.1903	-1.0000	0.0000	0.0000
1	! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)									
3	2	3		1.9682	-4.4628	1.7976	3.0000			