

Reactive MD-force field: C\H\Na by E. Hjertenæs, A.Q. Nguyen and H. Koch Phys. Chem. Chem. Phys., (2016), DOI:10.1039/c6cp06774c.

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39      ! Number of general parameters
50.0000 !Overcoordination parameter
 9.5469 !Overcoordination parameter
26.5405 !Valency angle conjugation parameter
 1.7224 !Triple bond stabilisation parameter
 6.8702 !Triple bond stabilisation parameter
60.4850 !C2-correction
 1.0588 !Undercoordination parameter
 4.6000 !Triple bond stabilisation parameter
12.1176 !Undercoordination parameter
13.3056 !Undercoordination parameter
-70.5044 !Triple bond stabilization energy
 0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
 2.8793 !Fe dimer correction
33.8667 !Valency undercoordination
 6.0891 !Valency angle/lone pair parameter
 1.0563 !Valency angle
 2.0384 !Valency angle parameter
 6.1431 !Fe dimer correction
 6.9290 !Double bond/angle parameter
 0.3989 !Double bond/angle parameter: overcoord
 3.9954 !Double bond/angle parameter: overcoord
-2.4837 !Fe dimer correction
 5.7796 !Torsion/BO parameter
10.0000 !Torsion overcoordination
 1.9487 !Torsion overcoordination
-1.2327 !Reserved
 2.1645 !Conjugation
 1.5591 !vdWaals shielding
 0.0010 !Cutoff for bond order (*100)
 2.1365 !Valency angle conjugation parameter
 0.6991 !Overcoordination parameter
50.0000 !Overcoordination parameter
 1.8512 !Valency/lone pair parameter
 0.5000 !ACKS2 softness parameter
20.0000 !Scale factor (d) in dispersion (LJ)
 5.0000 !Reserved
 0.0000 !1: disable undecoord term in val angle
 2.6962 !Valency angle conjugation parameter
3      ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
      alfa;gammavdW;valency;Eunder;Eover(n.u.);chiEEM;etaEEM;hbond
      cov r3;Elp;Heat inc.;bol131;bol132;bol133;n.u.;n.u.
      ov/un;vall1;n.u.;val3;vval4;rcore2;ecore2;acore2
C      1.3817  4.0000 12.0000  1.8903  0.1838  0.6544  1.1341  4.0000
      9.7559  2.1346  4.0000 34.9350 79.5548  5.4088  6.0000  0.0000
      1.2114  0.0000 202.2908  8.9539 34.9289 13.5366  0.8563  0.0000
      -2.8983 2.5000  1.0564  4.0000  2.9663  1.4000  0.0100 13.0000
H      0.8930  1.0000  1.0080  1.3550  0.0930  0.8203 -0.1000  1.0000
      8.2230 33.2894  1.0000  0.0000 121.1250  3.7248  9.6093  1.0000
      -0.1000 0.0000 61.6606  3.0408  2.4197  0.0003  1.0698  0.0000
      -19.4571 4.2733  1.0338  1.0000  2.8793  1.0000  0.2000 12.0000
Na     1.8000  1.0000 22.9898  2.8270  0.1872  1.1523 -1.0000  1.0000
      10.0000 2.5000  1.0000  0.0000  0.0000  1.9533  8.2770  0.0000
      -1.0000 0.0000 23.0445 100.0000  1.0000  0.0000  0.8563  0.0000
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-2.5000   3.9900   1.0338   8.0000   2.5791   1.1829   0.1998  13.0486
6   ! Nr of bonds; De(sigma);De(pi);De(pipi);pbe1;pbo5;13corr;pbo6;p(ovun1)
      pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr;n.u.
1  1  158.2004  99.1897  78.0000  -0.7738  -0.4550  1.0000  37.6117  0.4147
      0.4590  -0.1000  9.1628  1.0000  -0.0777  6.7268  1.0000  0.0000
1  2  169.4760  0.0000  0.0000  -0.6083  0.0000  1.0000  6.0000  0.7652
      5.2290  1.0000  0.0000  1.0000  -0.0500  6.9136  0.0000  0.0000
1  3  42.0386  0.0000  0.0000  0.7185  0.0000  0.0000  0.0000  0.1053
      7.2109  -0.6159  2.2890  1.0000  -0.1578  4.0000  0.0002  0.0000
2  2  153.3934  0.0000  0.0000  -0.4600  0.0000  1.0000  6.0000  0.7300
      6.2500  1.0000  0.0000  1.0000  -0.0790  6.0552  0.0000  0.0000
2  3  87.6869  0.0000  0.0000  -0.7276  -0.3000  0.0000  36.0000  0.2155
      1.1502  -0.3500  25.0000  1.0000  -0.2000  4.8137  0.0000  0.0000
3  3  60.0000  0.0000  0.0000  -0.3458  0.3000  0.0000  25.0000  0.2477
      2.4578  -0.4000  12.0000  1.0000  -0.0513  4.5180  0.0000  0.0000
3   ! Nr of off-diagonal terms; Ediss;Ro;alpha;rsigma;rpi;rpi2
1  2  0.1239  1.4004  9.8467  1.1210  -1.0000  -1.0000
1  3  0.3002  1.9234  10.8827  1.3909  0.6807  -1.0000
2  3  0.2944  1.5332  12.0465  1.7037  -1.0000  -1.0000
6   ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
1  1  1  59.0573  30.7029  0.7606  0.0000  0.7180  6.2933  1.1244
1  1  2  65.7758  14.5234  6.2481  0.0000  0.5665  0.0000  1.6255
1  2  1  0.0000  3.4110  7.7350  0.0000  0.0000  0.0000  1.0400
2  1  2  70.2607  25.2202  3.7312  0.0000  0.0050  0.0000  2.7500
1  2  2  0.0000  0.0000  6.0000  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
4   ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
1  1  1  1  -0.2500  34.7453  0.0288  -6.3507  -1.6000  0.0000  0.0000
1  1  1  2  -0.2500  29.2131  0.2945  -4.9581  -2.1802  0.0000  0.0000
2  1  1  2  -0.2500  31.2081  0.4539  -4.8923  -2.2677  0.0000  0.0000
0  2  2  0  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
0   ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1

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