

Reactive MD-force field: Pt/O (D. Fantauzzi 2014)

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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
-51.3259 !Triple bond stabilization energy
0.0000  !Lower Taper-radius
10.0000 !Upper Taper-radius
2.8793  !Not used
33.8667 !Valency undercoordination
6.0891  !Valency angle/lone pair parameter
1.0563  !Valency angle
2.0384  !Valency angle parameter
6.1431  !Not used
6.9290  !Double bond/angle parameter
0.3989  !Double bond/angle parameter: overcoord
3.9954  !Double bond/angle parameter: overcoord
-2.4837 !Not used
5.7796  !Torsion/BO parameter
10.0000 !Torsion overcoordination
1.9487  !Torsion overcoordination
-1.2327 !Conjugation 0 (not used)
2.1645  !Conjugation
1.5591  !vdWaals shielding
0.1000  !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  !Not used
20.0000 !Not used
5.0000  !Molecular energy (not used)
0.0000  !Molecular energy (not used)
2.6962  !Valency angle conjugation parameter
2      ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
      alfa;gammaavdW;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
O      1.2450  2.0000  15.9990  2.3890  0.1000  1.0898  1.0548  6.0000
      9.7300  13.8449  4.0000  37.5000  116.0768  8.5000  8.3122  2.0000
      0.9049  0.4056  59.0626  3.5027  0.7640  0.0021  0.9745  0.0000
      -3.5500  2.9000  1.0493  4.0000  2.9225  0.0000  0.0000  0.0000
Pt      1.9820  2.0000  195.0800  2.0423  0.3309  0.3500  -1.0000  2.0000
      12.3677  6.0083  2.0000  0.0000  0.0000  6.5824  7.6812  0.0000
      -1.0000  0.0000  133.1770  27.2704  1.8727  0.1586  0.8563  0.0000
      -13.0000  1.7416  1.0338  5.0000  2.5791  0.0000  0.0000  0.0000
3      ! Nr of bonds; Ediss1;LPpen;n.u.;pbe1;pbo5;l3corr;pbo6
      pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
1 1 142.2858 145.0000 50.8293 0.2506 -0.1000 1.0000 29.7503 0.6051
      0.3451 -0.1055 9.0000 1.0000 -0.1225 5.5000 1.0000 0.0000
1 2 169.9971 0.0000 0.0000 -0.5042 -0.2000 1.0000 16.0000 0.0200
      0.6890 -0.2000 15.0000 1.0000 -0.1319 5.2406 1.0000 0.0000
2 2 122.1369 0.0000 0.0000 -0.3578 -0.2000 0.0000 16.0000 0.2877
      0.9897 -0.2000 15.0000 1.0000 -0.0853 5.4801 0.0000 0.0000
1      ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
1 2 0.1065 1.9954 10.0000 1.5417 -1.0000 -1.0000
5      ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pvl;pvt
1 1 1 80.7324 30.4554 0.9953 0.0000 1.6310 50.0000 1.0783
2 1 2 93.0852 14.8589 9.8975 0.0000 0.6543 0.0000 1.4199
1 2 2 72.4925 49.2408 2.5133 0.0000 -0.1077 0.0000 2.0066
1 1 2 84.8578 15.4368 3.1947 0.0000 1.7040 0.0000 1.1000
1 2 1 1.0000 50.0000 8.2763 0.0000 0.0235 0.0000 3.0000
3      ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
1 1 1 1 -2.5000 -4.0000 1.0000 -2.5000 -1.0000 0.0000 0.0000
0 1 1 0 0.5511 25.4150 1.1330 -5.1903 -1.0000 0.0000 0.0000
2 1 1 2 -1.6582 50.0000 0.0100 -2.5000 -1.0000 0.0000 0.0000
0      ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
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