

Reactive MD-force field: Parameters from Josh Deetz and Roland Faller J. Phys. Chem. B, 2014, 118 (37), pp 10966-10978

```
39      ! Number of general parameters
50.0000 !Overcoordination parameter
11.0940 !Overcoordination parameter
26.5405 !Valency angle conjugation parameter
 1.5105 !Triple bond stabilisation parameter
 6.6630 !Triple bond stabilisation parameter
 0.0000 !C2-correction
 1.1770 !Undercoordination parameter
 4.6000 !Triple bond stabilisation parameter
13.0070 !Undercoordination parameter
13.5840 !Undercoordination parameter
-70.1292 !Triple bond stabilization energy
 0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
 2.8793 !Not used
38.1630 !Valency undercoordination
 6.2250 !Valency angle/lone pair parameter
 1.2120 !Valency angle
 1.9920 !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
 5.5360 !Torsion/BO parameter
 9.3570 !Torsion overcoordination
 1.7770 !Torsion overcoordination
-1.2327 !Conjugation 0 (not used)
 2.0960 !Conjugation
 1.5591 !vdWaals shielding
 0.1000 !Cutoff for bond order (*100)
 2.1365 !Valency angle conjugation parameter
 0.6300 !Overcoordination parameter
50.0001 !Overcoordination parameter
 1.6300 !Valency/lone pair parameter
 0.5000 !Not used
20.0000 !Not used
 5.0000 !Molecular energy (not used)
 0.0000 !Molecular energy (not used)
 2.7150 !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;val1;n.u.;val3,vval4
C      1.3825  4.0000  12.0000  1.9133  0.1853  0.7460
1.1359  4.0000
      9.7602  2.1346  4.0000  33.2433  79.5548  5.8070
6.5250  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 | 0.8690 | 1.0000 | 1.0080 | 1.7900 | 0.0420 | 1.0000 | - |
| 0.1000 | 1.0000 | | | | | | |
| | 9.3060 | 4.5180 | 1.0000 | 0.0000 | 121.1250 | 4.7340 | |
| 7.7690 | 1.0000 | | | | | | |
| | -0.1000 | 0.0000 | 62.4879 | 1.8210 | 3.5300 | 0.7530 | |
| 1.0698 | 0.0000 | | | | | | |
| | -17.8900 | 2.1360 | 1.0338 | 1.0000 | 2.6940 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| O | 1.0050 | 2.0000 | 15.9990 | 2.0930 | 0.0990 | 1.0000 | |
| 1.0420 | 6.0000 | | | | | | |
| | 9.9880 | 8.6620 | 4.0000 | 29.7160 | 116.0768 | 8.4960 | |
| 8.3930 | 2.0000 | | | | | | |
| | 0.9090 | 1.0000 | 60.8726 | 18.6790 | 3.2980 | 0.3480 | |
| 0.9745 | 0.0000 | | | | | | |
| | -3.0650 | 2.7640 | 1.0493 | 4.0000 | 2.2910 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| N | 1.2333 | 3.0000 | 14.0000 | 1.9324 | 0.1376 | 0.8596 | |
| 1.1748 | 5.0000 | | | | | | |
| | 10.0667 | 7.8431 | 4.0000 | 32.2482 | 100.0000 | 6.8418 | |
| 6.3404 | 2.0000 | | | | | | |
| | 1.0433 | 13.7673 | 119.9837 | 2.1961 | 3.0696 | 2.7683 | |
| 0.9745 | 0.0000 | | | | | | |
| | -4.3875 | 2.6192 | 1.0183 | 4.0000 | 2.8793 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| S | 1.9401 | 2.0000 | 32.0600 | 2.0629 | 0.2095 | 1.0316 | |
| 1.5483 | 6.0000 | | | | | | |
| | 9.9553 | 4.9055 | 4.0000 | 52.9998 | 112.1416 | 6.5181 | |
| 8.2345 | 2.0000 | | | | | | |
| | 1.4601 | 9.6977 | 71.1843 | 5.7487 | 23.2859 | 12.7147 | |
| 0.9745 | 0.0000 | | | | | | |
| | -11.0200 | 2.7266 | 1.0338 | 6.2998 | 2.8793 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| Si | 1.8340 | 4.0000 | 28.0600 | 1.9770 | 0.1330 | 1.0190 | |
| 1.5430 | 4.0000 | | | | | | |
| | 12.3020 | 1.5590 | 4.0000 | 13.2990 | 136.4845 | 1.9050 | |
| 6.8960 | 0.0000 | | | | | | |
| | -1.0000 | 0.0000 | 126.5182 | 3.2410 | 7.9170 | 0.2320 | |
| 0.8563 | 0.0000 | | | | | | |
| | -3.5720 | 3.9070 | 1.0338 | 6.8600 | 2.5490 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| Hc | 0.7853 | 1.0000 | 1.0080 | 1.5904 | 0.0419 | 1.0206 | - |
| 0.1000 | 1.0000 | | | | | | |
| | 9.3558 | 5.0519 | 1.0000 | 0.0000 | 121.1251 | 5.3201 | |
| 7.4367 | 1.0000 | | | | | | |
| | -0.1000 | 0.0000 | 62.4880 | 1.9772 | 3.3518 | 0.7572 | |
| 1.0699 | 0.0000 | | | | | | |
| | -15.7684 | 2.1489 | 1.0339 | 1.0000 | 2.8794 | 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 | |
| 15.0000 | 0.0000 | | | | | | |
| | -0.1000 | 0.0000 | 127.6226 | 8.7410 | 13.3640 | 0.6690 | |
| 0.9745 | 0.0000 | | | | | | |
| | -11.0000 | 2.7466 | 1.0338 | 6.2998 | 2.8793 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | |
| 24 | ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6 pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr | | | | | | |
| 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 | | | | | |
| 1 | 4 | 134.1215 | 140.2179 | 79.9745 | 0.0163 | -0.1428 | 1.0000 |
| 27.0617 | | 0.2000 | | | | | |
| | | 0.1387 | -0.3681 | 7.1611 | 1.0000 | -0.1000 | 5.0825 |
| 1.0000 | | 0.0000 | | | | | |
| 3 | 4 | 130.8596 | 169.4551 | 40.0000 | 0.3837 | -0.1639 | 1.0000 |
| 35.0000 | | 0.2000 | | | | | |
| | | 1.0000 | -0.3579 | 7.0004 | 1.0000 | -0.1193 | 6.8773 |
| 1.0000 | | 0.0000 | | | | | |
| 4 | 4 | 157.9384 | 82.5526 | 152.5336 | 0.4010 | -0.1034 | 1.0000 |
| 12.4261 | | 0.5828 | | | | | |
| | | 0.1578 | -0.1509 | 11.9186 | 1.0000 | -0.0861 | 5.4271 |
| 1.0000 | | 0.0000 | | | | | |
| 2 | 3 | 197.9250 | 0.0000 | 0.0000 | -0.6060 | 0.0000 | 1.0000 |
| 6.0050 | | 0.5514 | | | | | |
| | | 1.2450 | 1.0000 | 0.0000 | 1.0000 | -0.0570 | 4.0190 |
| 0.0000 | | 0.0000 | | | | | |
| 2 | 4 | 231.8173 | 0.0000 | 0.0000 | -0.3364 | 0.0000 | 1.0000 |
| 6.0000 | | 0.4402 | | | | | |
| | | 8.8910 | 1.0000 | 0.0000 | 1.0000 | -0.0327 | 6.5754 |
| 0.0000 | | 0.0000 | | | | | |
| 1 | 5 | 129.1942 | 74.3656 | 55.2528 | 0.1066 | -0.5211 | 1.0000 |
| 18.9617 | | 0.5950 | | | | | |

| | | | | | | | |
|---------|-----|----------|---------|---------|---------|---------|--------|
| | | 0.2950 | -0.2398 | 8.0314 | 1.0000 | -0.1019 | 5.6754 |
| 1.0000 | | 0.0000 | | | | | |
| | 2 5 | 151.3159 | 0.0000 | 0.0000 | -0.4644 | 0.0000 | 1.0000 |
| 6.0000 | | 0.5950 | | | | | |
| | | 9.4365 | 1.0000 | 0.0000 | 1.0000 | -0.0303 | 7.0100 |
| 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 | | | | | |
| | 1 6 | 90.9518 | 9.0694 | 0.0000 | 0.3171 | -0.5558 | 1.0000 |
| 17.2117 | | 0.5716 | | | | | |
| | | 0.7279 | -0.2078 | 7.7261 | 1.0000 | -0.1095 | 5.4535 |
| 1.0000 | | 0.0000 | | | | | |
| | 2 6 | 150.7718 | 0.0000 | 0.0000 | -0.3685 | 0.0000 | 1.0000 |
| 6.0000 | | 0.8896 | | | | | |
| | | 18.0431 | 1.0000 | 0.0000 | 1.0000 | -0.0592 | 6.3196 |
| 0.0000 | | 0.0000 | | | | | |
| | 3 6 | 220.2450 | 77.4510 | 44.5790 | -0.3420 | -0.3000 | 1.0000 |
| 36.5040 | | 0.3161 | | | | | |
| | | 0.9070 | -0.3490 | 5.0380 | 1.0000 | -0.3740 | 4.5070 |
| 1.0000 | | 0.0000 | | | | | |
| | 6 6 | 72.8867 | 50.0318 | 30.0000 | 0.9983 | -0.3000 | 1.0000 |
| 16.0000 | | 0.1000 | | | | | |
| | | 1.0538 | -0.0447 | 10.6176 | 1.0000 | -0.1452 | 8.0404 |
| 0.0000 | | 0.0000 | | | | | |
| | 1 7 | 170.2317 | 0.0000 | 0.0000 | -0.5932 | 0.0000 | 1.0000 |
| 6.0000 | | 0.7141 | | | | | |
| | | 5.2268 | 1.0000 | 0.0000 | 1.0000 | -0.0500 | 6.8316 |
| 0.0000 | | 0.0000 | | | | | |
| | 2 7 | 156.0974 | 0.0000 | 0.0000 | -0.1378 | 0.0000 | 1.0000 |
| 6.0000 | | 0.8241 | | | | | |
| | | 2.9908 | 1.0000 | 0.0000 | 1.0000 | -0.0594 | 4.8359 |
| 0.0000 | | 0.0000 | | | | | |
| | 7 7 | 156.0975 | 0.0000 | 0.0000 | -0.1379 | 0.0000 | 1.0000 |
| 6.0000 | | 0.8242 | | | | | |
| | | 2.9909 | 1.0000 | 0.0000 | 1.0000 | -0.0595 | 4.8360 |
| 0.0000 | | 0.0000 | | | | | |
| | 3 7 | 180.4374 | 0.0000 | 0.0000 | -0.8075 | 0.0000 | 1.0000 |
| 6.0000 | | 0.5515 | | | | | |
| | | 1.2491 | 1.0000 | 0.0000 | 1.0000 | -0.0658 | 5.0452 |
| 0.0000 | | 0.0000 | | | | | |
| | 6 7 | 146.7970 | 0.0000 | 0.0000 | -0.3420 | 0.0000 | 1.0000 |
| 6.0840 | | 0.8898 | | | | | |

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|--------|---|---|---|----------|---------|--------|----------|--------|---------|
| 1.0783 | 1 | 3 | 4 | 82.4890 | 31.4554 | 0.9953 | 0.0000 | 1.6310 | 0.0000 |
| 1.0783 | 3 | 3 | 3 | 80.7324 | 30.4554 | 0.9953 | 0.0000 | 1.6310 | 50.0000 |
| 1.0783 | 3 | 3 | 4 | 84.3637 | 31.4554 | 0.9953 | 0.0000 | 1.6310 | 0.0000 |
| 1.1519 | 4 | 3 | 4 | 89.7071 | 31.4554 | 0.9953 | 0.0000 | 1.6310 | 0.0000 |
| 1.2900 | 1 | 3 | 2 | 59.0670 | 27.7220 | 0.4270 | 0.0000 | 0.5560 | 0.0000 |
| 1.3023 | 2 | 3 | 3 | 84.9468 | 23.3540 | 1.5057 | 0.0000 | 2.6374 | 0.0000 |
| 1.0500 | 2 | 3 | 4 | 75.6201 | 18.7919 | 0.9833 | 0.0000 | 0.1218 | 0.0000 |
| 0.8820 | 2 | 3 | 2 | 84.2260 | 11.4170 | 1.1890 | 0.0000 | 1.0000 | 0.0000 |
| 1.0500 | 1 | 4 | 1 | 66.0330 | 22.0295 | 1.4442 | 0.0000 | 1.6777 | 0.0000 |
| 1.0500 | 1 | 4 | 3 | 103.3204 | 33.0381 | 0.5787 | 0.0000 | 1.6777 | 0.0000 |
| 1.0500 | 1 | 4 | 4 | 104.1335 | 8.6043 | 1.6495 | 0.0000 | 1.6777 | 0.0000 |
| 1.0500 | 3 | 4 | 3 | 74.1978 | 42.1786 | 1.7845 | -18.0069 | 1.6777 | 0.0000 |
| 1.0500 | 3 | 4 | 4 | 74.8600 | 43.7354 | 1.1572 | -0.9193 | 1.6777 | 0.0000 |
| 1.0500 | 4 | 4 | 4 | 75.0538 | 14.8267 | 5.2794 | 0.0000 | 1.6777 | 0.0000 |
| 1.0369 | 1 | 4 | 2 | 69.1106 | 25.5067 | 1.1003 | 0.0000 | 0.0222 | 0.0000 |
| 1.0369 | 2 | 4 | 3 | 81.3686 | 40.0712 | 2.2396 | 0.0000 | 0.0222 | 0.0000 |
| 1.0500 | 2 | 4 | 4 | 83.0104 | 43.4766 | 1.5328 | 0.0000 | 0.0222 | 0.0000 |
| 1.1243 | 2 | 4 | 2 | 70.8687 | 12.0168 | 5.0132 | 0.0000 | 0.0222 | 0.0000 |
| 1.0400 | 1 | 2 | 3 | 0.0000 | 25.0000 | 3.0000 | 0.0000 | 1.0000 | 0.0000 |
| 1.0400 | 1 | 2 | 4 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 |
| 1.0400 | 1 | 2 | 5 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 |
| 0.8550 | 3 | 2 | 3 | 0.0000 | 0.0140 | 7.9490 | 0.0000 | 0.0000 | 0.0000 |
| 1.0400 | 3 | 2 | 4 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 |
| 1.0400 | 4 | 2 | 4 | 0.0000 | 0.0019 | 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 | 2 | 2 | 4 | 0.0000 | 0.0019 | 6.0000 | 0.0000 | 0.0000 | 0.0000 |


```

48      ! Nr of
torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 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
 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 0.0830 0.0190 -2.4490 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 | | | | | | | | |
| 0 | 1 | 4 | 0 | -2.4242 | 128.1636 | 0.3739 | -6.6098 | -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 | 1.4816 | 55.6641 | 0.0004 | -7.0465 | -2.7831 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 4 | 4 | 0 | -0.3244 | 27.7086 | 0.0039 | -2.8272 | -2.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 4 | 1 | 4 | 4 | -5.5181 | 8.9706 | 0.0004 | -6.1782 | -2.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 1 | 5 | 0 | 0.1515 | 29.0501 | 0.0792 | -4.5064 | -1.0200 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 5 | 5 | 0 | -0.0054 | 0.1000 | 0.1715 | -2.2256 | -1.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 2 | 5 | 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 1 | 1 | 1 | 7 | -0.2500 | 31.2596 | 0.1709 | -4.6391 | -1.9002 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 1 | 1 | 7 | -0.1770 | 30.0252 | 0.4340 | -5.0019 | -2.0697 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 1 | 1 | 3 | -0.3568 | 22.6472 | 0.6045 | -4.0088 | -1.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 1 | 1 | 3 | 7 | -1.1953 | 42.1545 | -1.0000 | -8.0821 | -1.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 1 | 3 | 1 | -0.9284 | 34.3952 | 0.7285 | -2.5440 | -2.4641 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 1 | 3 | 7 | -2.5000 | 79.6980 | 1.0000 | -3.5697 | -2.7501 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 1 | 3 | 3 | -0.5583 | 80.0000 | 1.0000 | -4.4000 | -3.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 3 | 1 | 3 | 7 | 0.0345 | 78.9586 | -0.6810 | -4.1777 | -3.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 1 | 3 | 3 | 7 | -2.5000 | 3.3219 | 0.7180 | -5.2021 | -2.9330 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 3 | 3 | 7 | 2.2500 | -6.2288 | 1.0000 | -2.6189 | -1.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 7 | 3 | 3 | 3 | 0.4723 | -12.4144 | -1.0000 | -2.5000 | -1.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 1 | 7 | 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 7 | 7 | 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 0 | 7 | 3 | 0 | 0.0000 | 0.1000 | 0.0200 | -2.5415 | 0.0000 | |
| 0.0000 | 0.0000 | | | | | | | | |
| 10 | | | | ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1 | | | | | |
| 3 | 2 | 3 | | 1.2560 | -3.5540 | 1.4140 | 2.3840 | | |
| 3 | 7 | 3 | | 1.9682 | -4.4628 | 1.7976 | 3.0000 | | |
| 3 | 2 | 4 | | 2.0000 | -6.0000 | 1.7976 | 3.0000 | | |
| 4 | 2 | 3 | | 1.2000 | -2.0000 | 1.7976 | 3.0000 | | |
| 4 | 2 | 4 | | 1.2979 | -6.0000 | 1.7976 | 3.0000 | | |

| | | | | | | |
|---|---|---|--------|---------|--------|--------|
| 3 | 2 | 5 | 1.5000 | -2.0000 | 1.7976 | 3.0000 |
| 4 | 2 | 5 | 1.5000 | -2.0000 | 1.7976 | 3.0000 |
| 5 | 2 | 3 | 1.5000 | -2.0000 | 1.7976 | 3.0000 |
| 5 | 2 | 4 | 1.5000 | -2.0000 | 1.7976 | 3.0000 |
| 5 | 2 | 5 | 1.5000 | -2.0000 | 1.7976 | 3.0000 |