Supplementary Information

Interactions of graphene with oxidants in a mixed atmosphere: synergistic effects of O_2/H_2O and O_2/CO_2 on gasification reactivity and kinetics

Zeng Liang[1], Rita Khanna[2], Kejiang Li[1*], Yunfei Ma[3], Yuri Konyukhov[4], Yushan Bu[1], Jianliang Zhang[1], Alberto N. Conejo[1]

[1]School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, Beijing 100083, P.R. China.

[2]School of Materials Science and Engineering (ret.), The University of New South Wales, Sydney, NSW 2052, Australia

[3]School of Software Engineering, Xi'an Jiaotong University, Xi'an, 710049, PR China.

[4]Department of Functional Nanosystems and High-Temperature Materials, National University of Science and Technology "MISIS", Moscow, 119049, Russia.

***Corresponding author**: Kejiang Li

Address: 30 Xueyuan Rd., Haidian District, Beijing 100083, PR China.

E-mail: likejiang@ustb.edu.cn (Kejiang Li)

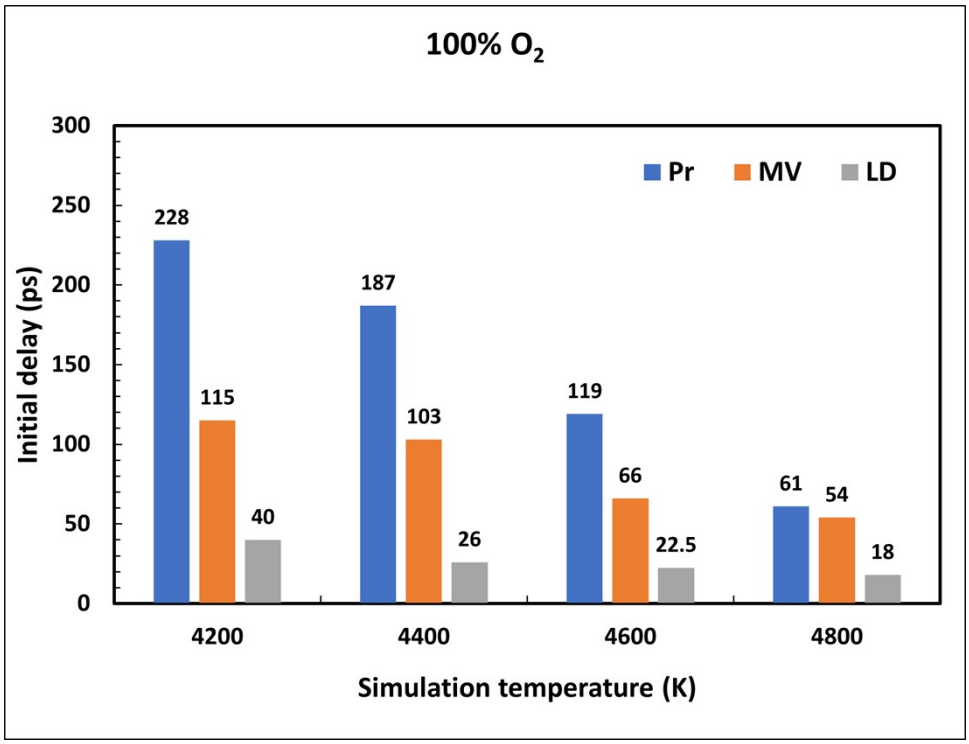

Fig. S1. Initial delays (ps) in carbon gasification of graphene under 100% O_2 environment. Data is provided for three graphene configurations: Pristine (Pr), Monovacant (MV) and line defect (LD) at a number of simulation temperatures.

Table. S1. Mixed Oxidant Composition. 13 groups of molecular number of the three gases (O_2, CO_2, H_2O) in each volume ratio component

NO	O_2	CO_2	H_2O	Cs	C:O	Remarks
1	0	0	800	800	1	100%H_2O
2	160	0	640	800	5/6	20%O_2:80%H_2O
3	320	0	480	800	5/7	40%O_2:60%H_2O
4	480	0	320	800	5/8	60%O_2:40%H_2O
5	560	0	240	800	0.59	70% O_2: 30% H_2O
6	640	0	160	800	5/9	80%O_2: 20%H_2O
7	720	0	80	800	0.53	90% O_2: 10% H_2O
8	0	800	0	800	1	100%CO_2
9	160	640	0	800	8/9	20%O_2:80%CO_2
10	320	480	0	800	4/5	40%O_2:60%CO_2
11	480	320	0	800	2/3	60%O_2:40%CO_2
12	640	160	0	800	3/5	80%O_2:20%CO_2
13	800	0	0	800	1/2	100%O_2

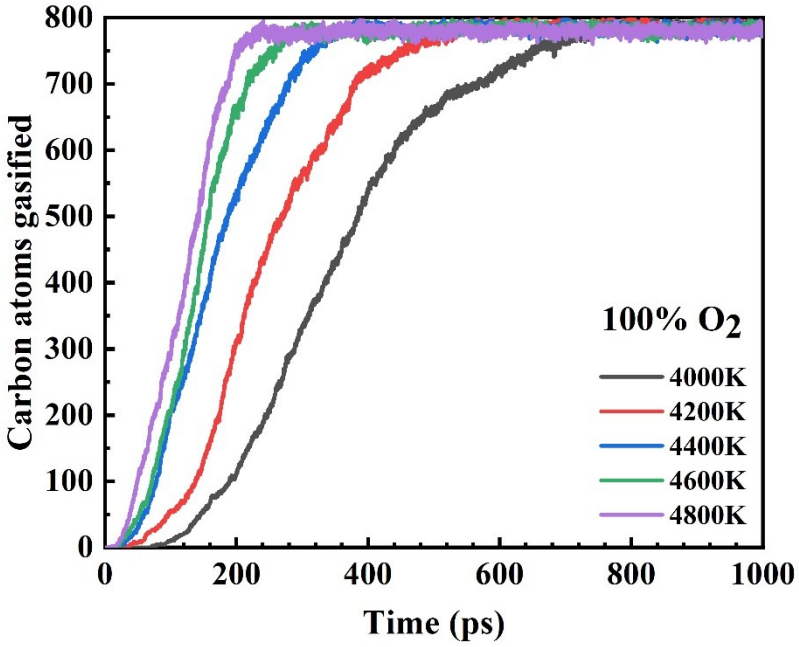

Fig. S2. Carbon gasification behavior of LD graphene under 100%O_2 at a range of temperatures.

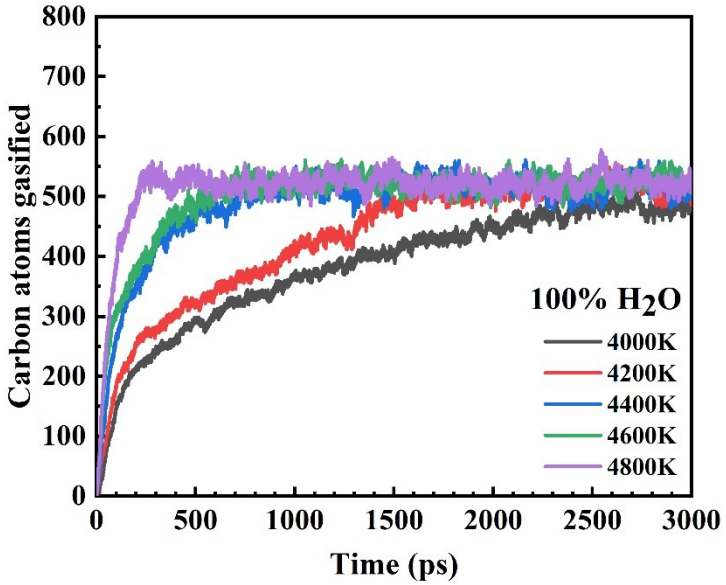

Fig. S3. Carbon gasification behavior of LD graphene under 100%H_2O at a range of temperatures.

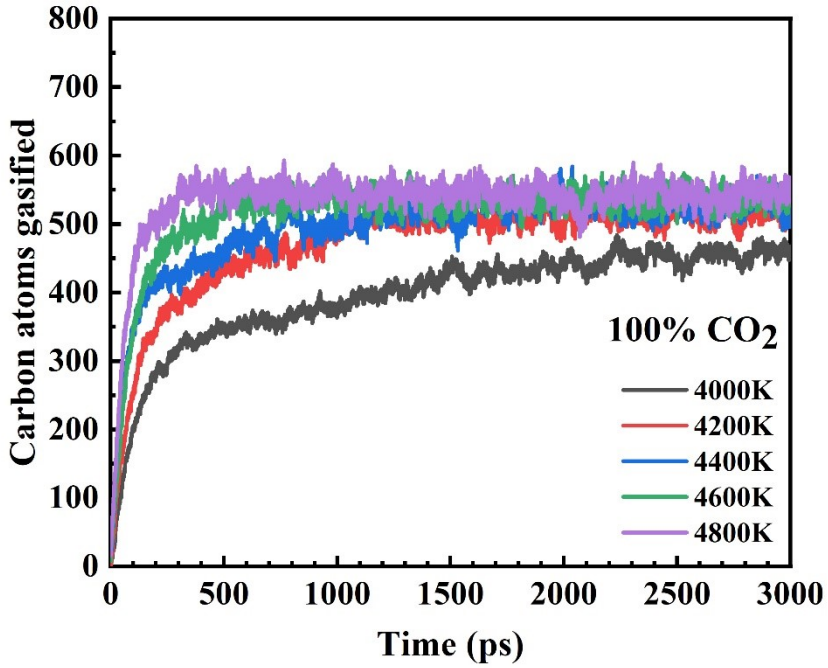

Fig. S4. Carbon gasification behavior of LD graphene under 100%CO_2 at a range of temperatures.

ReaxFF parameters

nitramines (RDX/HMX/TATB/PETN))+DMNA-barrier+innervdWaa An, Qi, et al. The Journal of Physical Chemistry C 117.50 (2013): 26551-26561.

```
 39       ! Number of general parameters
  50.0000 !Overcoordination parameter
   9.4514 !Overcoordination parameter
  29.8953 !Valency angle conjugation parameter
 216.5421 !Triple bond stabilisation parameter
  12.2245 !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
 -10.9834 !Triple bond stabilization energy
   0.0000 !Lower Taper-radius
  10.0000 !Upper Taper-radius
   2.8793 !Not used
  33.8667 !Valency undercoordination
   3.3976 !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
  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)
```

```
  4.8414 !Valency angle conjugation parameter
  3.5857 !Overcoordination parameter
 38.6472 !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)
  6.9784 !Valency angle conjugation parameter
 7    ! 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    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712   1.2385   4.0000
     8.7696   0.0000   4.0000  31.0823  79.5548   5.7254   6.9235   0.0000
     1.2104   0.0000 183.8108   5.7419  33.3951  11.9957   0.8563   0.0000
    -2.8983   4.7820   1.0564   4.0000   2.9663   1.6737   0.1421  14.0707
H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910  -0.1000   1.0000
     9.1506   0.0000   1.0000   0.0000 121.1250   3.8446  10.0839   1.0000
    -0.1000   0.0000  58.4369   3.8461   3.2540   1.0000   1.0698   0.0000
   -15.7683   2.1504   1.0338   1.0000   2.8793   1.2669   0.0139  12.4538
O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712   1.1139   6.0000
     9.9926   0.0000   4.0000  29.5271 116.0768   8.5000   7.1412   2.0000
     0.9909  14.7235  69.2921   9.1371   1.6258   0.1863   0.9745   0.0000
    -3.5965   2.5000   1.0493   4.0000   2.9225   1.7221   0.1670  13.9991
N    1.2456   3.0000  14.0000   2.0437   0.1035   0.8712   1.1911   5.0000
     9.8823   0.0000   4.0000  32.4758 100.0000   6.8453   6.8349   2.0000
     1.0636   0.0276 127.9672   2.2169   2.8632   2.4419   0.9745   0.0000
    -4.0959   2.0047   1.0183   4.0000   2.8793   1.5967   0.1649  13.9888
S    1.9647   2.0000  32.0600   2.0783   0.2176   1.0336   1.5386   6.0000
     9.9676   0.0000   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   1.8000   0.1000  14.0000
Si   1.9006   4.0000  28.0600   1.8610   0.2074   0.6295   1.2962   4.0000
```

12.2693 0.0000 4.0000 24.9985 139.9309 2.9124 7.4273 0.0000

1.2000 0.0000 128.2031 5.3697 18.4627 0.1712 0.8563 0.0000

-5.8495 2.2852 1.0338 4.0000 2.5791 1.8737 0.0421 12.0707

X -0.1000 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 6.0000

10.0000 0.0000 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 1.6737 0.1421 14.0707

20 ! 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 3 159.7219 116.8921 77.9315 -0.4324 -0.1742 1.0000 15.0019 0.5160

1.2934 -0.3079 7.0252 1.0000 -0.1543 4.5116 0.0000 0.0000

3 3 108.9631 158.3501 42.0558 0.1226 -0.1324 1.0000 28.5716 0.2545

1.0000 -0.2656 8.6489 1.0000 -0.1000 6.8482 1.0000 0.0000

1 4 128.9104 171.2945 100.5836 -0.1306 -0.4948 1.0000 26.7458 0.4489

0.3746 -0.3549 7.0000 1.0000 -0.1248 4.9232 1.0000 0.0000

3 4 85.0402 118.8680 75.7263 0.7080 -0.1062 1.0000 16.6913 0.2407

0.3535 -0.1906 8.4054 1.0000 -0.1154 5.6575 1.0000 0.0000

4 4 160.6599 73.3721 154.2849 -0.7107 -0.1462 1.0000 12.0000 0.6826

0.9330 -0.1434 10.6712 1.0000 -0.0890 4.6486 1.0000 0.0000

2 3 219.7016 0.0000 0.0000 -0.6643 0.0000 1.0000 6.0000 0.9854

5.1146 1.0000 0.0000 1.0000 -0.0532 5.1189 0.0000 0.0000

2 4 208.0443 0.0000 0.0000 -0.3923 0.0000 1.0000 6.0000 0.3221

10.5505 1.0000 0.0000 1.0000 -0.0690 6.2949 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

1 6 100.2834 27.9207 0.0000 0.1119 -0.5558 1.0000 17.2117 0.5923

0.9528 -0.2353 9.9655 1.0000 -0.1218 5.7788 1.0000 0.0000

2 6 235.5112 0.0000 0.0000 -0.7467 0.0000 1.0000 6.0000 0.5536

19.6541 1.0000 0.0000 1.0000 -0.0438 6.8851 0.0000 0.0000

3 6 277.9031 21.9498 0.0000 -0.7494 -0.3000 1.0000 36.0000 0.7564

8.2632 -0.4502 23.7800 1.0000 -0.1377 7.1295 1.0000 0.0000

4 6 185.4488 39.2832 43.3991 -0.1922 -0.3000 1.0000 36.0000 0.8217

0.8538 -0.3887 4.4334 1.0000 -0.5241 4.4529 1.0000 0.0000

6 6 90.1889 47.8775 30.0000 0.6567 -0.3000 1.0000 16.0000 0.0147

0.3287 -0.1777 4.6512 1.0000 -0.0592 7.7781 0.0000 0.0000

12 ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2

1 2 0.0464 1.8296 9.9214 1.0029 -1.0000 -1.0000

2 3 0.0403 1.6913 10.4801 0.8774 -1.0000 -1.0000

2 4 0.0524 1.7325 10.1306 0.9982 -1.0000 -1.0000

1 3 0.1028 1.9277 9.1521 1.3399 1.1104 1.1609

1 4 0.2070 1.7366 9.5916 1.2960 1.2008 1.1262

3 4 0.0491 1.7025 10.6101 1.3036 1.1276 1.0173

1 6 0.1295 1.6787 11.0825 1.7116 1.5500 -1.0000

2 6 0.0670 1.4906 12.7773 1.3322 -1.0055 -1.0000

3 6 0.1091 1.9544 11.1442 1.6740 1.3888 -1.0000

4 6 0.1365 1.9123 11.1784 -1.7095 -1.4858 -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

82 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2

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 1.0400

1 1 3 65.1700 8.0170 7.5000 0.0000 0.2028 10.0000 1.0400

3 1 3 71.7582 26.7070 6.0466 0.0000 0.2000 0.0000 1.8525

1 1 4 65.4228 43.9870 1.5602 0.0000 0.2000 10.0000 1.8525

3 1 4 73.7046 23.8131 3.9811 0.0000 0.2000 0.0000 1.8525

4 1 4 65.6602 40.5852 1.8122 0.0000 0.2000 0.0000 1.8525

2 1 3 56.4426 17.6020 5.3044 0.0000 0.9699 0.0000 1.1272

2 1 4 71.0777 9.1462 3.4142 0.0000 0.9110 0.0000 1.0400

1 2 4 0.0000 0.0019 6.3000 0.0000 0.0000 0.0000 1.0400

1 3 1 72.1018 38.4720 1.3926 0.0000 0.4785 0.0000 1.2984

1 3 3 89.9987 44.9806 0.5818 0.0000 0.7472 0.0000 1.2639

1 3 4 70.3281 12.9371 7.5000 0.0000 0.7472 0.0000 1.2639

3 3 3 84.2807 24.1938 2.1695 -10.0000 0.7472 0.0000 1.2639

3 3 4 84.2585 44.1039 0.9185 0.0000 0.7472 0.0000 1.2639

4 3 4 74.2312 25.7005 4.3943 0.0000 0.7472 0.0000 1.2639

1 3 2 89.0416 36.9460 0.4569 0.0000 2.7636 0.0000 2.0494

2 3 3 81.1709 4.2886 6.5904 0.0000 3.0000 0.0000 1.2618

2 3 4 75.9203 44.9675 0.8889 0.0000 3.0000 0.0000 1.2618

2 3 2 82.2020 12.7165 3.9296 0.0000 0.2765 0.0000 1.0470

1 4 1 68.3788 18.3716 1.8893 0.0000 2.4132 0.0000 1.3993

1 4 3 86.5585 37.6814 1.1611 0.0000 1.7325 0.0000 1.0440

1 4 4 74.4818 12.0954 7.5000 0.0000 1.7325 0.0000 1.0440

3 4 3 78.5850 44.3389 1.3239 -26.2246 1.7325 40.0000 1.0440

3 4 4 77.6245 32.0866 1.8889 -0.9193 1.7325 0.0000 1.0440

4 4 4 66.4718 15.9087 7.5000 0.0000 1.7325 0.0000 1.0440

1 4 2 90.0000 33.6636 1.1051 0.0000 0.2638 0.0000 1.1376

2 4 3 83.8493 44.9000 1.3580 0.0000 0.5355 0.0000 2.5279

2 4 4 78.7452 24.2010 3.7481 0.0000 0.5355 0.0000 2.5279

2 4 2 55.8679 14.2331 2.9225 0.0000 0.2000 0.0000 2.9932

1 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 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 1.0400

3 2 3 0.0000 0.0019 6.0000 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 0.0019 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 1.0400

1 1 5 74.4180 33.4273 1.7018 0.1463 0.5000 0.0000 1.6178

1 5 1 79.7037 28.2036 1.7073 0.1463 0.5000 0.0000 1.6453

2 1 5 63.3289 29.4225 2.1326 0.0000 0.5000 0.0000 3.0000

1 5 2 85.9449 38.3109 1.2492 0.0000 0.5000 0.0000 1.1000

1 5 5 85.6645 40.0000 2.9274 0.1463 0.5000 0.0000 1.3830

2 5 2 83.8555 5.1317 0.4377 0.0000 0.5000 0.0000 3.0000

2 5 5 97.0064 32.1121 2.0242 0.0000 0.5000 0.0000 2.8568

6 6 6 76.2257 38.6984 0.8301 0.0000 0.0005 0.0000 1.3036

2 6 6 79.2712 10.2508 2.4946 0.0000 2.6950 0.0000 1.2160

2 6 2 77.4183 10.2268 4.0230 0.0000 3.2555 0.0000 1.0400

3 6 6 75.0505 22.1873 1.3013 0.0000 4.0000 0.0000 1.1770

2 6 3 64.2067 18.3649 4.0936 0.0000 3.4106 0.0000 1.0400

3 6 3 98.1116 32.8740 0.3463 0.0000 0.2200 0.0000 1.2221

6 3 6 55.8974 1.8196 0.3930 0.0000 2.7790 0.0000 1.0920

2 3 6 71.3545 4.4881 5.8566 0.0000 3.5827 0.0000 1.0900

3 3 6 68.4721 18.1831 2.3112 0.0000 1.1055 0.0000 1.0400

2 2 6 0.0000 47.1300 6.0000 0.0000 1.6371 0.0000 1.0400

6 2 6 0.0000 27.4206 6.0000 0.0000 1.6371 0.0000 1.0400

3 2 6 0.0000 7.0550 3.9236 0.0000 1.6371 0.0000 1.0400

2 2 5 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400

1 1 6 72.5239 22.3583 2.0393 0.0000 1.0031 0.0000 1.0400

1 6 1 68.7380 13.0736 7.7287 0.0000 1.0031 0.0000 1.0000

6 1 6 69.3369 18.9270 2.0703 0.0000 1.0031 0.0000 1.0400

1 6 6 69.3369 19.6964 2.0703 0.0000 1.0031 0.0000 1.0400

2 1 6 84.1550 32.8355 0.6419 0.0000 1.0000 0.0000 1.0000

1 6 2 72.5949 14.8347 2.4952 0.0000 1.0000 0.0000 1.0400

4 6 6 64.4297 13.1239 1.1830 0.0000 2.1459 0.0000 1.0400

4 6 4 78.4992 7.8594 2.3011 0.0000 0.7689 0.0000 1.0400

3 6 4 77.4641 4.5724 1.0849 0.0000 0.7689 0.0000 1.0400

6 4 6 25.5269 3.0725 0.2486 0.0000 4.1125 0.0000 1.0400

2 6 4 77.4079 16.0992 2.2665 0.0000 0.8613 0.0000 1.0400

2 4 6 74.6462 4.7671 1.6524 0.0000 1.6982 0.0000 1.0400

4 4 6 76.8202 12.7851 0.6196 0.0000 2.2466 0.0000 1.0400

3 4 6 69.8728 32.7155 1.5875 0.0000 2.2466 0.0000 1.0400

4 3 6 74.8601 21.1475 13.2496 0.0000 1.4170 0.0000 1.3151

4 2 6 0.0000 31.0427 4.5625 0.0000 1.6371 0.0000 1.0400

1 3 6 70.0000 12.0356 1.0943 0.0000 1.0000 0.0000 3.0000

1 6 3 97.8539 19.3628 1.9813 0.0000 1.0000 0.0000 1.7348

3 1 6 49.0987 14.0291 1.2540 0.0000 1.0000 0.0000 1.0000

1 2 6 0.0000 2.5000 1.0000 0.0000 1.0000 0.0000 1.2500

37 ! 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 1.7254 86.0769 0.3440 -4.2330 -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 1.2314 116.5137 0.5599 -4.1412 0.0000 0.0000 0.0000

0 1 4 0 -1.3258 149.8644 0.4790 -7.1541 -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 1.3168 57.0732 0.2679 -4.1516 -2.0000 0.0000 0.0000

0 4 4 0 2.0000 75.3685 -0.7852 -9.0000 -2.0000 0.0000 0.0000

0 1 1 0 0.0930 18.6070 -1.3191 -9.0000 -1.0000 0.0000 0.0000

4 1 4 4 -2.0000 20.6655 -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 1.2707 21.6200 1.5000 -9.0000 -2.0000 0.0000 0.0000

1 3 3 1 -1.8804 79.9255 -1.5000 -4.1940 -2.0000 0.0000 0.0000

3 1 3 3 -2.0000 22.5092 1.5000 -8.9500 -2.0000 0.0000 0.0000

1 4 4 3 0.1040 70.1152 0.5284 -3.5026 -2.0000 0.0000 0.0000

1 1 3 4 1.5571 150.0000 -1.5000 -6.2992 -2.0000 0.0000 0.0000

2 1 3 4 -2.0000 156.6604 1.1004 -7.3729 -2.0000 0.0000 0.0000

1 3 4 3 2.0000 96.6281 -1.5000 -3.8076 -2.0000 0.0000 0.0000

1 1 4 2 -2.0000 147.2445 -1.5000 -7.0142 -2.0000 0.0000 0.0000

1 1 4 3 -2.0000 47.8326 -1.5000 -9.0000 -2.0000 0.0000 0.0000

2 3 4 3 -0.2997 152.9040 -1.5000 -4.4564 -2.0000 0.0000 0.0000

2 4 4 3 0.1040 70.1152 0.5284 -3.5026 -2.0000 0.0000 0.0000

2 6 6 2 0.0000 0.0000 0.0640 -2.4426 0.0000 0.0000 0.0000

2 6 6 6 0.0000 0.0000 0.1587 -2.4426 0.0000 0.0000 0.0000

0 4 6 0 0.0000 0.0000 0.0000 -2.4426 0.0000 0.0000 0.0000

6 1 3 4 2.2432 70.4121 0.7831 -3.8898 -2.0000 0.0000 0.0000

4 1 3 6 -0.0199 98.6767 0.1000 -4.2582 -2.0000 0.0000 0.0000

3 1 3 6 0.9384 100.4942 -1.2731 -3.5147 -2.0000 0.0000 0.0000

9 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1

3 2 3 2.1845 -2.3549 3.0582 19.1627

3 2 4 1.6658 -3.8907 3.0582 19.1627

4 2 3 1.8738 -3.5421 3.0582 19.1627

4 2 4 1.8075 -4.1846 3.0582 19.1627

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