Electronic Supplementary Information

Initial Stage of Titanium Oxidation in Ti/CuO Thermites: a Molecular Dynamics Study using ReaxFF Forcefield

Hicham Jabraoui[a], Alain Estève[a], Sungwook Hong[b], Carole Rossi[a, †]

a. LAAS-CNRS, University of Toulouse, 31077 Toulouse, France

b. Department of Physics and Engineering, California State University, Bakersfield, Bakersfield, California 93311, United States of America

† Corresponding Author Carole Rossi E-mail: rossi@laas.fr

SI. 1. NEB CALCULATIONS FOR OXYGEN DIFFUSION

Here we combine minimization using Damped Dynamics (DD) method[1] and Climbing image-nudged elastic band (CI-NEB) calculations[2] implemented in LAMMPS packages[3] to compute oxygen diffusion barrier energy in CuO materials. By comparing the value obtained by ReaxFF and our previous DFT calculations[4], our main objective is to check if the ReaxFF parameters used allow studying the nanothermite ignition context. For a reasonable comparison, we put the two approaches namely DFT/CI-NEB and minimization energy/CI-NEB under the same conditions using the same number of images between the initial and final state on the diffusion channels. oxygen and the same structure CuO, see the detail of the CuO structure in our previous DFT calculations **Ref**[4]. Two approaches show that CuO bulk diffusion (either as a Frenkel defect or as an interstitial) is not possible at low temperature (below 600 K), since the barrier energy of this diffusion is higher than 3 eV (see **Figure S1 a**). ReaxFF reports an almost similar barrier energy of diffusion oxygen in perfect CuO with a value at around 4 eV. This means that the presence of an oxygen vacancy is necessary to reasonably activate the diffusion of oxygen during the deoxygenation of CuO and its decomposition during the ignition of nanothermite. In the presence of oxygen vacancy, DFT has previously reported that oxygen diffusion via the oxygen vacancy in bulk CuO can only be feasible in two favorable crystallographic orientations, namely [110] and [001]. Similar to what is obtained with DFT, ReaxFF approach shows a barrier energy less than 2 eV, while compared to DFT calculations for [110], ReaxFF is overestimating the barrier. Note also that for the [001] direction, ReaxFF is underestimating the barrier (see **Figure S1 b**). Coming from the bulk towards the layers close to the surface, ReaxFF shows that the oxygen diffusion barrier energy decreases along two favorable crystallographic directions, by around 0.2 eV (see **Figure S1 c**). On both surfaces, namely (001) and (111), preoxy diffusion results in a barrier energy of about 2 (eV) (see **Figure S1 d**). Compared to DFT calculations, ReaxFF gives an overestimated barrier energy onto the surface (001) and an underestimated barrier energy onto the (111) surface. Generating an O_2 molecule from the surface, ReaxFF shows a formation energy of 7.11 eV) from the (111) (6.88 eV for DFT) surface and 0.28 eV from the (001) surface (1.53 eV for DFT). On the surface (001),

ReaxFF shows a shift with DFT which can be correlated by the fact that with DFT the (001) surface is strongly reconstructed whereas with the minimization energy in the ReaxFF framework this reconstruction is less pronounced.

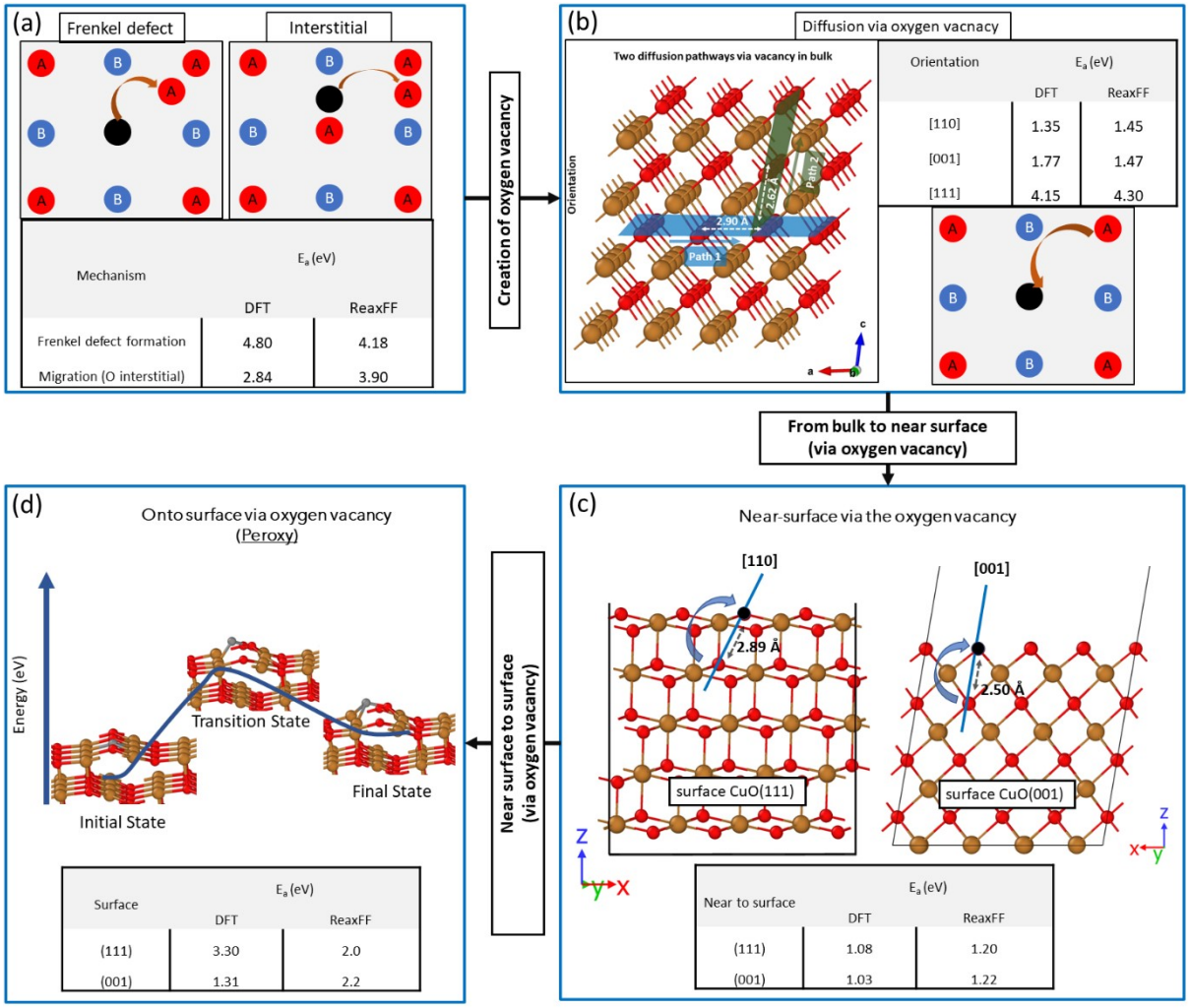

Figure S1. Oxygen diffusion pathways in CuO at different levels, (a) into bulk without defect, (b) into bulk via oxygen vacancy in two favorable crystallographic orientations, (c) near surface via vacancy oxygen and (d) onto the surface as peroxy. The red and light brown balls represent oxygen and copper atoms, respectively.

SII. Ti/CuO DETAILS

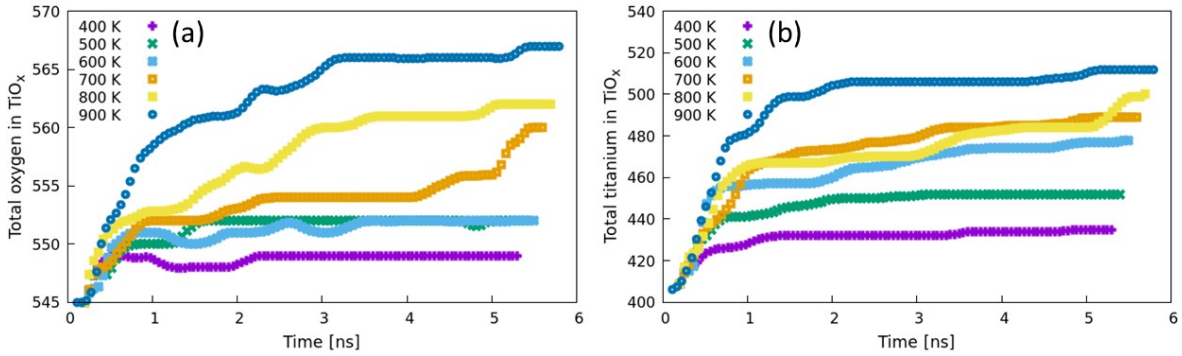

Figure S2. (a-b) The temporal evolution of the total amount of oxygen and the total amount of titanium in the TiO_x region over annealing simulation times at different temperatures, respectively.

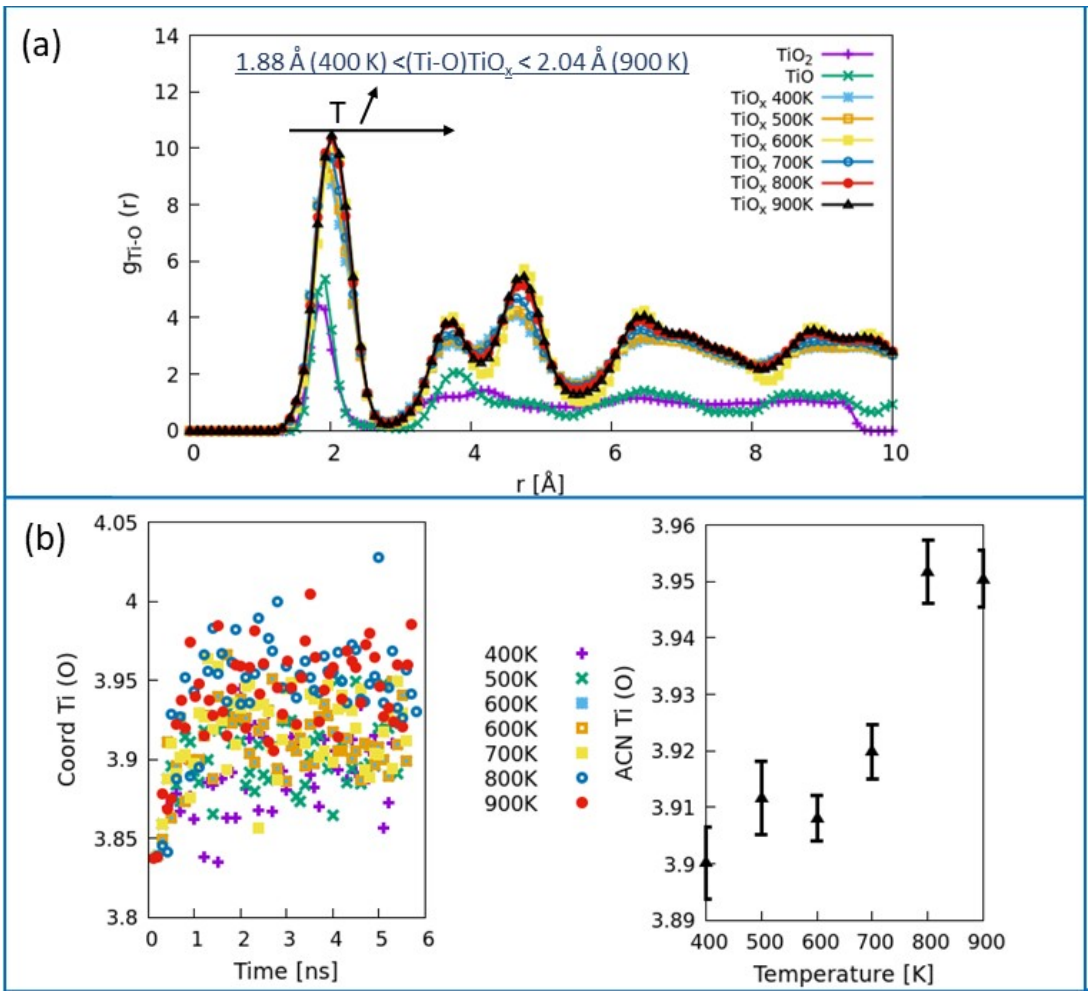

Figure S3. (a-b) Radial distribution function (RDF) of Ti-O and the average coordination number (ACN) of Ti with respect to O in pristine TiO, pristine TiO_2 and the newly created TiO_x at different temperatures, respectively. ACN and RDF were determined over the last 1ns of 5 ns of annealing.

SIII. Al/CuO DETAILS

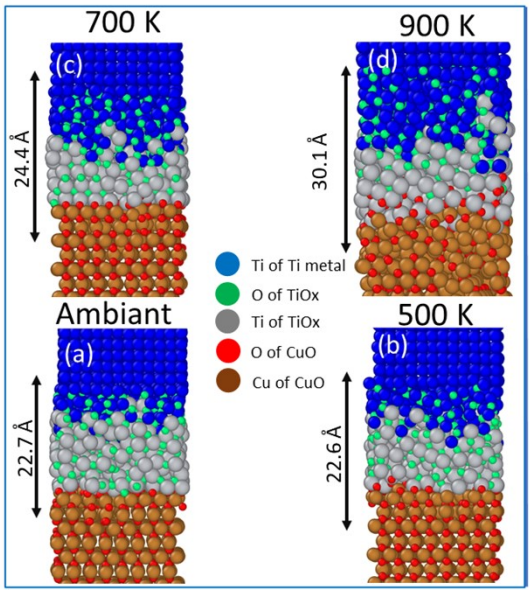

Figure S4. (a-d) represent two-dimensional snapshots of the initial (pre-annealed) and final (post-annealed) structures of Al/*am*Al_xO_y/CuO at different selected temperatures (ambient, 500, 700, and 900 K), respectively. Noteworthy, Defective CuO is considered in this study.

Table S1. The total Al_xO_y thickness, its depth extension into the Al metallic fuel region and into the CuO region, and its Stoichiometry as a function of temperature. Average values were computed over the last 100 ps of 5 ns of annealing.

T (K)	Al_xO_y thickness (Å)	Al_xO_y into metal Al (Å)	Al_xO_y into CuO (Å)	Al_xO_y Stoichiometry
Ambiant	22.74	0	0	$Al_{2.8}O_3$
400	22.82 ± 0.02	0.20 ± 0.01	0.01 ± 0.02	$Al_{2.9}O_3$
500	22.86 ± 0.02	0.22 ± 0.01	0.07 ± 0.01	$Al_{2.7}O_3$
600	23.87 ± 0.02	1.21 ± 0.01	0.07 ± 0.04	$Al_{3.5}O_3$
700	25.05 ± 0.07	2.20 ± 0.02	0.12 ± 0.02	$Al_{3.6}O_3$
800	26.40 ± 0.02	2.93 ± 0.01	0.80 ± 0.07	$Al_{3.6}O_3$
900	30.10 ± 0.07	4.34 ± 0.03	3.00 ± 0.07	$Al_{3.6}O_3$

SIV. REAXFF PARAMETERS

Reactive MD-force field: H/O/Si/Al/Cu, G.M. Psofogiannakis et al., J. Phys. Chem. C, 2015, 119 (12), pp 6678-6686, http://dx.doi.org/10.1021/acs.jpcc.5b00699; add TiO2 from Sung-Yup Kim and Adri C. T. van Duin, 2013, http://dx.doi.org/10.1021/jp4031943

```
 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 !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
16    ! 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    1.3817   4.0000  12.0000   1.8903   0.1838   0.9000   1.1341   4.0000
     9.7559   2.1346   4.0000  34.9350  79.5548   5.9666   7.0000   0.0000
     1.2114   0.0000 202.5551   8.9539  34.9289  13.5366   0.8563   0.0000
    -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
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   0.0000   0.0000   0.0000
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

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 1.9405 2.0000 32.0600 2.0677 0.2099 1.0336 1.5479 6.0000

9.9575 4.9055 4.0000 52.9998 112.1416 6.5000 8.2545 2.0000

1.4601 9.7177 71.1843 5.7487 23.2859 12.7147 0.9745 0.0000

-11.0000 2.7466 1.0338 6.2998 2.8793 0.0000 0.0000 0.0000

Si 2.0175 4.0000 28.0600 2.0473 0.1835 0.8925 1.2962 4.0000

12.3588 1.2523 4.0000 21.7115 139.9309 4.6988 6.0000 0.0000

-1.0000 0.0000 128.2031 8.7895 23.9298 0.8381 0.8563 0.0000

-4.7525 2.1607 1.0338 4.0000 2.5791 0.0000 0.0000 0.0000

Ca 1.9927 2.0000 40.0870 2.7005 0.1848 0.7939 1.0000 2.0000

10.6123 27.5993 3.0000 38.0000 0.0000 -1.9372 6.5275 0.0000

-1.3000 0.0000 220.0000 49.9248 0.3370 0.0000 0.0000 0.0000

-2.0000 4.0000 1.0564 6.2998 2.9663 1.4000 0.0100 13.0000

Cs 2.5411 1.0000 132.9054 2.1409 0.3507 0.9824 -1.0000 1.0000

14.0000 2.5000 1.0000 0.0000 0.0000 -4.1130 8.7265 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-2.5000 3.9900 1.0338 8.0000 2.5791 1.0000 0.0100 13.0000

K 2.1000 1.0000 39.0983 2.6480 0.1676 0.3343 -1.0000 1.0000

9.0047 2.5000 1.0000 0.0000 0.0000 -5.0000 10.4546 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-2.5000 3.9900 1.0338 8.0000 2.5791 1.0000 0.0100 13.0000

Sr 2.1997 2.0000 87.6200 2.5141 0.3839 0.3983 1.0000 2.0000

11.1452 27.5993 3.0000 0.0000 0.0000 -4.2868 6.5000 0.0000

-1.3000 0.0000 220.0000 49.9248 0.3370 0.0000 0.0000 0.0000

-25.0000 4.0000 1.0564 6.2998 2.9663 1.0000 0.1000 13.0000

Na 1.8000 1.0000 22.9898 2.8270 0.1872 0.4000 -1.0000 1.0000

10.0000 2.5000 1.0000 0.0000 0.0000 -0.9871 6.7728 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-2.5000 3.9900 1.0338 8.0000 2.5791 0.0000 0.0000 0.0000

Mg 1.8278 2.0000 24.3050 2.2494 0.1830 0.4805 1.0000 2.0000

10.8448 4.4030 3.0000 38.0000 0.0000 0.1595 6.1918 0.0000

-1.3000 0.0000 34.5160 49.9248 0.3370 0.0000 0.0000 0.0000

-16.6849 2.3663 1.0564 6.0000 2.9663 0.0000 0.0000 0.0000

Al 2.1967 3.0000 26.9820 2.3738 0.2328 0.4873 -1.6836 3.0000

9.4002 2.6409 3.0000 0.0076 16.5151 -0.7626 6.4941 0.0000

-1.0000 0.0000 78.4675 20.0000 0.2500 0.0000 0.8563 0.0000

-23.1826 1.5000 1.0338 8.0000 2.5791 1.4000 0.2000 13.0000

Cu 1.9202 2.0000 63.5460 1.9221 0.2826 1.0000 0.1000 1.0000

10.9889 100.0000 1.0000 0.0000 0.0000 2.7875 6.0000 0.0000

-1.0000 0.0000 80.7000 34.9555 0.4988 0.0000 0.8563 0.0000

-5.1872 3.1491 1.0000 4.0000 2.5791 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 1.5000 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

Ti 2.0254 4.0000 47.8800 2.2105 0.1574 0.6311 0.1000 4.0000

12.7041 16.6482 4.0000 0.1000 0.0000 -1.3647 6.8406 0.0000

-1.0000 0.0000 143.1770 27.6505 -0.0753 0.0064 0.8563 0.0000

-15.0000 3.8359 1.0338 12.0000 2.2632 0.0000 0.0000 0.0000

76 ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6

pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr

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

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

1 3 158.6946 107.4583 23.3136 -0.4240 -0.1743 1.0000 10.8209 1.0000

0.5322 -0.3113 7.0000 1.0000 -0.1447 5.2450 0.0000 0.0000

3 3 142.2858 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 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 3 160.0000 0.0000 0.0000 -0.5725 0.0000 1.0000 6.0000 0.5626

1.1150 1.0000 0.0000 1.0000 -0.0920 4.2790 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 5 128.9942 74.5848 55.2528 0.1035 -0.5211 1.0000 18.9617 0.6000

0.2949 -0.2398 8.1175 1.0000 -0.1029 5.6731 1.0000 0.0000

2 5 151.5159 0.0000 0.0000 -0.4721 0.0000 1.0000 6.0000 0.6000

9.4366 1.0000 0.0000 1.0000 -0.0290 7.0050 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 6 108.3910 95.0233 0.0000 0.1129 -0.5558 1.0000 17.2117 0.4568

0.2424 -0.2378 10.1163 1.0000 -0.1020 5.7156 1.0000 0.0000

2 6 250.0000 0.0000 0.0000 -0.7128 0.0000 1.0000 6.0000 0.1186

18.5790 1.0000 0.0000 1.0000 -0.0731 7.4983 0.0000 0.0000

3 6 272.8709 18.4462 0.0000 -0.6107 -0.3000 1.0000 36.0000 0.8270

10.2334 -0.5495 29.9954 1.0000 -0.1277 7.5863 1.0000 0.0000

4 6 119.7136 41.2405 43.3991 -0.2060 -0.3000 1.0000 36.0000 0.7957

0.8189 -0.2614 9.4060 1.0000 -0.1245 6.1856 1.0000 0.0000

6 6 78.0276 54.0531 30.0000 0.5398 -0.3000 1.0000 16.0000 0.0476

0.2865 -0.8055 7.1248 1.0000 -0.0681 8.6957 0.0000 0.0000

2 7 0.0000 0.0000 0.0000 -0.0203 -0.1418 1.0000 13.1260 0.0230

8.2136 -0.1310 0.0000 1.0000 -0.2692 6.4254 0.0000 24.4461

3 7 50.8757 0.0000 43.3991 1.0000 -0.3000 1.0000 36.0000 0.0025

0.7609 -0.2500 12.0000 1.0000 -0.0515 8.9041 1.0000 24.4461

5 7 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

6 7 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

7 7 36.9494 0.0000 0.0000 -0.0412 -0.2000 0.0000 16.0000 0.3233

0.3708 -0.2000 10.0000 1.0000 -0.0822 4.2104 0.0000 0.0000

2 8 0.0000 0.0000 0.0000 -0.0203 -0.1418 1.0000 13.1260 0.0230

8.2136 -0.1310 0.0000 1.0000 -0.2692 6.4254 0.0000 24.4461

3 8 20.2042 0.0000 43.0000 0.8725 -0.3000 1.0000 36.0000 0.9891

1.1717 -0.3500 25.0000 1.0000 -0.0535 7.4006 1.0000 0.0000

8 8 23.4317 0.0000 0.0000 0.0743 0.3000 0.0000 25.0000 0.5292

0.7716 -0.4000 12.0000 1.0000 -0.0584 4.5750 0.0000 0.0000

2 9 0.0000 0.0000 0.0000 -1.0000 -0.3000 1.0000 36.0000 0.7000

10.1151 -0.3500 25.0000 1.0000 -0.1053 8.2003 1.0000 0.0000

3 9 22.6146 0.0000 43.0000 0.6651 -0.3000 1.0000 36.0000 1.0000

0.9166 -0.3500 25.0000 1.0000 -0.0583 7.3861 1.0000 0.0000

9 9 22.6628 0.0000 0.0000 0.3272 0.3000 0.0000 25.0000 0.5944

0.9915 -0.4000 12.0000 1.0000 -0.0517 4.5075 0.0000 0.0000

2 10 0.0000 0.0000 0.0000 -0.0203 -0.1418 1.0000 13.1260 0.0230

8.2136 -0.1310 0.0000 1.0000 -0.2692 6.4254 0.0000 24.4461

3 10 40.0000 0.0000 43.3991 1.0000 -0.3000 1.0000 36.0000 1.0000

0.9111 -0.2500 12.0000 1.0000 -0.0746 8.2827 1.0000 24.4461

10 10 25.4008 0.0000 0.0000 0.2399 -0.2000 0.0000 16.0000 0.4158

0.5220 -0.2000 10.0000 1.0000 -0.0848 4.0000 0.0000 0.0000

4 7 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

4 8 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

4 9 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

4 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

5 8 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

5 9 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

5 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

6 8 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

6 9 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

6 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

7 8 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

7 9 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

7 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

8 9 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

8 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

9 10 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

2 11 0.0000 0.0000 0.0000 -1.0000 -0.3000 1.0000 36.0000 0.7000
10.1151 -0.3500 25.0000 1.0000 -0.1053 8.2003 1.0000 0.0000
3 11 45.8933 0.0000 0.0000 -0.1511 -0.3000 1.0000 36.0000 0.3105
5.8448 -0.3500 25.0000 1.0000 -0.0659 7.9140 1.0000 0.0000
6 11 0.1000 0.0000 0.0000 0.2500 -0.5000 1.0000 35.0000 0.6000
0.5000 -0.5000 20.0000 1.0000 -0.2000 10.0000 1.0000 0.0000
11 11 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
2 12 58.6896 0.0000 0.0000 -0.0203 -0.1418 1.0000 13.1260 0.0230
8.2136 -0.1310 0.0000 1.0000 -0.2692 6.4254 0.0000 24.4461
3 12 60.0341 0.0000 43.3991 1.0000 -0.3000 1.0000 36.0000 0.0038
1.0000 -0.2500 12.0000 1.0000 -0.0884 6.7572 1.0000 24.4461
12 12 27.2865 0.0000 0.0000 0.3694 -0.2000 0.0000 16.0000 0.2631
0.7983 -0.2000 10.0000 1.0000 -0.1135 4.5200 0.0000 0.0000
2 13 92.8579 0.0000 0.0000 -0.6528 -0.3000 0.0000 36.0000 0.1551
10.0663 -0.3500 25.0000 1.0000 -0.0842 7.1758 0.0000 0.0000
3 13 182.0654 0.0000 0.0000 -0.0920 -0.3000 0.0000 36.0000 0.1688
0.0010 -0.3500 25.0000 1.0000 -0.1959 6.0894 0.0000 0.0000
6 13 0.0000 0.0000 0.0000 1.0000 0.3000 0.0000 26.0000 1.0000
0.5000 0.0000 12.0000 1.0000 -0.2000 10.0000 0.0000 0.0000
7 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000
0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000
8 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000
0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000
9 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000
0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000
10 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000
0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000
11 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000
0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000
12 13 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

```
      0.5000  -0.2500  15.0000   1.0000  -0.1000   9.0000   0.0000   0.0000
13 13  34.0777   0.0000   0.0000   0.4832  -0.3000   0.0000  16.0000   0.5154
      6.4631  -0.4197  14.3085   1.0000  -0.1463   6.1608   0.0000   0.0000
 2 14   0.0000   0.0000   0.0000   0.2000  -0.1418   1.0000  13.1260   0.5000
      0.5000  -0.2000  20.0000   1.0000  -0.1000   9.0000   0.0000   0.0000
 3 14  81.4346   0.0000   0.0000  -0.1594  -0.3000   1.0000  36.0000   0.0025
      0.2904  -0.2500  12.0000   1.0000  -0.0742   9.3638   0.0000   0.0000
14 14  73.6263   0.0000   0.0000   0.0209  -0.2000   0.0000  16.0000   0.3414
      0.4703  -0.2000  15.0000   1.0000  -0.1319   5.9254   0.0000   0.0000
 6 14   0.0000   0.0000   0.0000   1.0000   0.3000   0.0000  26.0000   1.0000
      0.5000  -0.1000  12.0000   1.0000  -0.2000  25.0000   0.0000   0.0000
13 14   0.0000   0.0000   0.0000   1.0000   0.3000   0.0000  26.0000   1.0000
      0.5000  -0.1000  12.0000   1.0000  -0.2000  10.0000   0.0000   0.0000
 3 16 130.5629  37.6984   0.0000   0.9228  -0.3000   0.0000  36.0000   0.0850
      0.1150  -0.2818  16.1571   1.0000  -0.1343   6.8264   0.0000   0.0000
16 16  80.1930   0.0000   0.0000  -0.8469  -0.2000   0.0000  16.0000   0.2022
      0.7528  -0.1924  14.9725   1.0000  -0.0885   5.0000   0.0000   0.0000
13 16   0.0000   0.0000   0.0000   1.0000   0.3000   0.0000  26.0000   1.0000
      0.5000  -0.1000  12.0000   1.0000  -0.2000  10.0000   0.0000   0.0000
14 16   0.0000   0.0000   0.0000   1.0000   0.3000   0.0000  26.0000   1.0000
      0.5000  -0.1000  12.0000   1.0000  -0.2000  10.0000   0.0000   0.0000
44    ! Nr of off-diagonal terms;   Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.1239   1.4004   9.8467   1.1210  -1.0000  -1.0000
 2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
 2  4   0.1059   1.8290   9.7818   0.9598  -1.0000  -1.0000
 1  3   0.1156   1.8520   9.8317   1.2854   1.1352   1.0706
 1  4   0.1447   1.8766   9.7990   1.3436   1.1885   1.1363
 3  4   0.1048   2.0003  10.1220   1.3173   1.1096   1.0206
 1  6   0.0541   2.0811  13.5179   1.7778   1.5840  -1.0000
 2  6   0.1659   1.4000  11.7054   1.3437  -1.0000  -1.0000
 3  6   0.1330   2.0545  10.8315   1.7043   1.3773  -1.0000
```

4	6	0.1297	1.9384	10.9856	1.6175	1.4045	-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
1	7	0.1000	1.9000	11.5000	-1.0000	-1.0000	-1.0000
2	7	0.0100	1.6000	13.2979	-1.0000	-1.0000	-1.0000
3	7	0.0955	1.7587	11.9417	1.9052	-1.0000	-1.0000
5	7	0.1000	1.9000	11.0000	-1.0000	-1.0000	-1.0000
6	7	0.1000	1.9000	11.0000	-1.0000	-1.0000	-1.0000
2	8	0.2961	1.7153	13.7662	-1.0000	-1.0000	-1.0000
3	8	0.1924	1.7793	11.9109	1.9358	-1.0000	-1.0000
2	9	0.3000	1.5647	13.3924	-1.0000	-1.0000	-1.0000
3	9	0.1832	1.7503	12.6152	1.6986	-1.0000	-1.0000
2	10	0.0274	1.6386	13.6906	0.0010	-1.0000	-1.0000
3	10	0.2033	1.7974	11.2834	1.8164	-1.0000	-1.0000
5	8	0.2500	1.9000	12.0000	-1.0000	-1.0000	-1.0000
6	8	0.2500	1.9000	11.0000	-1.0000	-1.0000	-1.0000
5	9	0.2500	2.1000	10.5000	-1.0000	-1.0000	-1.0000
6	9	0.2500	2.1000	9.5000	-1.0000	-1.0000	-1.0000
5	10	0.3000	2.2000	11.5000	-1.0000	-1.0000	-1.0000
6	10	0.3000	2.2000	10.5000	-1.0000	-1.0000	-1.0000
3	11	0.0825	1.5904	11.3396	1.5905	-1.0000	-1.0000
6	11	0.1757	2.0409	13.7267	-1.0000	-1.0000	-1.0000
2	12	0.0200	1.4000	9.0000	1.8670	-1.0000	-1.0000
3	12	0.0702	1.7500	12.0414	1.4636	-1.0000	-1.0000
6	12	0.1000	1.8500	11.0000	-1.0000	-1.0000	-1.0000
2	13	0.0564	1.4937	12.0744	1.7276	-1.0000	-1.0000
3	13	0.1960	1.8464	11.1461	1.5646	-1.0000	-1.0000
6	13	0.0980	1.7870	10.6898	-1.0000	-1.0000	-1.0000
2	14	0.0300	1.5200	12.5000	0.1000	-1.0000	-1.0000
3	14	0.0348	1.7637	12.3562	1.7228	-1.0000	-1.0000
13	14	0.0341	0.7870	9.0714	-1.0000	-1.0000	-1.0000

```
 6 14   0.0650   1.3563   9.7035  -1.0000  -1.0000  -1.0000
 3 16   0.1200   1.8000  10.5000   1.6526   1.4718  -1.0000
13 16   0.0341   0.7870   9.0714  -1.0000  -1.0000  -1.0000
14 16   0.0341   0.7870   9.0714  -1.0000  -1.0000  -1.0000
141    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2;val(bo)
 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
 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
 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  49.6811   7.1713   4.3889   0.0000   0.7171  10.2661   1.0463
 3  1  3  77.7473  40.1718   2.9802 -25.3063   1.6170 -46.1315   2.2503
 1  1  4  66.1305  12.4661   7.0000   0.0000   3.0000  50.0000   1.1880
 3  1  4  73.9544  12.4661   7.0000   0.0000   3.0000   0.0000   1.1880
 4  1  4  64.1581  12.4661   7.0000   0.0000   3.0000   0.0000   1.1880
 2  1  3  65.0000  13.8815   5.0583   0.0000   0.4985   0.0000   1.4900
 2  1  4  74.2929  31.0883   2.6184   0.0000   0.0755   0.0000   1.0500
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  73.5312  44.7275   0.7354   0.0000   3.0000   0.0000   1.0684
 1  3  3  79.4761  36.3701   1.8943   0.0000   0.7351  67.6777   3.0000
 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   1.0783
 4  3  4  89.7071  31.4554   0.9953   0.0000   1.6310   0.0000   1.1519
 1  3  2  70.1880  20.9562   0.3864   0.0000   0.0050   0.0000   1.6924
 2  3  3  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000   1.1680
 2  3  4  75.6201  18.7919   0.9833   0.0000   0.1218   0.0000   1.0500
 2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000   1.5800
 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	1.0500
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	1.0369
2	4	4	83.0104	43.4766	1.5328	0.0000	0.0222	0.0000	1.0500
2	4	2	70.8687	12.0168	5.0132	0.0000	0.0222	0.0000	1.1243
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	1.0400
3	2	3	0.0000	15.0000	2.8900	0.0000	0.0000	0.0000	2.8774
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	8.5744	3.0000	0.0000	0.0000	0.0000	1.0421
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	5	74.9397	25.0560	1.8787	0.1463	0.0559	0.0000	1.0400
1	5	1	86.9521	36.9951	2.0903	0.1463	0.0559	0.0000	1.0400
2	1	5	74.9397	25.0560	1.8787	0.0000	0.0000	0.0000	1.0400
1	5	2	86.1791	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
1	5	5	85.3644	36.9951	2.0903	0.1463	0.0559	0.0000	1.0400
2	5	2	93.1959	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
2	5	5	84.3331	36.9951	2.0903	0.0000	0.0000	0.0000	1.0400
6	6	6	71.0490	32.4076	1.2648	0.0000	0.0133	0.0000	1.2899
2	6	6	77.2616	5.0190	7.8944	0.0000	4.0000	0.0000	1.0400
2	6	2	75.7983	14.4132	2.8640	0.0000	4.0000	0.0000	1.0400
3	6	6	99.8997	26.6610	2.1237	0.0000	0.0100	0.0000	1.4341
2	6	3	73.6998	40.0000	1.8782	0.0000	4.0000	0.0000	1.1290
3	6	3	98.2184	38.9429	0.7727	0.0000	1.1658	0.0000	2.2641
6	3	6	39.2858	1.3068	5.6478	0.0000	3.8972	0.0000	3.0000
2	3	6	79.2126	4.8973	8.0000	0.0000	1.0859	0.0000	2.1209

3 3 6 82.7397 32.1198 1.8862 0.0000 0.1058 0.0000 1.5443

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 69.1709 18.9268 2.1226 0.0000 1.0031 0.0000 1.0400

6 1 6 68.6453 18.7377 2.0496 0.0000 1.0031 0.0000 1.0400

1 6 6 68.9902 19.7021 2.0587 0.0000 1.0031 0.0000 1.0400

2 1 6 72.6403 13.6964 2.4702 0.0000 1.0000 0.0000 1.0400

1 6 2 71.8708 14.6864 2.4702 0.0000 1.0000 0.0000 1.0400

4 6 6 60.6199 17.7559 1.0576 0.0000 2.1459 0.0000 1.0400

4 6 4 74.1294 20.6494 2.1244 0.0000 0.7689 0.0000 1.0400

3 6 4 57.0650 9.4985 0.3423 0.0000 0.7689 0.0000 1.0400

6 4 6 24.1137 1.7457 0.2198 0.0000 4.1125 0.0000 1.0400

2 6 4 68.7410 15.5851 1.8545 0.0000 0.8613 0.0000 1.0400

2 4 6 80.9040 4.0560 1.2284 0.0000 1.6982 0.0000 1.0400

4 4 6 60.0000 10.0000 0.7500 0.0000 1.0000 0.0000 1.0400

3 4 6 69.8728 32.7155 1.5875 0.0000 2.2466 0.0000 1.0400

4 3 6 69.8728 27.1273 1.5875 0.0000 2.2466 0.0000 1.0400

4 2 6 0.0000 31.0427 4.5625 0.0000 1.6371 0.0000 1.0400

1 3 6 85.8521 12.6881 1.0112 0.0000 1.0000 0.0000 1.3220

1 6 3 71.7524 35.8987 1.5000 0.0000 1.0000 0.0000 1.0487

3 1 6 70.0000 5.0250 1.0000 0.0000 1.0000 0.0000 1.2500

1 2 6 0.0000 2.5000 1.0000 0.0000 1.0000 0.0000 1.2500

3 7 3 1.0000 4.9611 2.4541 0.0000 0.5754 0.0000 1.0000

7 3 7 9.5066 4.2640 3.1438 0.0000 1.9819 0.0000 1.6463

2 3 7 51.3829 2.5000 0.2500 0.0000 0.0500 0.0000 1.0000

3 3 7 70.0000 25.0000 1.0000 0.0000 1.0000 0.0000 1.2500

3 8 3 45.7222 4.2175 3.5761 0.0000 0.6153 0.0000 2.3668

2 3 8 94.0770 2.0922 6.0000 0.0000 0.7307 0.0000 1.0135

8 3 8 75.6996 5.2610 3.9306 0.0000 1.9091 0.0000 1.1965

3 9 3 100.0000 1.2360 6.8249 0.0000 3.2930 0.0000 1.0000

2 3 9 100.0000 1.0007 9.7740 0.0000 1.4276 0.0000 1.0000

9 3 9 98.5744 2.1499 1.6268 0.0000 3.7347 0.0000 2.8271

3 10 3 40.5067 9.9705 4.0000 0.0000 0.0500 0.0000 1.5730

10 3 10 40.0000 9.5071 4.0000 0.0000 3.7118 0.0000 1.4108

2 3 10 81.1078 2.0823 5.0000 0.0000 0.7032 0.0000 1.0000

3 3 10 70.0000 25.0000 1.0000 0.0000 1.0000 0.0000 1.2500

5 3 7 40.0000 5.0000 2.0000 0.0000 1.0000 0.0000 1.2500

6 3 7 30.0000 10.0000 2.0000 0.0000 1.0000 0.0000 1.2500

5 3 8 40.0000 10.0000 2.0000 0.0000 1.0000 0.0000 1.2500

6 3 8 30.0000 15.0000 2.0000 0.0000 1.0000 0.0000 1.2500

5 3 9 40.0000 4.0000 2.0000 0.0000 1.0000 0.0000 1.2500

6 3 9 30.0000 8.0000 2.0000 0.0000 1.0000 0.0000 1.2500

5 3 10 40.0000 15.0000 2.0000 0.0000 1.0000 0.0000 1.2500

6 3 10 30.0000 22.5000 2.0000 0.0000 1.0000 0.0000 1.2500

2 12 2 0.0000 49.8261 0.2093 0.0000 2.0870 0.0000 2.2895

2 2 12 0.0000 40.0366 3.1505 0.0000 1.1296 0.0000 1.1110

12 2 12 0.0000 0.5047 0.8000 0.0000 0.8933 0.0000 4.6650

2 12 12 0.0000 8.7037 0.0827 0.0000 3.5597 0.0000 1.1198

3 12 3 16.6660 25.0000 1.4129 0.0000 0.3049 0.0000 1.2391

12 3 12 58.7093 23.5645 8.1273 0.0000 3.9792 0.0000 1.6907

2 3 12 47.5370 6.3596 2.6766 0.0000 2.7588 0.0000 2.6720

2 12 3 0.0000 35.0000 0.3447 0.0000 1.0000 0.0000 1.9494

3 3 12 70.0000 20.0000 1.0000 0.0000 1.0000 0.0000 1.2500

6 3 12 30.0000 10.0000 2.0000 0.0000 1.0000 0.0000 1.2500

3 2 13 0.0000 4.2750 1.0250 0.0000 1.3750 0.0000 1.4750

2 2 13 0.0000 3.0000 1.0000 0.0000 1.0000 0.0000 1.2500

13 2 13 0.0000 20.2391 0.1328 0.0000 2.9860 0.0000 1.0870

2 3 13 88.6163 10.1310 1.6896 0.0000 3.0000 0.0000 1.0000

3 3 13 34.4326 25.9544 5.1239 0.0000 2.7500 0.0000 1.7141

13 3 13 13.8580 12.3669 4.4355 0.0000 0.6619 0.0000 1.1908
2 13 2 67.4229 4.5148 5.9702 0.0000 3.0000 0.0000 2.6879
2 13 3 41.8108 17.3800 2.6618 0.0000 0.7372 0.0000 1.0100
3 13 3 55.4358 22.1089 3.7402 0.0000 3.0000 0.0000 2.2064
3 13 13 32.1032 2.3304 4.5935 0.0000 0.5894 0.0000 1.0140
2 13 13 180.0000 -26.7860 7.3549 0.0000 1.0000 0.0000 1.0252
2 13 13 78.2279 37.6504 0.4809 0.0000 1.0000 0.0000 2.9475
6 3 13 7.1670 11.9291 3.9535 0.0000 1.0000 0.0000 3.4258
3 14 3 96.2265 4.5610 12.0000 0.0000 0.3211 0.0000 1.5204
3 14 3 0.0000 9.1552 7.9919 0.0000 0.1660 0.0000 1.5386
14 3 14 100.0000 10.1065 6.0000 0.0000 1.0000 0.0000 3.6601
2 3 14 55.0417 3.5032 3.9979 0.0000 1.5171 0.0000 1.0400
3 3 14 70.0000 30.0000 2.0000 0.0000 1.0000 0.0000 1.2500
3 14 14 66.7783 14.3146 0.7911 0.0000 1.0000 0.0000 1.2333
13 3 14 68.0314 6.5925 10.1832 0.0000 3.3231 0.0000 0.8395
6 3 14 113.9913 7.3197 0.3892 0.0000 3.2258 0.0000 1.1530
3 16 3 90.0000 30.4624 2.1468 0.0000 0.0500 0.0000 1.9485
16 3 16 90.0000 5.7486 5.0000 0.0000 2.0000 0.0000 1.1000
3 3 16 62.9344 15.0215 4.3743 0.0000 0.6168 0.0000 1.1673
3 16 16 33.7127 8.0623 3.4580 0.0000 0.0500 0.0000 2.6065
13 3 16 68.0314 6.5925 10.1832 0.0000 3.3231 0.0000 0.8395
14 3 16 68.0314 6.5925 10.1832 0.0000 3.3231 0.0000 0.8395
42 ! 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
1 1 1 3 -0.3495 22.2142 -0.2959 -2.5000 -1.9066 0.0000 0.0000
2 1 1 3 0.0646 24.3195 0.6259 -3.9603 -1.0000 0.0000 0.0000
3 1 1 3 -0.5456 5.5756 0.8433 -5.1924 -1.0180 0.0000 0.0000
1 1 3 1 1.7555 27.9267 0.0072 -2.6533 -1.0000 0.0000 0.0000
1 1 3 2 -1.4358 36.7830 -1.0000 -8.1821 -1.0000 0.0000 0.0000

2 1 3 1 -1.3959 34.5053 0.7200 -2.5714 -2.1641 0.0000 0.0000

2 1 3 2 -2.5000 70.0597 1.0000 -3.5539 -2.9929 0.0000 0.0000

1 1 3 3 0.6852 11.2819 -0.4784 -2.5000 -2.1085 0.0000 0.0000

2 1 3 3 0.1933 80.0000 1.0000 -4.0590 -3.0000 0.0000 0.0000

3 1 3 1 -1.9889 76.4820 -0.1796 -3.8301 -3.0000 0.0000 0.0000

3 1 3 2 0.2160 72.7707 -0.7087 -4.2100 -3.0000 0.0000 0.0000

3 1 3 3 -2.5000 71.0772 0.2542 -3.1631 -3.0000 0.0000 0.0000

1 3 3 1 2.5000 -0.6002 1.0000 -3.4297 -2.8858 0.0000 0.0000

1 3 3 2 -2.5000 -3.3822 0.7004 -5.4467 -2.9586 0.0000 0.0000

2 3 3 2 2.5000 -4.0000 0.9000 -2.5000 -1.0000 0.0000 0.0000

1 3 3 3 1.2329 -4.0000 1.0000 -2.5000 -1.7479 0.0000 0.0000

2 3 3 3 0.8302 -4.0000 -0.7763 -2.5000 -1.0000 0.0000 0.0000

3 3 3 3 -2.5000 -4.0000 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

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 -2.7203 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 3.3423 30.3435 0.0365 -2.7171 0.0000 0.0000 0.0000

0 5 5 0 -0.0555 -42.7738 0.1515 -2.2056 0.0000 0.0000 0.0000

0 2 5 0 0.0000 0.0000 0.0000 0.0000 0.0000 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 2 6 0 0.0000 0.0000 0.1200 -2.4847 0.0000 0.0000 0.0000

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

1 1 3 3 -2.0000 73.0530 1.5000 -9.0000 -2.0000 0.0000 0.0000

1 3 3 1 0.0002 80.0000 -1.5000 -2.5000 -2.0000 0.0000 0.0000

3 1 3 3 -1.8835 20.0000 1.5000 -9.0000 -2.0000 0.0000 0.0000

2 3 14 3 -1.5000 6.8333 -0.1978 -1.4683 0.0000 0.0000 0.0000

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

3 2 3 2.1200 -3.5800 1.4500 19.5000