SUPPORTING INFORMATION

Development of a ReaxFF reactive force field for Fe/Cr/O/S and application to oxidation of butane over a pyrite-covered Cr_2O_3 catalyst

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Figure Captions

Figure S1 Initial configurations of the (a) C4H10/O2, (b) C4H10/O2/Cr2O3 and (c) C4H10/O2/Cr2O3/FeS2 systems. Gray and white colors represent C and H of hydrocarbon, respectively. Cyan, red, green and yellow colors represent Cr, O, Fe and S of Cr-oxide and pyrite, respectively.

Figure S2 Equations of state for single crystals of Cr metal (bcc, fcc and a15) at 0 K. A cohesive energy of bcc Cr is 93.7 kcal/mol in ReaxFF, compared to an experimental value of 94.6 kcal/mol and the QM value of 93.9 kcal/mol.

Figure S3 Number of products during the NVT-MD simulation of C4H10/O2 system at 2500 K.

Figure S4 Dehydrogenation of C4H10 on Cr-oxide, forming a hydroxyl group and a butane radical. The reaction was observed at 1000 K.

Figure S5 Number of hydroxyl group formed on the Cr2O3 and Cr2O3/FeS2 surfaces during the oxidation of C4H10. In the presence of pyrite, SOH species is also generated.

Figure S6 Number of carbon atoms in the carbon-containing intermediates bound to the Cr2O3 and FeS2/Cr2O3 surface.

Figure S7 The amount of Cr atoms with low coordination number (≤ 4) and bulk oxide-like coordination number (> 4) during the butane oxidation in (a) Cr oxide and (b) pyrite-modified Cr oxide.

Figure S8 The number of reactive oxygen species evolved during the butane oxidation on (a) the clean Cr oxide and (b) the pyrite-modified Cr oxide at 1600 K.

Figure S9 The amount of sulfur species released from pyrite during the butane dehydrogenation reaction without O2 at 2000 K.

Figures

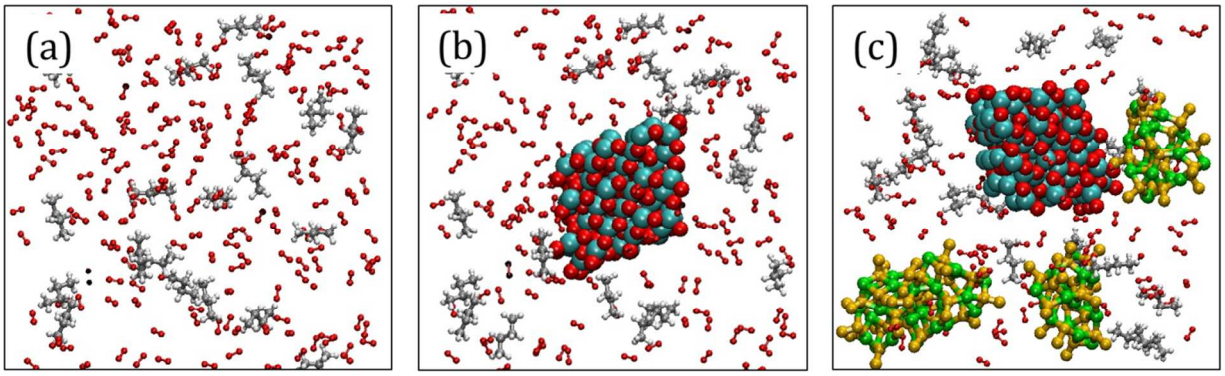

Figure S1 Initial configurations of the (a) C_4H_{10}/O_2, (b) $C_4H_{10}/O_2/Cr_2O_3$ and (c) $C_4H_{10}/O_2/Cr_2O_3/FeS_2$ systems. Gray and white colors represent C and H of hydrocarbon, respectively. Cyan, red, green and yellow colors represent Cr, O, Fe and S of Cr-oxide and pyrite, respectively.

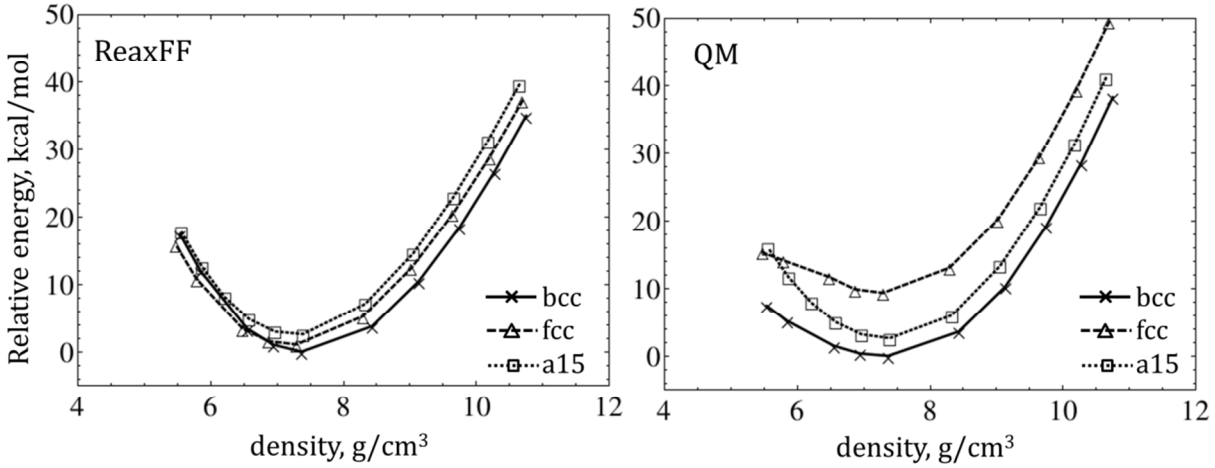

Figure S2 Equations of state for single crystals of Cr metal (bcc, fcc and a15) at 0 K. A cohesive energy of bcc Cr is 93.7 kcal/mol in ReaxFF, compared to an experimental value of 94.6 kcal/mol and the QM value of 93.9 kcal/mol.

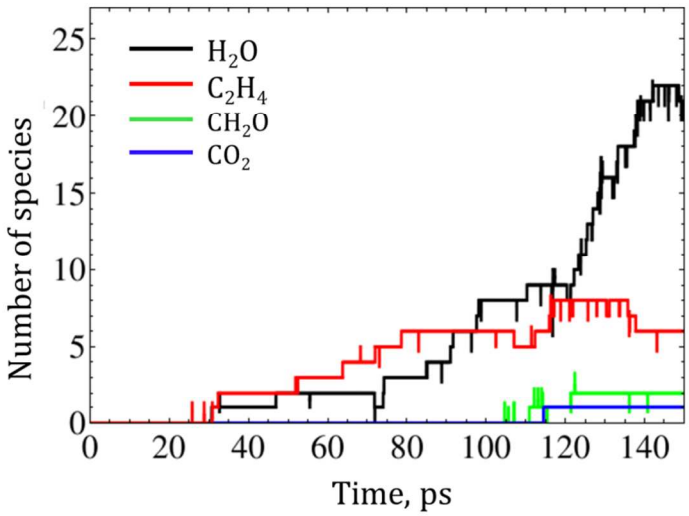

Figure S3 Number of products during the NVT-MD simulation of C_4H_{10}/O_2 system at 2500 K.

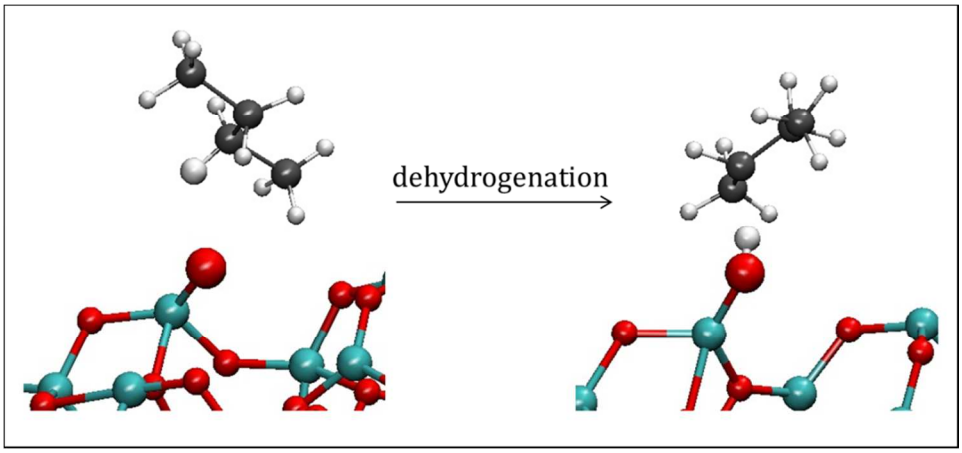

Figure S4 Dehydrogenation of C_4H_{10} on Cr-oxide, forming a hydroxyl group and a butane radical. The reaction was observed at 1000 K.

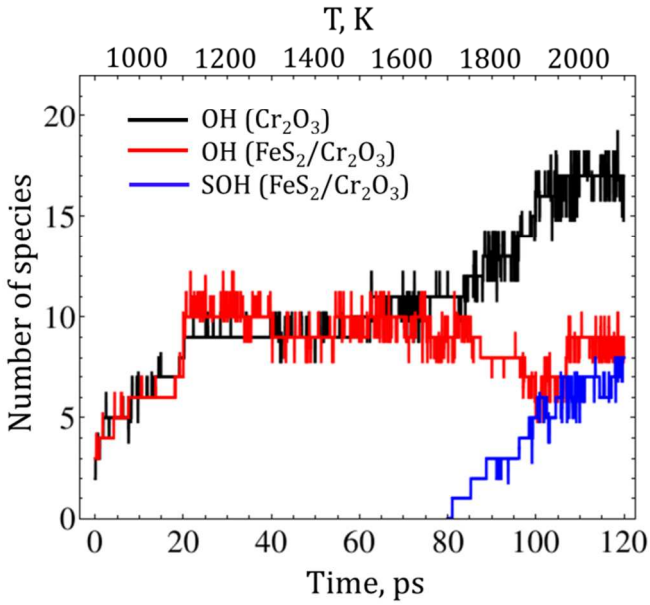

Figure S5 Number of hydroxyl group formed on the Cr_2O_3 and Cr_2O_3/FeS_2 surfaces during the oxidation of C_4H_{10}. In the presence of pyrite, SOH species is also generated.

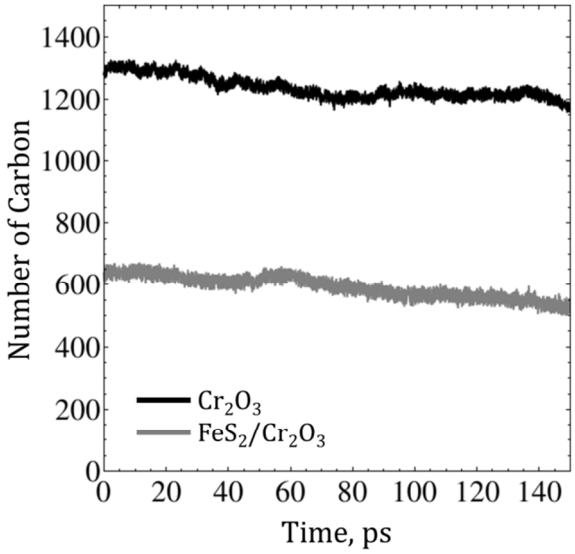

Figure S6 Number of carbon atoms in the carbon-containing intermediates bound to the Cr_2O_3 and FeS_2/Cr_2O_3 surface.

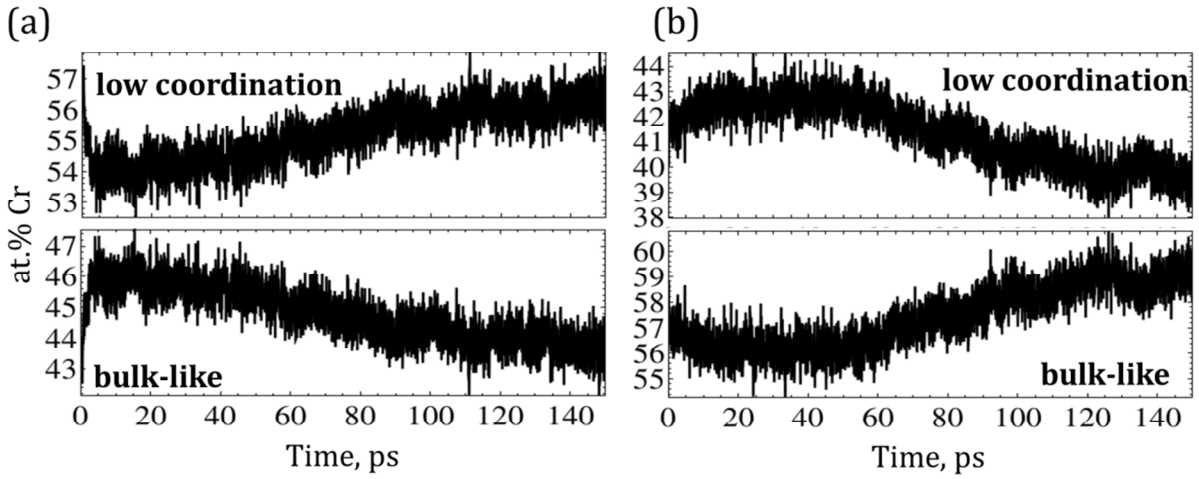

Figure S7 The amount of Cr atoms with low coordination number (≤ 4) and bulk oxide-like coordination number (> 4) during the butane oxidation in (a) Cr oxide and (b) pyrite-modified Cr oxide.

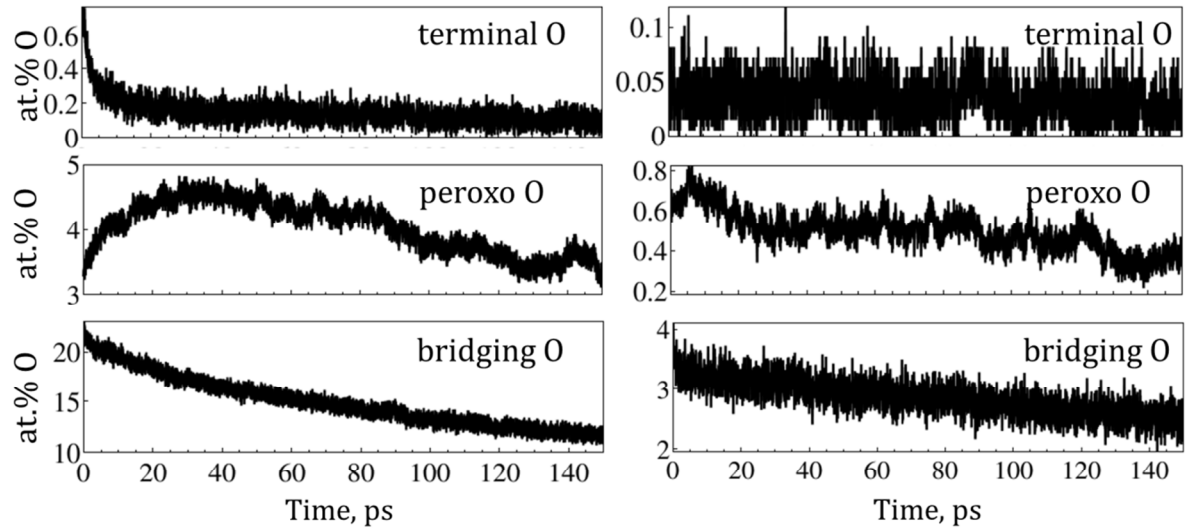

Figure S8 The number of reactive oxygen species evolved during the butane oxidation on (a) the clean Cr oxide and (b) the pyrite-modified Cr oxide at 1600 K.

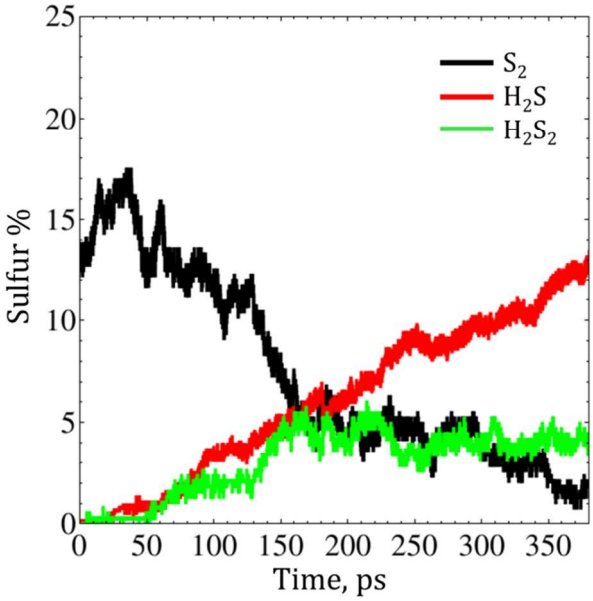

Figure S9 The amount of sulfur species released from pyrite during the butane dehydrogenation reaction without O_2 at 2000 K.

The ReaxFF Reactive Force Field parameters for Cr/O/Fe/S/C/H

This force field can be used with the standalone ReaxFF program, as well as with the LAMMPS open-source MD-program and the ADF-program.

```
Reactive MD-force field: Cr/O/Fe/S/C/H force field 2014
 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
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  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
 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    1.3817   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
Fe   1.9029   3.0000  55.8450   2.0990   0.1181   0.4744  -1.6836   3.0000
    10.8548   2.6084   3.0000   0.0000  18.3725   1.7785   8.6281   0.0000
    -1.2000   0.0000 102.1000  25.3430  10.1260   0.7590   0.8563   0.0000
   -16.0573   2.6997   1.0338   6.0000   2.5791   0.0000   0.0000   0.0000
S    1.8328   2.0000  32.0600   1.8815   0.3236   0.7530   1.6468   6.0000
     9.0000   4.9055   4.0000  30.0000 112.1416   6.5745   9.0000   2.0000
     1.0000   3.4994  65.0000  12.0000  22.1978  15.3230   0.9745   0.0000
   -15.7363   2.8802   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
Cr   1.8921   6.0000  51.9962   2.3712   0.2336   0.5639  -1.6836   6.0000
    10.3177   2.8702   6.0000   0.0000  18.3190   1.4546   8.9500   0.0000
    -1.2000   0.0000 102.1000  25.3430  10.1260   0.7590   0.8563   0.0000
   -11.1953   2.6997   1.0338   6.0000   2.5791   0.0000   0.0000   0.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   0.0100  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   5.00009999.9999   0.0000
    -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   2.0000   2.8793   0.0000   0.0000   0.0000
21      ! 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  3 164.4303  82.6772  60.8077  -0.3739  -0.2351   1.0000  10.5036   1.0000
        0.4475  -0.2288   7.0250   1.0000  -0.1363   4.8734   0.0000   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   0.0000  -0.0920   4.2790   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  4 109.5214   0.0000   0.0000   0.6663  -0.3000   1.0000  36.0000   0.0100
        1.0648  -0.3500  15.0000   1.0000  -0.1512   4.1708   1.0000   0.0000
```

```
  2  4  78.2669   0.0000   0.0000   0.4668   0.0000   1.0000   6.0000   0.1766
        0.5673   1.0000   0.0000   1.0000  -0.1543   5.4965   0.0000   0.0000
  3  4  67.5128   0.0000   0.0000   0.1301  -0.3000   0.0000  36.0000   0.0852
        1.0000  -0.3500  15.0000   1.0000  -0.0629   7.1208   0.0000   0.0000
  4  4  41.4611   0.0000   0.0000   0.2931  -0.2000   0.0000  16.0000   0.2682
        0.6294  -0.2000  15.0000   1.0000  -0.0512   6.8013   0.0000   0.0000
  1  5 192.1462  90.5383  55.2528  -0.5652  -0.5211   1.0000  18.9617   0.1958
        2.0000  -0.1016  13.8750   1.0000  -0.1579   5.5813   1.0000   0.0000
  2  5 188.3744   0.0000   0.0000  -0.6562   0.0000   1.0000   6.0000   0.3870
       11.8360   1.0000   0.0000   1.0000  -0.0762   5.0961   1.0000   0.0000
  3  5 107.2917 202.9813  40.0000   0.4728  -0.2406   1.0000  22.1005   0.0500
        0.6528  -0.3341   7.9877   1.0000  -0.0909   6.9512   1.0000   0.0000
  4  5  75.5280   0.0000   0.0000  -0.4815  -0.3390   0.0000  16.0000   0.1769
        0.2800  -0.1838  15.0000   1.0000  -0.0758   6.3424   0.0000   0.0000
  5  5  86.8868  69.1367   0.0000  -0.9993  -0.4781   1.0000  17.8574   0.0999
        0.2799  -0.1677   8.2557   1.0000  -0.1131   6.1440   1.0000   0.0000
  2  6   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000   0.5000
        0.3000  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000   0.0000
  3  6 114.0666   0.0000   0.0000   0.2305  -0.3000   1.0000  36.0000   0.6591
        0.5793  -0.3500  15.0000   1.0000  -0.1989   4.8803   1.0000   0.0000
  5  6  88.6258   0.0000   0.0000   0.6879  -0.3891   1.0000  36.0000   0.0835
        0.2900  -0.2339  12.1279   1.0000  -0.1166   5.6660   1.0000   0.0000
  6  6  57.5947   0.0000   0.0000  -1.0000  -0.3000   0.0000  16.0000   0.0100
        0.0842  -0.3000  16.0000   1.0000  -0.1098   5.3349   0.0000   0.0000
  4  6  41.4444   0.0000   0.0000   0.9374  -0.1000   0.0000  16.0000   0.0106
        0.2209  -0.2000  15.0000   1.0000  -0.0925   6.1220   0.0000   0.0000
  1  6   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000   0.5000
        0.3000  -0.3500  15.0000   1.0000  -0.2000   8.0000   1.0000   0.0000
 15    ! 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
  1  3   0.1345   1.8422   9.7725   1.2835   1.1576   1.0637
  2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
  1  4   0.4204   1.4900  11.0144   1.4071  -1.0000  -1.0000
  2  4   0.0200   1.9451  10.8595   1.4157  -1.0000  -1.0000
  3  4   0.1000   1.8000   9.1989   1.7050  -1.0000  -1.0000
  1  5   0.3314   1.7976  10.5605   1.6918   1.4000  -1.0000
  2  5   0.1020   1.7528   9.6276   1.3714  -1.0000  -1.0000
  3  5   0.2832   1.8196  10.2295   1.4502   1.4557  -1.0000
  4  5   0.0854   1.7474  12.7924   1.9838  -1.0000  -1.0000
  2  6   0.1000   1.5000  11.0000  -1.0000  -1.0000  -1.0000
  3  6   0.0582   1.7000  11.6513   1.5924  -1.0000  -1.0000
  5  6   0.2523   1.9844  10.1396   1.8938  -1.0000  -1.0000
  4  6   0.3236   2.1670  10.1297   1.9025  -1.0000  -1.0000
  1  6   0.1000   1.5000  11.0000  -1.0000  -1.0000  -1.0000
120    ! 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
  2  1  2  70.2607  25.2202   3.7312   0.0000   0.0050   0.0000   2.7500
  1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
  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
  1  1  3  53.9517   7.8968   2.6122   0.0000   3.0000  58.6562   1.0338
  3  1  3  76.9627  44.2852   2.4177 -25.3063   1.6334 -50.0000   2.7392
  1  3  1  72.6199  42.5510   0.7205   0.0000   2.9294   0.0000   1.3096
  1  3  3  81.9029  32.2258   1.7397   0.0000   0.9888  68.1072   1.7777
  3  3  3  80.7324  30.4554   0.9953   0.0000   3.0000  50.0000   1.0783
  2  1  3  65.0000  16.3141   5.2730   0.0000   0.4448   0.0000   1.4077
  1  3  2  70.1101  13.1217   4.4734   0.0000   0.8433   0.0000   3.0000
  2  3  3  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000   1.1680
  2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000   1.5800
  1  2  3   0.0000  25.0000   3.0000   0.0000   1.0000   0.0000   1.0400
  2  2  3   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000   1.0421
  3  2  3   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000   2.8774
```

1	4	1	0.1000	42.2980	0.3169	0.0000	1.1069	0.0000	2.3466
1	1	4	74.8790	30.0000	2.0000	0.0000	2.0334	0.0000	1.0928
1	4	4	47.9341	1.0246	7.9341	0.0000	2.8853	0.0000	1.0000
4	1	4	33.2812	34.6443	3.0111	0.0000	0.1701	0.0000	1.0510
2	4	2	20.3683	0.0100	2.2825	0.0000	0.7660	0.0000	1.3788
2	2	4	0.0000	0.0100	1.0568	0.0000	1.8595	0.0000	3.6142
4	2	4	0.0000	10.4428	7.9607	0.0000	2.3717	0.0000	1.1970
2	4	4	48.4128	4.0632	0.6773	0.0000	2.2274	0.0000	1.8605
2	1	4	2.6539	32.1638	0.9167	0.0000	0.0240	0.0000	1.1158
1	4	2	42.7140	0.1451	0.2500	0.0000	0.0851	0.0000	2.8955
1	2	4	0.0000	0.0100	2.2066	0.0000	1.9789	0.0000	1.4466
1	3	4	90.0000	42.4716	6.6776	0.0000	2.4560	0.0000	1.6221
3	1	4	54.6900	12.6123	2.3543	0.0000	2.0000	0.0000	1.2513
1	4	3	38.2755	19.3103	0.1151	0.0000	0.7569	0.0000	2.3113
2	3	4	26.0012	49.6772	0.0500	0.0000	1.1589	0.0000	1.0000
3	2	4	0.0000	0.0100	3.2567	0.0000	2.0582	0.0000	1.3513
2	4	3	38.5594	11.2599	0.1898	0.0000	0.1904	0.0000	1.4041
4	3	4	63.0740	14.8127	2.9929	0.0000	0.7552	0.0000	1.3634
3	3	4	73.6721	32.6330	1.7223	0.0000	1.0221	0.0000	1.4351
3	4	3	76.5431	0.0583	0.0500	0.0000	0.4968	0.0000	2.2792
3	4	4	69.4895	5.7742	8.0001	0.0000	1.7794	0.0000	2.7889
5	5	5	84.2345	15.5790	3.7715	0.0000	1.3066	0.0000	1.6270
2	5	2	90.0601	42.2756	0.5302	0.0000	0.3707	0.0000	1.0071
2	5	5	66.1035	8.0885	1.0424	0.0000	0.7355	0.0000	3.0000
1	1	5	71.4462	27.2223	6.7228	0.0000	0.0050	0.0000	2.6454
1	5	1	92.6710	15.6798	3.1104	0.0000	0.3458	0.0000	2.3207
2	1	5	43.6595	11.8933	0.5449	0.0000	0.0050	0.0000	1.9326
1	5	2	99.1897	14.1666	2.5588	0.0000	0.3542	0.0000	2.5990
1	5	5	89.3910	5.0000	7.0000	0.0000	1.0050	0.0000	1.5000
3	5	3	83.5231	37.5859	0.9881	-0.0100	1.4725	0.0000	1.0641
1	5	3	79.9791	29.5117	7.0000	0.0000	0.0050	0.0000	1.2255
1	3	5	83.1032	23.4174	0.7741	0.0000	1.2168	0.0000	2.7365
3	3	5	60.2631	30.0701	2.1707	0.0000	1.3323	0.0000	1.0192
3	5	5	55.9402	38.2990	3.6930	0.0000	2.2673	0.0000	1.0000
2	3	5	35.9099	19.1501	1.9918	0.0000	0.9342	0.0000	2.7883
1	2	5	0.0000	0.2500	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	5	0.0000	1.0000	6.0000	0.0000	0.0000	0.0000	1.0400
5	2	5	0.0000	7.5000	2.0000	0.0000	0.0000	0.0000	1.0400
5	4	5	0.2000	7.5083	1.3736	0.0000	0.0412	0.0000	1.8149
4	5	4	100.0000	9.2519	0.7752	0.0000	0.1221	0.0000	2.2142
4	4	5	33.4003	16.6274	0.1076	0.0000	0.0825	0.0000	1.0000
4	5	5	77.0475	7.4569	4.9579	0.0000	0.7548	0.0000	2.3345
2	5	4	84.8837	16.4865	0.8240	0.5000	0.5428	0.0000	1.1398
4	2	5	0.0000	10.0000	1.0000	0.5000	0.2500	0.0000	1.5000
3	4	5	29.3282	8.1452	2.8121	0.0000	0.2287	0.0000	1.9412
4	3	5	4.8461	5.5458	2.9681	0.0000	1.0491	0.0000	1.4836
3	5	4	89.9073	7.0973	1.3919	0.0000	0.8210	0.0000	2.9921
3	6	3	63.9878	12.9742	3.0000	0.0000	0.5058	0.0000	3.0000
6	3	6	54.9212	26.4957	1.1780	0.0000	2.0000	0.0000	2.2398
3	3	6	44.9499	30.0000	4.2281	0.0000	1.6672	0.0000	1.2000
3	6	6	51.2416	17.2148	0.3698	0.0000	1.5585	0.0000	1.5755
2	3	6	70.0000	20.0000	2.0000	0.0000	1.0000	0.0000	1.0500
2	6	3	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0500
3	2	6	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0500
2	6	6	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0500
2	6	2	70.0000	20.0000	2.0000	0.0000	1.0000	0.0000	1.0500
6	2	6	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0500
2	2	6	70.0000	20.0000	2.0000	0.0000	1.0000	0.0000	1.0500
5	6	5	70.0000	20.0000	2.0000	0.0000	1.0000	0.0000	1.0000
6	5	6	87.7418	23.5125	2.9950	0.0000	0.5199	0.0000	1.6571
5	5	6	70.0000	20.0000	2.0000	0.0000	1.0000	0.0000	1.0000
5	6	6	50.5809	19.2597	0.3584	0.0000	0.2153	0.0000	1.6345
2	5	6	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0500

```
 1  5  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 5  3  5  76.3546  40.0000   3.3161   0.0005   1.9473   0.0000   1.0000
 4  3  6  61.0461   0.2600   1.3988   0.0000   0.9535   0.0000   3.0000
 3  6  4  44.3862  26.6099   2.0221   0.0000   1.9212   0.0000   3.0000
 3  4  6  41.9243  20.0000   2.9881   0.0000   1.2678   0.0000   2.6481
 3  6  5  19.4072  10.4590   2.8285   0.0000   1.0074   0.0000   2.3949
 3  5  6  83.6415  19.7500   2.9247   0.0000   1.9437   0.0000   1.0348
 5  3  6  89.6617  15.3276   2.7567   0.0000   1.6031   0.0000   1.0781
 5  4  6   0.2000   7.5083   1.3736   0.0000   0.0412   0.0000   1.8149
 4  6  5  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0000
 4  5  6  93.8709  16.3822   1.8851   0.0000   0.3210   0.0000   1.9357
 1  4  5  60.3275  30.0000   1.0871   0.0000   1.3106   0.0000   1.6977
 1  5  4  67.5806  21.4421   0.9049   0.0000   0.7789   0.0000   1.2000
 4  1  5  89.6657  30.0000   3.0000   0.0000   2.0000   0.0000   1.2000
 1  2  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  6  2  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 2  1  6  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 1  6  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  6  1  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 6  1  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  1  6  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 1  6  3  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 3  1  6  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 1  3  6  63.7706  34.5234   0.9493   0.0000   2.4647   0.0000   1.7747
 1  6  4   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  4  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 4  1  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 2  6  4   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 2  4  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 4  2  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  2  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  6  2   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 2  1  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 1  5  6  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 1  6  5  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 5  1  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
 2  6  5  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 2  5  6  70.0000  20.0000   2.0000   0.0000   1.0000   0.0000   1.0500
 5  2  6   0.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.0500
38    ! 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   1.2799  20.7787  -0.5249  -2.5000  -1.0000   0.0000   0.0000
 2  1  1  3   1.9159  19.8113   0.7914  -4.6995  -1.0000   0.0000   0.0000
 3  1  1  3  -1.4477  16.6853   0.6461  -4.9622  -1.0000   0.0000   0.0000
 1  1  3  1   0.4816  19.6316  -0.0057  -2.5000  -1.0000   0.0000   0.0000
 1  1  3  2   1.2044  80.0000  -0.3139  -6.1481  -1.0000   0.0000   0.0000
 2  1  3  1  -2.5000  31.0191   0.6165  -2.7733  -2.9807   0.0000   0.0000
 2  1  3  2  -2.4875  70.8145   0.7582  -4.2274  -3.0000   0.0000   0.0000
 2  1  3  3  -1.4383  80.0000   1.0000  -3.6877  -2.8000   0.0000   0.0000
 3  1  3  1  -1.1390  78.0747  -0.0964  -4.5172  -3.0000   0.0000   0.0000
 3  1  3  2  -2.5000  70.3345  -1.0000  -5.5315  -3.0000   0.0000   0.0000
 3  1  3  3  -0.1583  20.0000   1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  3  3  1   0.0002  80.0000  -1.5000  -4.4848  -2.0000   0.0000   0.0000
 1  3  3  2  -2.5000   0.1181   0.0268  -5.4085  -2.9498   0.0000   0.0000
 2  3  3  2   0.1995   5.0000   0.2000  -2.6000   0.0000   0.0000   0.0000
 1  3  3  3   0.4118   0.5219   0.9706  -2.5004  -0.9972   0.0000   0.0000
 2  3  3  3   0.1000  43.1840   0.5000  -6.6539   0.0000   0.0000   0.0000
 3  3  3  3   0.1000   1.0000   0.1000  -2.5000  -0.9000   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   0.0000   0.0000   0.0000
0  3  3  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000   0.0000
1  1  3  3  -0.0002  20.1851   0.1601  -9.0000  -2.0000   0.0000   0.0000
2  1  4  4   0.0000   0.0000   0.0000  -5.0000   0.0000   0.0000   0.0000
0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
5  5  5  5   2.4661  71.9719   0.0100  -8.0000   0.0000   0.0000   0.0000
2  5  5  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000   0.0000
2  3  5  3   2.5000   2.5000   0.2237 -10.0000   0.0000   0.0000   0.0000
0  1  5  0   0.5000  50.0000   0.5000 -10.0000   0.0000   0.0000   0.0000
0  3  5  0   0.5000  50.0000   0.5000  -8.0000   0.0000   0.0000   0.0000
3  5  5  5   0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000   0.0000
3  5  5  3   0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000   0.0000
1  5  5  1   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000   0.0000
1  5  5  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000   0.0000
2  5  5  2   0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000   0.0000
4     ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
3  2  3   2.1200  -3.5800   1.4500  19.5000
3  2  5   2.5000  -1.0000   1.4500  19.5000
5  2  3   2.5000  -1.0000   1.4500  19.5000
5  2  5   2.5000  -2.0000   1.4500  19.5000
```