Supplementary information for:

Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO_2/Al_2O_3 Electrodes of Li-ion Batteries: ReaxFF Reactive Force Field Modeling

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Tables and Figures:

Figure S1. Diffusion coefficient of Li in a-SiO2at different Li concentration. MSD versus time.

Figure S2. Representative structure of *a*-SiO_2 and diffusion of Li

Figure S3. Lithiation and dilithiation of *a*-Si

Table S1: ReaxFF potential parameters for Li/Si/O/Al interactions.

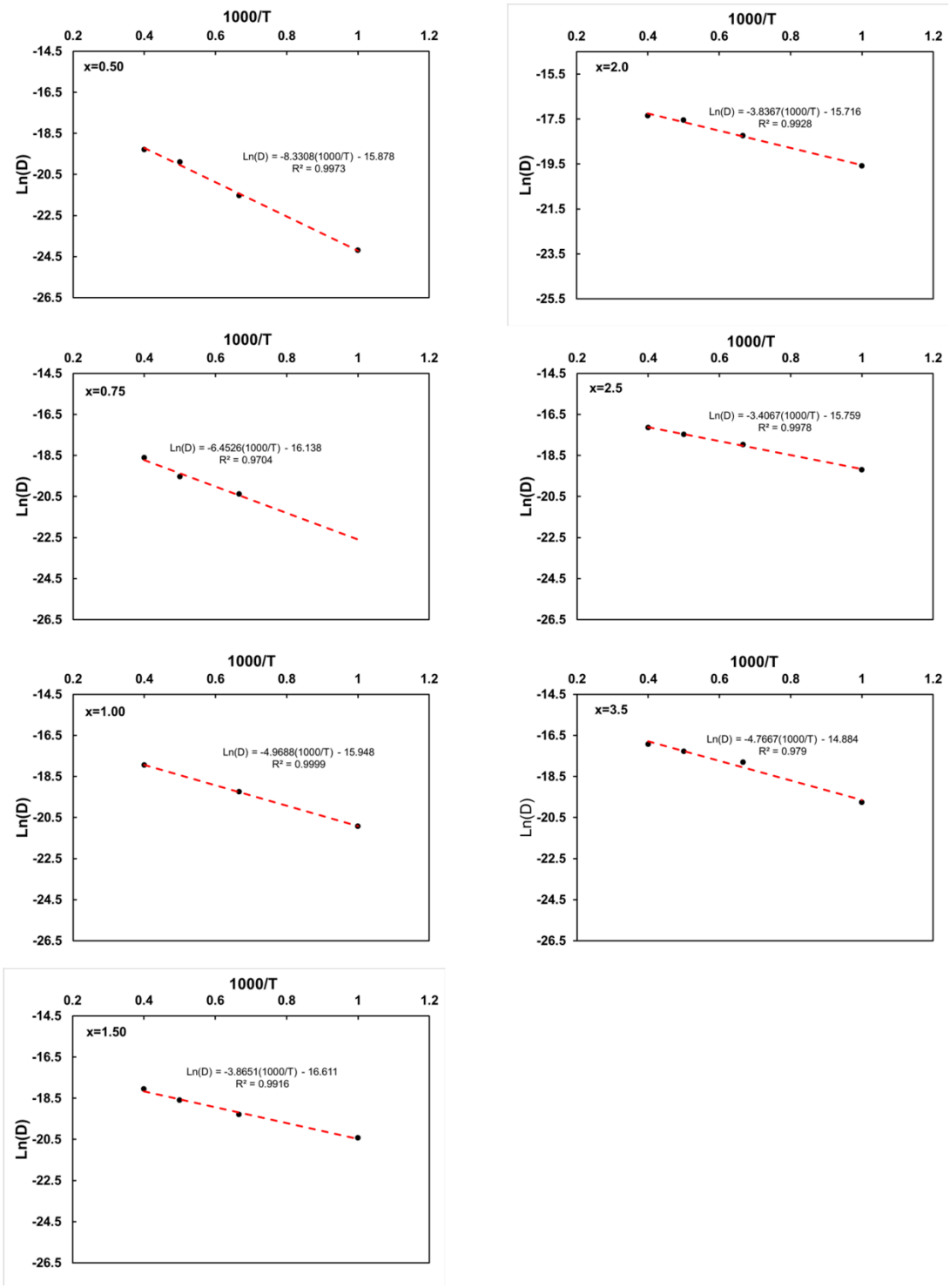

Figure S1. Diffusion coefficient of Li in *a*-SiO_2 at different Li concentration. MSD versus time.

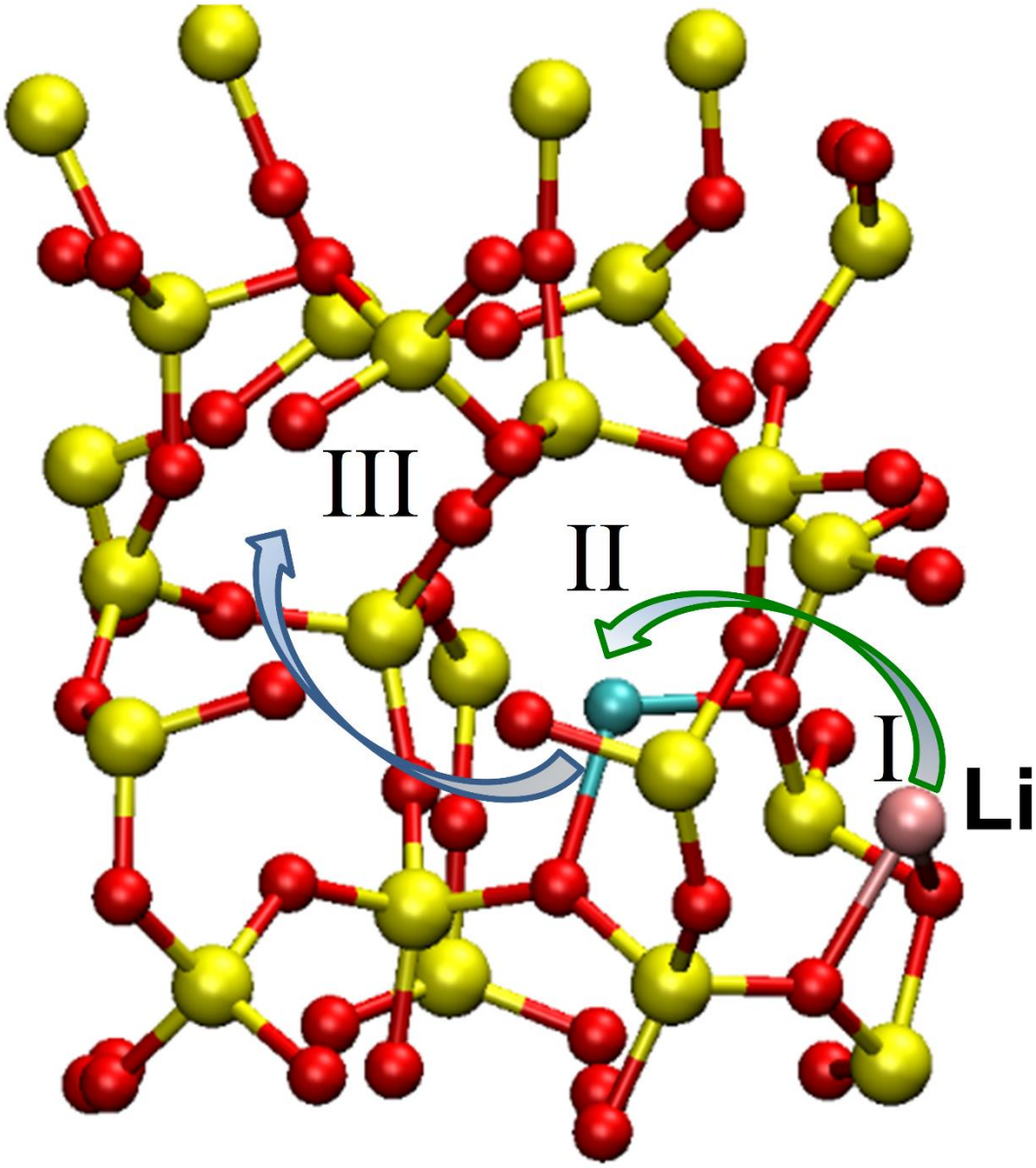

Figure S2. Representative structure of *a*-SiO_2 and diffusion of Li

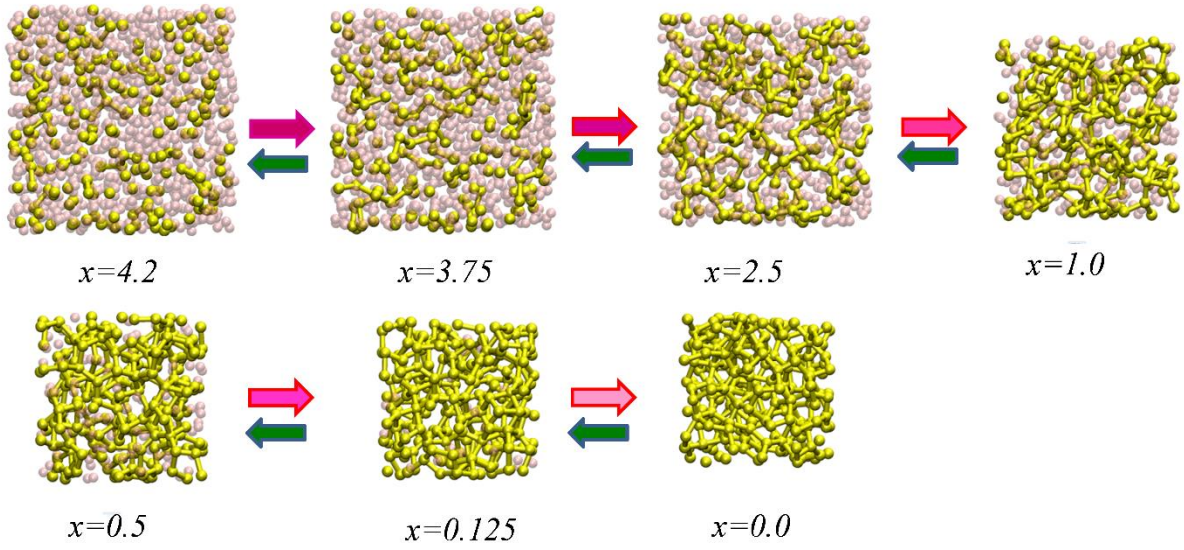

Figure S3. Lithiation and dilithiation of *a*-Si

Table S1:

```
Reactive MD-force field: Li/Si/Al/O force field March 2016_JPCA
 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
   15.0000 !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
    0.0010 !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
  6    ! 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
 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   1.0000   0.2000
12.0000
 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   1.3000   0.2000
13.0000
 Si   2.2977   4.0000  28.0600   1.8329   0.1837   0.5947   1.2962
4.0000
     11.7318   5.2054   4.0000  21.7115 139.9309   4.2033   5.5558
0.0000
     -1.0000   0.0000 104.0000   9.0751  23.8188   0.8381   0.8563
0.0000
     -4.1684   2.0754   1.0338   4.0000   2.5791   1.4000   0.2000
13.0000
 Al   2.1967   3.0000  26.9820   2.3738   0.2328   0.4961  -1.6836
3.0000
      9.4002   1.6831   3.0000   0.0076  16.5151  -0.3343   6.5000
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
 Li   1.9255   1.0000   6.9410   1.7722   0.1109   0.4634  -0.1000
1.0000
      9.3147   1.2063   1.0000   0.0000   0.0000  -6.9345  15.0000
0.0000
     -1.0000   0.0000  37.5000   5.4409   6.9107   0.1973   0.8563
0.0000
    -25.0000   2.2989   1.0338   1.0000   2.8103   1.3000   0.2000
13.0000
 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   5.0000 900.0000
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   0.0500   0.0010
10.0000
 15      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                        pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
  1  1 153.3934   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
  2  2 142.2858 145.0000  50.8293   0.2506  -0.1000   1.0000  29.7503
0.6051
```

```
         0.3451  -0.1055   9.0000   1.0000  -0.1225   5.5000   1.0000
0.0000
  1  2 160.0000   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
  1  3 101.1840   0.0000   0.0000  -0.1751   0.0000   1.0000   6.0000
1.1044
         7.3549   1.0000   0.0000   1.0000  -0.0450   7.9080   0.0000
0.0000
  2  3 273.4986   5.0000   0.0000  -0.3682  -0.3000   1.0000  36.0000
0.1000
        10.2378  -0.2158  28.6984   1.0000  -0.1451   8.0936   1.0000
0.0000
  3  3  70.3209  54.0531  30.0000   0.2206  -0.3000   1.0000  16.0000
0.0159
         0.0035  -0.8055   7.1248   1.0000  -0.0965   8.7733   0.0000
0.0000
  1  4  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
  2  4 181.1998   0.0000   0.0000  -0.2276  -0.3000   0.0000  36.0000
0.1925
         0.2086  -0.3500  25.0000   1.0000  -0.2000   6.1462   0.0000
0.0000
  3  4   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
  4  4  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
  1  5  63.4649   0.0000   0.0000   0.0294   0.0000   0.0000   6.0000
0.4868
         0.3090   0.0000  12.0000   1.0000  -0.0800   5.1033   0.0000
0.0000
  2  5  76.3632  -0.0200   0.0000  -0.4309   0.3000   0.0000   6.0000
0.1271
         0.4301  -0.2500  11.9965   1.0000  -0.2188   6.6027   0.0000
0.0000
  3  5  23.2383   0.0000   0.0000   0.6079   0.3000   0.0000  26.0000
0.7696
         0.0781   0.0000  12.0000   1.0000  -0.1658   5.2531   0.0000
0.0000
  4  5   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
  5  5  52.4319   0.0000   0.0000   0.2219   0.3000   0.0000  26.0000
0.5355
```

```
         0.9010   0.0000  12.0000   1.0000  -0.1497   4.0597   0.0000
0.0000
 10    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
  1  3   0.1035   1.3327  11.5963   1.3977  -1.0000  -1.0000
  2  3   0.1547   1.9047  10.7461   1.6501   1.3386  -1.0000
  1  4   0.0564   1.4937  12.0744   1.7276  -1.0000  -1.0000
  2  4   0.2017   1.8458  11.0700   1.6009  -1.0000  -1.0000
  3  4   0.1000   1.8500  10.3237  -1.0000  -1.0000  -1.0000
  1  5   0.2966   1.2550  10.2920   1.1989  -1.0000  -1.0000
  2  5   0.1112   1.6982  11.0473   1.5212  -1.0000   1.0000
  3  5   0.0800   2.0062  11.5806   1.7679   1.0000   1.0000
  4  5   0.0209   1.5000   9.0666  -1.0000   1.0000   1.0000
 36    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2;val(bo)
  1  1  1   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000
1.0400
  2  2  2  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000
1.0783
  1  2  2  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000
1.1680
  1  2  1  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000
1.5800
  2  1  2   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000
2.8774
  1  1  2   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000
1.0421
  3  3  3  78.5339  36.4328   1.0067   0.0000   0.1694   0.0000
1.6608
  1  3  3  68.5501  19.4239   2.3592   0.0000   0.2029   0.0000
1.0000
  1  3  1  70.7499  11.4850   4.6606   0.0000   1.5647   0.0000
1.0902
  2  3  3  91.0715  41.9975   3.5577   0.0000   1.6017   0.0000
3.0000
  1  3  2  73.6998  40.0000   1.8782   0.0000   4.0000   0.0000
1.1290
  2  3  2  80.6181  38.2534   7.5388   0.0000   0.0050   0.0000
2.4899
  2  3  3  91.0715  41.9975   3.5577   0.0000   1.6017   0.0000
3.0000
  3  2  3 103.8959  13.2049   2.7392   0.0000   1.6076   0.0000
1.9673
  1  2  3  90.0000   6.6857   1.6689   0.0000   2.5771   0.0000
1.0400
  2  2  3 107.9279  37.5298   8.0000   0.0000   1.7014   0.0000
2.2487
  1  1  3   0.0000   0.0100   1.0000   0.0000   1.0000   0.0000
2.0000
  3  1  3   0.0000   4.4216   0.8596   0.0000   0.9624   0.0000
1.0000
  2  1  3   0.0000   5.0000   1.0000   0.0000   1.0000   0.0000
1.2500
```

```
  2  1  4   0.0000   4.2750   1.0250   0.0000   1.3750   0.0000
1.4750
  1  1  4   0.0000   3.0000   1.0000   0.0000   1.0000   0.0000
1.2500
  4  1  4   0.0000  20.2391   0.1328   0.0000   2.9860   0.0000
1.0870
  1  2  4  88.1144  13.2143   1.5068   0.0000   3.0000   0.0000
1.0100
  2  2  4  34.4326  25.9544   5.1239   0.0000   2.7500   0.0000
1.7141
  4  2  4  20.7204  13.4875   4.0000   0.0000   0.6619   0.0000
1.4098
  1  4  1  67.4229   4.5148   5.9702   0.0000   3.0000   0.0000
2.6879
  1  4  2  41.8108  17.3800   2.6618   0.0000   0.7372   0.0000
1.0100
  2  4  2  69.3665  17.7549   3.1750   0.0000   3.0000   0.0000
1.1304
  1  4  4 180.0000 -26.7860   7.3549   0.0000   1.0000   0.0000
1.0252
  1  4  4  78.2279  37.6504   0.4809   0.0000   1.0000   0.0000
2.9475
  2  5  2  83.7146   8.7579   4.0000   0.0000   0.2652   0.0000
1.2463
  2  2  5  81.6233  30.0000   2.0000   0.0000   1.0000   0.0000
1.0000
  5  2  5  86.6874  22.4076   4.0000   0.0000   0.1000   0.0000
1.3084
  4  2  5  13.6525  12.0927   4.0000   0.0000   1.0000   0.0000
3.0818
  3  2  4  18.0953   5.3220   4.0000   0.0000   1.0000   0.0000
1.0139
  3  2  5  86.9269  18.2323   2.8071   0.0000   0.9102   0.0000
2.9549
  8    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  2  2  2   0.8302  -4.0000  -0.7763  -2.5000  -1.0000   0.0000
0.0000
  2  2  2  2  -2.5000  -4.0000   1.0000  -2.5000  -1.0000   0.0000
0.0000
  0  1  1  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000
  0  1  2  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000
0.0000
  0  2  2  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000
0.0000
  1  3  3  1   0.0000   0.0000   0.0640  -2.4426   0.0000   0.0000
0.0000
  1  3  3  3   0.0000   0.0000   0.1587  -2.4426   0.0000   0.0000
0.0000
  0  1  3  0   0.0000   0.0000   0.1200  -2.4847   0.0000   0.0000
0.0000
  1    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
```

```
2  1  2   2.1200  -3.5800   1.4500  19.5000
```