Supplemental Information for "Interfacial Structure and Evolution of the Water-Silica Gel System by Reactive Force Field Based Molecular Dynamics Simulations"

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Short range structure features such as bond distances, bond angles of the initial silica, gel, water (SGW) interfacial structures and those equilibrated at four different temperatures are summarized in Table S1.

Interatomic distances and bond angles were calculated from the bond angle distribution (BAD) and pair distribution function (PDF) from the final 50ps of the 300K run at the end of the simulation. The BAD and PDF account for the vibrations and variation in the bond lengths and angles due to the amorphous structure and temperature of the system. Many of the bond angles and distances inside the SiO_4 tetrahedron and the water molecule are stable across the different phases and level of structural evolution and are consistent with experiment. This includes the Si-O, O-O, Si-Si, and O_w-H_w interatomic distances and O-Si-O, Si-O-Si, and H_w-O_w-H_w bond angles, and the peak of the PDF and BAD is reported in Tables S1.

The structural parameters for the SiO_4 tetrahedron in the silica and gel regions of the model (Si-O, O-O, and Si-Si interatomic distances and O-Si-O and Si-O-Si bond angles) have differences of less than 1%, indicating that there is limited distortion of the silica structure. A similar trend is observed for the water molecules, with comparable O_w-H_w and H_w-H_w interatomic distances and H_w-O_w-H_w bond angles for molecules in both the gel and the bulk water which are comparable to experimental values (Table S1). There is a slight transition in the O_w-H_w-O_w bond angle for the water molecules in both the gel and bulk water regions towards the bulk water value of 164^o, but is consistent with previous computational investigations of the

structure of water in increasing cluster size[1]. The O_w-O_w interatomic distances are similar to the value for bulk water simulated with ReaxFF of 165° [2]. In the bulk water there is a decrease in the O_w-O_w interatomic distance of ~0.1Å as the system evolves, which may account for interactions between the water with the dissolved silica content. Water in close contact with silica, termed nanoconfined water, exhibits lower O_w-O_w interatomic distances by ~0.12Å from the experimentally reported bulk values [3-4]. Overall, the short range structure around silicon and oxygen such as the bond angle and decreases bond distances remain largely unchanged suggesting that the SiO_4 tetrahedrons and water molecules do not experience any drastic changes in the evolution of the gel structures.

Table S1: Short-range structural features in the SGW models and the initial structures. The peak of the bond angle distributions (BAD) and pair distribution functions (PDF) are reported with the full-width-at-half-max (FWHM_ value as the error. Experimental values from literature are included for comparison.

		Initial	SGW-1	SGW-2	SGW-3	SGW-4	Expt.
Si-O dist. (Å)	Silica	1.60±0.10	1.59±0.10	1.59±0.11	1.59±0.11	1.59±0.12	1.61[a]
	Gel	1.58±0.09	1.58±0.09	1.58±0.09	1.58±0.11	1.58±0.11	
O-O dist. (Å)	Silica	2.57±0.30	2.57±0.30	2.57±0.31	2.57±0.32	2.57±0.32	2.65[b]
	Gel	2.59±0.25	2.59±0.22	2.59±0.24	2.57±0.24	2.58±0.25	
Si-Si dist. (Å)	Silica	3.14±0.14	3.14±0.14	3.13±0.15	3.13±0.17	3.13±0.17	3.1[c]
	Gel	3.12±0.13	3.12±0.11	3.12±0.12	3.12±0.13	3.11±0.13	
O-Si-O angle (°)	Silica	109±13	109±12	109±12	109±14	109±14	109.4[b]
	Gel	109±13	109±12	109±12	109±14	109±14	
Si-O-Si angle (°)	Silica	157±26	156±26	156±27	156±28	156±28	153[b]
	Gel	158±25	160±23	159±23	159±24	158±25	
O_w-H_w dist. (Å)	Gel	0.97±0.07	0.97±0.07	0.97±0.08	0.97±0.07	0.97±0.08	0.98[d]
	Water	0.98±0.05	0.97±0.07	0.97±0.07	0.97±0.08	0.97±0.08	
O_w-O_w dist. (Å)	Gel	2.84±0.67	2.84±0.44	2.84±0.49	2.86±0.60	2.87±0.70	2.85[e]
	Water	2.74±0.36	2.76±0.42	2.72±0.52	2.67±0.98	2.64±0.69	
O_w-H_w-O_w angle (°)	Gel	162±30	164±49	162±29	160±36	160±32	174[e]
	Water	167±23	165±24	164±27	161±30	160±32	
H_w-O_w-H_w angle (°)	Gel	104±17	104±15	104±16	103±17	104±16	104.5[d]
	Water	105±13	104±15	104±16	104±16	104±16	

[a]Neutron diffraction[5], [b]Electron diffraction[6], [c]Large angle x-ray scattering[7], [d]Electron diffraction[8], [e]Molecular beam electric resonance spectroscopy[9]

The interatomic potentials used in this work was originally from Ref. 10 and 11. The ReaxFF parameters are listed in the below table.

Table S2: ReaxFF potential parameters for the water/silica interactions[10,11]

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Reactive MD-force field: Si/SiO/SiN interactions with water and Na+ Fogarty et al.
 39      ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
    1.6725 !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
  -40.0000 !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)
    1.7602 !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)
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  0.7903 !Valency angle conjugation parameter
10    ! 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   0.6544   1.1341   4.0000
     9.7559   2.1346   4.0000  34.9350  79.5548   5.4088   6.0000   0.0000
     1.2114   0.0000 202.2908   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  55.1878   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  68.0152   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   2.2403   0.1102   0.9928   1.1748   5.0000
     9.8276  12.0698   4.0000  30.2790 100.0000   6.1112   6.6645   2.0000
     1.0433   0.1000 119.9837   0.7382   6.7108   2.7268   0.9745   0.0000
    -2.0000   4.0000   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   0.6632   1.2962   4.0000
    12.3588   1.2523   4.0000  21.7115 139.9309   4.6461   6.0005   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
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
F    1.1846   1.0000  18.9984   1.7922   0.1267   0.4038  -0.1000   7.0000
    10.3184   7.5000   1.0000   9.2533   0.2000   9.3891   6.5612   2.0000
    -1.0000   3.5571  18.0000   6.9821   4.1799   1.0561   0.0000   0.0000
    -7.3000   2.6656   1.0493   4.0000   2.9225   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
P    1.5994   3.0000  30.9738   1.7000   0.1743   1.0000   1.3000   5.0000
     9.1909  14.9482   5.0000   0.0000   0.0000   1.6676   7.0946   0.0000
    -1.0000  25.0000 125.6300   0.2187  21.4305  15.1425   0.0000   0.0000
    -3.9294   3.4831   1.0338   5.0000   2.8793   0.0000   0.0000   0.0000
39     ! 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 -0.0553 6.9316 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 3 100.9167 136.3836 65.3877 0.3895 -0.3906 1.0000 18.8159 0.6674
1.1202 -0.3411 9.1099 1.0000 -0.1966 5.6975 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 4 165.1874 148.6965 87.7249 -1.3237 -0.3504 1.0000 27.5446 0.1473
0.1449 -0.2871 7.2074 1.0000 -0.2565 4.4890 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 0.0000 -0.0920 4.2790 0.0000 0.0000
2 4 208.1369 0.0000 0.0000 -0.3949 0.0000 1.0000 6.0000 0.3340
6.0174 1.0000 0.0000 1.0000 -0.1026 5.5235 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 5 107.2917 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 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 6 228.6887 0.0000 0.0000 -0.4125 0.0000 1.0000 6.0000 0.1504
18.1084 1.0000 0.0000 1.0000 -0.0980 7.4442 0.0000 0.0000
3 6 292.0110 25.7380 0.0000 -0.6150 -0.3000 1.0000 36.0000 1.0000
11.1536 -0.5377 30.0000 1.0000 -0.1399 7.0398 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
5 6 0.0000 0.0000 0.0000 1.0000 -0.3000 1.0000 36.0000 0.5000
0.2350 -0.3500 15.0000 1.0000 -0.2000 8.0000 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 -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 7 45.8933 0.0000 0.0000 -0.1511 -0.3000 1.0000 36.0000 0.3105

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      5.8448  -0.3500  25.0000   1.0000  -0.0659   7.9140   1.0000   0.0000
 6  7   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
 7  7  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
 1  8 233.5531   0.0000   0.0000  -0.8902  -0.5000   1.0000  35.0000   0.4347
      2.5511  -0.2500  15.0000   1.0000  -0.0865   5.3191   1.0000   0.0000
 2  8 149.7505   0.0000   0.0000  -0.4042  -0.2000   0.0000  16.0000   0.9446
      5.6404  -0.2000  15.0000   1.0000  -0.2500   6.2346   0.0000   0.0000
 3  8   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
      1.0001  -0.2000  15.0000   1.0000  -0.1000  15.0000   0.0000   0.0000
 4  8   0.0000   0.0000   0.0000  -0.4643   0.0000   1.0000   6.0000   0.6151
     12.3710   1.0000   0.0000   1.0000  -0.0098   8.5980   0.0000   0.0000
 5  8   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
      0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 6  8 329.4806   0.0000   0.0000  -1.3973  -0.3500   1.0000  25.0000   0.8000
      0.5397  -0.2500  15.0000   1.0000  -0.1597   5.0000   1.0000   0.0000
 7  8   0.0000   0.0000   0.0000   0.2500  -0.5000   1.0000  45.0000   0.6000
      0.4000  -0.2500  15.0000   1.0000  -0.1000  10.0000   1.0000   0.0000
 8  8 123.0018   0.0000   0.0000  -0.5940  -0.3500   1.0000  25.0000   0.6976
      1.8101  -0.2500  15.0000   1.0000  -0.0694   6.3418   1.0000   0.0000
 1 10 110.0000  92.0000   0.0000   0.2171  -0.1418   1.0000  13.1260   0.6000
      0.3601  -0.1310  10.7257   1.0000  -0.0869   5.3302   1.0000   0.0000
 2 10   0.1466   0.0000   0.0000   0.2250  -0.1418   1.0000  13.1260   0.6000
      0.3912  -0.1310   0.0000   1.0000  -0.1029   9.3302   0.0000   0.0000
 3 10 201.0058 194.1410   0.0000   1.0000  -0.5000   1.0000  25.0000   0.4873
      0.4358  -0.1571  15.8745   1.0000  -0.2431   6.3823   1.0000   0.0000
 6 10   0.0000   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
 7 10   0.0000   0.0000   0.0000   0.2171  -0.5000   1.0000  35.0000   0.6000
      0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
10 10   0.0000   0.0000   0.0000   0.2171  -0.5000   1.0000  35.0000   0.6000
      0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
23    ! 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   0.1275   1.3000   9.8924   1.0418  -1.0000  -1.0000
 1  3   0.0647   2.0109  10.0105   1.3177   1.2052   1.0682
 1  4   0.1952   1.8813   9.7734   1.3434   1.2545   1.1533
 3  4   0.1201   2.4775   9.0171   1.5285   1.0682   1.2716
 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
 3  5   0.2832   1.8196  10.2295   1.4502   1.4557  -1.0000
 4  5   0.1505   1.9000  10.5104   1.8000   1.4000  -1.0000
 1  6   0.0541   2.0811  13.5179   1.7778   1.5840  -1.0000
 2  6   0.1190   1.7901  10.7337   1.3946  -1.0000  -1.0000
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 3  6   0.1293   2.1561  10.5766   1.7129   1.3690  -1.0000
 4  6   0.1297   1.9384  10.9856   1.6175   1.4045  -1.0000
 5  6   0.0600   1.7000  11.0000  -1.0000  -1.0000  -1.0000
 3  7   0.0825   1.5904  11.3396   1.5905  -1.0000  -1.0000
 6  7   0.1757   2.0409  13.7267  -1.0000  -1.0000  -1.0000
 1  8   0.1394   1.6575  11.1294   1.3470  -1.0000  -1.0000
 2  8   0.2500   0.9047   9.2682   1.0500  -1.0000  -1.0000
 3  8   0.1547   2.1287   9.6188  -1.0000  -1.0000  -1.0000
 6  8   0.1386   1.6000  13.7429   1.4464  -1.0000  -1.0000
 3 10   0.0534   1.7520  10.4281   1.8000   1.4498  -1.0000
 6 10   0.1130   1.7570   9.3000  -0.1000  -1.0000  -1.0000
131    ! 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  66.0686  28.5756   1.4793   0.0000   2.9950  58.6562   1.0000
 3  1  3  84.3310  21.5172   5.4724  -1.0000   1.5183   0.0000   2.9776
 1  1  4  66.8437  45.0000   1.2491   0.0000   1.1834   0.0000   3.0000
 3  1  4  82.7022  45.0000   0.5769   0.0000   1.1019   0.0000   1.0000
 4  1  4  90.0000  43.1792   0.5055   0.0000   1.1155   0.0000   1.0204
 2  1  3  64.3088  32.5434   2.1997   0.0000   0.1000   0.0000   1.2995
 2  1  4  63.9629  41.6246   1.4921   0.0000   0.2000   0.0000   2.8070
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  68.4903  45.0000   1.3617   0.0000   2.8294   0.0000   1.0000
 1  3  3  80.6161  45.0000   1.4073   0.0000   1.0572  68.1072   1.4451
 1  3  4  69.5983  45.0000   1.4248   0.0000   2.9000   0.0000   2.3286
 3  3  3  89.9934  17.9465   1.7798   0.0000   2.9881   0.0000   1.0538
 3  3  4  83.5202  33.7933   1.0337   0.0000   2.9000   0.0000   1.3398
 3  3  5  60.2631  30.0701   2.1707   0.0000   1.3323   0.0000   1.0192
 4  3  4  67.1317  42.3748   1.7873   0.0000   3.0072   0.0000   1.5832
 1  3  2  90.0000   7.1513   7.5000   0.0000   1.3111   0.0000   3.0000
 2  3  3  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000   1.1680
 2  3  4  72.7348  20.1071   7.5000   0.0000   0.1000   0.0000   1.0746
 2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000   1.5800
 1  4  1  70.6778  12.3495   3.0486   0.0000   2.8702   0.0000   1.0000
 1  4  3  73.9745  21.1329   2.3337   0.0000   2.8701   0.0000   1.7170
 1  4  4  71.4579  14.0942   2.8540   0.0000   2.8701   0.0000   1.0631
 3  4  3  74.2613  20.9008   2.8607 -18.0069   3.0701   0.0000   1.3874
 3  4  4  74.2615  27.8669   1.6736  -0.9193   3.0117   0.0000   1.4381
 4  4  4  73.3189  24.9685   2.2561   0.0000   2.9983   0.0000   2.1573
 1  4  2  70.2498  13.6111   2.6311   0.0000   0.2025   0.0000   1.0000
 2  4  3  74.5739  45.0000   1.4078   0.0000   0.3956   0.0000   3.0000
 2  4  4  79.7136  45.0000   0.5316   0.0000   0.5437   0.0000   1.0000
```

2	4	2	80.2201	6.8385	7.5000	0.0000	0.1000	0.0000	1.0000
1	2	3	0.0000	8.9481	0.5983	0.0000	0.0000	0.0000	1.0000
1	2	4	0.0000	0.2694	2.1363	0.0000	0.0000	0.0000	1.8036
1	2	5	0.0000	15.0000	3.0000	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	1.0574	0.1000	0.0000	0.0000	0.0000	2.7676
3	2	5	0.0000	1.0000	6.0000	0.0000	0.0000	0.0000	1.0400
4	2	4	0.0000	0.0100	1.0929	0.0000	0.0000	0.0000	2.1728
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	74.4180	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	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
2	2	5	0.0000	0.0019	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	3	5	76.3546	40.0000	3.3161	0.0005	1.9473	0.0000	1.0000
5	4	5	62.0000	33.4273	1.7018	0.1463	0.5000	0.0000	1.0500
5	5	5	84.2345	15.5790	3.7715	0.0000	1.3066	0.0000	1.6270
3	5	3	83.5231	37.5859	0.9881	-0.0100	1.4725	0.0000	1.0641
3	5	5	55.9402	38.2990	3.6930	0.0000	2.2673	0.0000	1.0000
1	5	3	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
1	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
3	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
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	99.7692	37.1505	1.3922	0.0000	0.0100	0.0000	1.3119
2	6	3	76.8040	40.0000	8.0000	0.0000	1.1072	0.0000	1.0400
3	6	3	99.1665	35.3379	0.8098	0.0000	1.9119	0.0000	1.0400
6	3	6	20.0000	1.3008	0.5929	0.0000	4.0000	0.0000	3.0000
2	3	5	35.9099	19.1501	1.9918	0.0000	0.9342	0.0000	2.7883
2	3	6	62.0763	39.6267	1.7913	0.0000	0.4595	0.0000	3.0000
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	40.0000	4.8986	0.0000	4.0000	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
1	1	8	72.2937	34.6301	6.9379	0.0000	0.1000	0.0000	4.0000
8	1	8	73.5980	38.7521	6.2303	0.0000	3.9063	0.0000	2.3075
1	8	1	0.0000	22.5817	3.8557	0.0000	3.4497	0.0000	2.5900
1	8	8	0.0000	26.2476	1.0288	0.0000	1.9253	0.0000	1.7848
2	1	8	69.6421	10.0000	2.0000	0.0000	1.0000	0.0000	1.0400
3	1	8	61.8207	37.7572	8.0000	0.0000	1.6293	0.0000	4.0000
5	1	8	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
6	6	8	70.5736	50.0000	1.2563	0.0000	0.1000	0.0000	1.2052
8	6	8	77.7691	49.9881	4.3411	0.0000	7.9949	0.0000	2.3018
6	8	6	0.0000	25.0000	5.5234	0.0000	0.1000	0.0000	1.1737
6	8	8	0.0000	18.2841	9.0327	0.0000	7.9884	0.0000	1.0838
8	8	8	0.0000	30.0000	20.0000	0.0000	0.1000	0.0000	1.1577
5	5	6	0.0000	10.0000	1.0000	0.5000	0.2500	0.0000	1.5000
6	6	5	0.0000	10.0000	1.0000	0.5000	0.2500	0.0000	1.5000
6	5	6	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
5	6	5	70.0000	25.0000	1.0000	0.0000	1.0000	0.0000	1.2500
2	6	8	69.4699	32.8373	1.9685	0.0000	0.7394	0.0000	3.0000
3	6	8	87.3549	38.6733	2.2786	0.0000	1.2018	0.0000	1.2328
3	2	8	0.0000	1.8088	0.0100	0.0000	0.0000	0.0000	1.2229
2	8	2	0.0000	10.0000	5.0000	0.0000	0.0000	0.0000	1.9555
6	8	2	21.2734	2.6664	5.2500	0.0000	0.7927	0.0000	2.9500
6	2	8	21.0771	44.1825	0.8441	0.0000	3.0612	0.0000	1.0500
8	2	8	0.0000	6.1464	2.9766	0.0000	0.0000	0.0000	2.9536
2	8	8	0.0000	4.2419	0.0568	0.0000	0.0000	0.0000	1.8781
3	10	3	90.0000	18.4167	0.6799	-8.0000	0.1310	0.0000	2.2321
2	3	10	72.6004	9.6150	0.8905	0.0000	3.5473	0.0000	1.0400
3	3	10	60.0000	40.0000	4.0000	0.0000	1.0000	0.0000	1.0400
3	2	10	0.0000	10.0000	1.0000	0.0000	1.0000	0.0000	1.0400
6	3	10	67.3176	9.1175	2.2677	0.0000	1.0000	0.0000	1.0000
10	3	10	62.1312	7.5931	0.1000	0.0000	0.5154	0.0000	2.1744
1	3	10	74.5094	2.5288	2.0377	0.0000	1.0000	0.0000	2.7779

```
 2 10  3  75.0000  25.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 3 10 10  70.0000  25.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 1 10  3  82.8511  35.1702   2.2155   0.0000   1.0000   0.0000   1.0400
 3  1 10  50.2929  41.6249   2.8868   0.0000   1.0000   0.0000   1.0400
 2  1 10  75.0000  30.0000   3.0000   0.0000   0.0050   0.0000   1.1400
76    ! 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  -0.5740  22.4215   0.8787  -2.7603  -1.1000   0.0000   0.0000
 2  1  1  3   1.8164  18.8479   0.5134  -7.0513  -1.0978   0.0000   0.0000
 3  1  1  3  -2.5000  56.1599  -1.0000  -4.3607  -0.8614   0.0000   0.0000
 1  1  3  1   2.5000  14.6490   1.0000  -2.5209  -0.9000   0.0000   0.0000
 1  1  3  3  -0.0002  20.1851   0.1601  -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
 3  1  3  3  -0.1583  20.0000   1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  1  3  2  -2.2946  11.6826  -1.0000  -2.5000  -0.9000   0.0000   0.0000
 2  1  3  1  -1.0402  26.8401   0.6384  -2.5000  -0.9000   0.0000   0.0000
 2  1  3  2  -1.0000  66.0304   0.7580  -5.4593  -1.1000   0.0000   0.0000
 2  1  3  3   2.1531  45.9655   1.0000  -2.5000  -2.8274   0.0000   0.0000
 3  1  3  1   0.6706  80.0000  -0.2443  -4.7181  -3.0437   0.0000   0.0000
 3  1  3  2  -1.0000  91.6742  -0.5000  -3.9849  -3.0476   0.0000   0.0000
 1  3  3  2  -2.5000  -0.5181   0.0268  -5.4085  -2.9498   0.0000   0.0000
 2  3  3  2  -2.1995 -25.0000  -1.0000  -2.6000  -0.9921   0.0000   0.0000
 1  3  3  3   2.4118 -24.8219   0.9706  -2.5004  -0.9972   0.0000   0.0000
 2  3  3  3  -2.5000  43.1840  -0.6826  -6.6539  -1.2407   0.0000   0.0000
 3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -0.9000   0.0000   0.0000
 1  1  4  2  -1.0000  71.4280  -0.5000  -8.0000  -1.9825   0.0000   0.0000
 2  1  4  2  -1.0000  63.9914   0.7449  -8.0000  -2.1051   0.0000   0.0000
 3  1  4  2  -1.0000  24.9527   1.0000  -4.6063  -2.5261   0.0000   0.0000
 3  1  1  4   1.0000  25.3373   1.0000  -4.1453  -0.9511   0.0000   0.0000
 4  1  1  4  -1.0000  21.8427   1.0000  -4.0686  -1.7241   0.0000   0.0000
 1  1  4  1   1.0000  83.8750   1.0000  -6.5279  -1.6589   0.0000   0.0000
 3  1  4  1  -1.0000  48.6477   1.0000  -8.0000  -1.8038   0.0000   0.0000
 2  1  1  4   1.0000  98.8297  -0.2745  -4.9954  -1.9000   0.0000   0.0000
 4  1  4  2   0.5000   2.8273  -0.1650  -7.9605  -2.0202   0.0000   0.0000
 2  1  4  1  -1.0000  92.9120  -0.4541  -7.7688  -1.5996   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   0.2176  40.4126   0.3535  -3.9875  -2.0051   0.0000   0.0000
 0  2  4  0   0.0000   0.1032   0.3000  -5.0965   0.0000   0.0000   0.0000
 0  3  4  0   1.1397  61.3225   0.5139  -3.8507  -2.7831   0.0000   0.0000
 0  4  4  0   0.7265  44.3155   1.0000  -4.4046  -2.0000   0.0000   0.0000
```

```
 4  1  4  4 -0.0949   8.7582   0.3310  -7.9430  -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  3  5  0  0.5000  50.0000   0.5000  -8.0000   0.0000   0.0000   0.0000
 0  5  5  0 -0.0170 -56.0786   0.6132  -2.2092   0.0000   0.0000   0.0000
 2  5  5  2  0.0000  50.0000   0.0000  -8.0000   0.0000   0.0000   0.0000
 3  5  5  3  0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000   0.0000
 3  5  5  5  0.2500  90.0000   0.5000  -6.0000   0.0000   0.0000   0.0000
 5  5  5  5  2.4661  71.9719   0.0100  -8.0000   0.0000   0.0000   0.0000
 0  2  5  0  0.0000   0.0000   0.0000   0.0000   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
 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  1  8 -0.7001   2.9144   1.0000  -2.6026  -1.7255   0.0000   0.0000
 2  1  1  8  0.0000   5.0000  -0.2000  -8.0000  -1.7255   0.0000   0.0000
 8  1  1  8 -0.0036  22.6930   0.0763  -2.6712  -1.7255   0.0000   0.0000
 0  1  8  0  0.2763  58.2831   0.9030  -3.3268   0.0000   0.0000   0.0000
 0  8  8  0  0.7648  43.2514   0.8294  -4.0355   0.0000   0.0000   0.0000
 8  1  3  1  0.0000   5.0000   0.2410  -8.0000   0.0000   0.0000   0.0000
 3  1  1  8  0.0000  16.9798   0.5678  -5.5057  -1.0000   0.0000   0.0000
 8  6  6  8  0.9000  90.0000   1.0000  -3.6535   0.0000   0.0000   0.0000
 2  6  6  8  0.0000  90.0000   0.1048  -2.5000   0.0000   0.0000   0.0000
 3  6  6  8  0.0000  79.3385   0.9357  -2.5000   0.0000   0.0000   0.0000
 6  6  6  8 -0.9000  79.3917  -0.0446  -2.5000   0.0000   0.0000   0.0000
 1  1  1 10  0.0000  19.3871   0.0103 -25.5765  -1.7255   0.0000   0.0000
10  1  1 10  0.0000  80.5586   0.1104  -8.0928  -1.7255   0.0000   0.0000
 0  1 10  0  4.0000  45.8264   0.9000  -4.0000   0.0000   0.0000   0.0000
 0 10 10  0  4.0000  45.8264   0.9000  -4.0000   0.0000   0.0000   0.0000
 2  1  3 10 -1.5000  18.9285   0.3649  -6.1208   0.0000   0.0000   0.0000
 2  3 10  3  1.5000  -1.0000   0.2575  -6.2100   0.0000   0.0000   0.0000
 1  3 10  3 -1.4375  -0.8700   0.9861  -2.5424   0.0000   0.0000   0.0000
10  3 10  3 -1.5000  21.5086  -1.0000  -4.8869   0.0000   0.0000   0.0000
 3  1  1  6 -0.5740  22.4215   0.8787  -2.7603  -1.1000   0.0000   0.0000
 1  1  6  3 -0.5740  22.4215   0.8787  -2.7603  -1.1000   0.0000   0.0000
12    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   2.1200  -3.5800   1.4500  19.5000
 3  2  4   2.1215  -7.5000   1.4500  19.5000
 4  2  3   1.7500  -4.3286   1.4500  19.5000
 4  2  4   2.4000  -2.3575   1.4500  19.5000
 3  2  5   2.5000  -1.0000   1.4500  19.5000
 4  2  5   1.5000  -2.0000   1.4500  19.5000
 5  2  3   2.5000  -1.0000   1.4500  19.5000
 5  2  4   1.5000  -2.0000   1.4500  19.5000
 5  2  5   2.5000  -2.0000   1.4500  19.5000
```

```
  3  2  8   1.5033  -0.0100   1.4500  19.5000
  8  2  3   1.7547  -0.2589   1.4500  19.5000
  8  2  8   1.5061  -7.5000   1.4500  19.5000
################################################################################
#
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