Calculation of the OH frequencies including the correction for anharmonicity.

Use of a quadratic fit to energy versus displacement for small changes in bond length allows a straightforward estimation of the vibrational frequencies within the harmonic approximation. This is, however, a bad approximation to calculate OH frequencies and a more suitable mathematical function to describe better the OH bond is needed, so that a better behaviour is achieved as the OH bond length elongates further from the equilibrium position. The Morse function below provides a reasonable approach:

$$E = A \cdot \left(1 - e^{-\alpha (x - x_0)}\right)^2 + B$$

where 'x' is the O-H length, 'x_0' its equilibrium distance, 'A' is the well depth, and ' ' is the width of the potential.

The force constant of the bond, 'k_e', can be found by taking the second derivative of the potential energy function, from which it follows:

$$\alpha = \sqrt{\frac{k_e}{2A}}$$

For the estimation of the anharmonicity, the Morse function can be approximated at small displacements from the equilibrium as a third order polynomial:

$$E = -A\alpha^3 \cdot (x - x_0)^3 + A\alpha^2 \cdot (x - x_0)^2 + B$$

And from this fit, the parameters A, B, and x_0 can be obtained.

The harmonic frequency, ν_0, can be obtained from:

$$\nu_0 = \frac{\alpha}{2\pi} \sqrt{\frac{2A}{\mu}}$$

where 'μ' is the reduced mass of the OH system.

Then, the stationary states of the OH system defined by the Morse hamiltonian are given by:

$$E_n = (n+\frac{1}{2})h\nu_0 - \left(n+\frac{1}{2}\right)^2\left(\frac{h^2\alpha^2}{8\pi^2\mu}\right)$$

where the fundamental frequency, ν, will be given by the transition 0→1 : (E_1-E_0)/h, from which it follows:

$$\nu = \nu_0(1-\frac{h\alpha^2}{4\pi^2\mu\nu_0})$$

In order to calculate ν and ν_0, from the computational viewpoint we can rewrite the third order polynomial as:

$$E = -A_0(x-x_0)^3 + A_1(x-x_0)^2 + A_2$$

and then, if energy is in eV, distance in Å, and atomic mass in atomic units, we can use the following straightforward equations, which only need the parameters A_0 and A_1 from the fit:

$$\nu_0 = 520.9863\cdot\sqrt{\frac{2A_1}{\mu}}$$

$$\nu = \nu_0(1-33.682\frac{A_0^2}{\mu\nu_0 A_1^2})$$

from which the harmonic, ν_0, and anharmonic, ν, frequencies can be easily obtained.

Table 3s. Supplemetary structural data to Table 3.

labels	O-T-O	O-T-O	O-T-O	O-T-O
O1-Si-O2	111(46)	111(46)	111(47)	111(47)
O1-Si-O3	110(46)	110(47)	110(46)	110(47)
O1-Si-O4	109(46)	109(47)	109(47)	109(46)
O2-Si-O3	109(47)	108(46)	108(46)	109(47)
O2-Si-O4	109(47)	109(46)	109(47)	109(46)
O3-Si-O4	110(47)	110(47)	110(46)	110(46)
O1H-Si-O2	109(1)	--	--	--
O1H-Si-O3	108(1)	--	--	--
O1H-Si-O4	102(1)	--	--	--
O2H-Si-O1	--	109(1)	--	--
O2H-Si-O3	--	108(1)	--	--
O2H-Si-O4	--	102(1)	--	--
O3H-Si-O1	--	--	108(1)	--
O3H-Si-O2	--	--	104(1)	--
O3H-Si-O4	--	--	107(1)	--
O4H-Si-O1	--	--	--	102(1)
O4H-Si-O2	--	--	--	107(1)
O4H-Si-O3	--	--	--	107(1)
O1H-Al-O2	106(1)	--	--	--
O1H-Al-O3	105(1)	--	--	--
O1H-Al-O4	99(1)	--	--	--
O2H-Al-O1	--	107(1)	--	--
O2H-Al-O3	--	105(1)	--	--
O2H-Al-O4	--	98(1)	--	--
O3H-Al-O1	--	--	104(1)	--
O3H-Al-O2	--	--	97(1)	--
O3H-Al-O4	--	--	107(1)	--
O4H-Al-O1	--	--	--	99(1)
O4H-Al-O2	--	--	--	105(1)
O4H-Al-O3	--	--	--	107(1)
O1-Al-O2	--	--	114(1)	113(1)
O1-Al-O3	--	112(1)	--	115(1)
O1-Al-O4	--	115(1)	111(1)	--
O2-Al-O3	115(1)	--	--	112(1)
O2-Al-O4	112(1)	--	117(1)	--
O3-Al-O4	114(1)	114(1)	--	--

Table X1. Cif file corresponding to the $Si_{48}O_{96}$ unit cell.

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_audit_creation_method        'generated by GS'

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_cell_length_b              17.343
_cell_length_c              17.343
_cell_angle_alpha           60.00
_cell_angle_beta            60.00
_cell_angle_gamma           60.00

_symmetry_space_group_name_H-M   'P 1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Si    0.2157    0.8562    0.0356
Si    0.8562    0.2157    0.3926
Si    0.3926    0.0355    0.8562
Si    0.0355    0.3926    0.2157
Si    0.0355    0.2157    0.8562
Si    0.8562    0.0355    0.2157
Si    0.2158    0.0355    0.3926
Si    0.2157    0.3926    0.8562
Si    0.3926    0.8562    0.2157
Si    0.0355    0.8562    0.3926
Si    0.8562    0.3926    0.0355
Si    0.3926    0.2157    0.0356
Si    0.7843    0.1438    0.9645
Si    0.1438    0.7843    0.6074
Si    0.6074    0.9645    0.1438
Si    0.9644    0.6074    0.7843
Si    0.9644    0.7843    0.1438
Si    0.1438    0.9645    0.7843
Si    0.7843    0.9644    0.6074
Si    0.7843    0.6074    0.1438
Si    0.6074    0.1438    0.7843
Si    0.9645    0.1438    0.6074
Si    0.1438    0.6074    0.9645
Si    0.6074    0.7843    0.9645
Si    0.2157    0.0355    0.8562
Si    0.0356    0.2157    0.3926
Si    0.3926    0.8562    0.0355
Si    0.8561    0.3926    0.2157
Si    0.8562    0.2157    0.0355
Si    0.0355    0.8562    0.2157
Si    0.2157    0.8562    0.3926
Si    0.2157    0.3926    0.0356
Si    0.3926    0.0356    0.2157
Si    0.8562    0.0355    0.3926
Si    0.0355    0.3926    0.8562
Si    0.3926    0.2157    0.8562
Si    0.7843    0.9645    0.1438
Si    0.9645    0.7843    0.6074
Si    0.6074    0.1438    0.9645
Si    0.1439    0.6074    0.7843
```

Si	0.1438	0.7843	0.9645
Si	0.9645	0.1438	0.7843
Si	0.7843	0.1438	0.6074
Si	0.7843	0.6074	0.9645
Si	0.6074	0.9644	0.7843
Si	0.1438	0.9645	0.6074
Si	0.9645	0.6074	0.1438
Si	0.6074	0.7843	0.1438
O	0.2133	0.0000	0.7867
O	0.0000	0.2133	0.5000
O	0.5000	0.7867	1.0000
O	0.7867	0.5000	0.2133
O	0.7867	0.2133	1.0000
O	0.0000	0.7867	0.2133
O	0.2133	0.7867	0.5000
O	0.2133	0.5000	0.0001
O	0.5000	0.0000	0.2133
O	0.7867	1.0000	0.5000
O	1.0000	0.5000	0.7867
O	0.5000	0.2133	0.7867
O	0.7867	0.0000	0.2133
O	1.0000	0.7867	0.5000
O	0.5000	0.2133	0.0000
O	0.2133	0.5000	0.7867
O	0.2133	0.7867	1.0000
O	1.0000	0.2133	0.7867
O	0.7867	0.2133	0.5000
O	0.7867	0.5000	0.9999
O	0.5000	1.0000	0.7867
O	0.2133	0.0000	0.5000
O	0.0000	0.5000	0.2133
O	0.5000	0.7867	0.2133
O	0.1414	0.1414	0.8518
O	0.1414	0.1414	0.3653
O	0.3654	0.8518	0.1414
O	0.8518	0.3654	0.1414
O	0.8518	0.1414	0.1414
O	0.1414	0.8518	0.1414
O	0.1414	0.8518	0.3654
O	0.1414	0.3653	0.1414
O	0.3653	0.1414	0.1414
O	0.8518	0.1414	0.3654
O	0.1414	0.3654	0.8518
O	0.3654	0.1414	0.8518
O	0.8586	0.8586	0.1482
O	0.8586	0.8586	0.6347
O	0.6346	0.1482	0.8586
O	0.1482	0.6346	0.8586
O	0.1482	0.8586	0.8586
O	0.8586	0.1482	0.8586
O	0.8586	0.1482	0.6346
O	0.8586	0.6347	0.8586
O	0.6347	0.8586	0.8586
O	0.1482	0.8586	0.6346
O	0.8586	0.6346	0.1482
O	0.6346	0.8586	0.1482
O	0.1872	0.9649	0.9649
O	0.9649	0.1872	0.3830
O	0.3830	0.9649	0.9649
O	0.9649	0.3830	0.1872
O	0.9649	0.1872	0.9649

O	0.9649	0.9649	0.1872
O	0.1872	0.9649	0.3830
O	0.1872	0.3830	0.9649
O	0.3830	0.9649	0.1872
O	0.9649	0.9649	0.3830
O	0.9649	0.3829	0.9649
O	0.3830	0.1872	0.9649
O	0.8128	0.0351	0.0351
O	0.0351	0.8128	0.6170
O	0.6170	0.0351	0.0351
O	0.0351	0.6170	0.8128
O	0.0351	0.8128	0.0351
O	0.0351	0.0351	0.8128
O	0.8128	0.0351	0.6170
O	0.8128	0.6170	0.0351
O	0.6170	0.0351	0.8128
O	0.0351	0.0351	0.6170
O	0.0351	0.6170	0.0351
O	0.6170	0.8128	0.0351
O	0.3217	0.0356	0.8210
O	0.0355	0.3218	0.3218
O	0.3217	0.8210	0.0356
O	0.8210	0.3217	0.3217
O	0.8210	0.3217	0.0356
O	0.0356	0.8210	0.3217
O	0.3217	0.8210	0.3217
O	0.3217	0.3217	0.0356
O	0.3218	0.0356	0.3218
O	0.8210	0.0356	0.3217
O	0.0356	0.3217	0.8210
O	0.3217	0.3217	0.8210
O	0.6783	0.9644	0.1790
O	0.9645	0.6782	0.6783
O	0.6783	0.1790	0.9644
O	0.1790	0.6783	0.6783
O	0.1790	0.6783	0.9644
O	0.9644	0.1790	0.6783
O	0.6783	0.1790	0.6783
O	0.6782	0.6783	0.9644
O	0.6782	0.9644	0.6783
O	0.1790	0.9644	0.6783
O	0.9644	0.6783	0.1790
O	0.6783	0.6783	0.1790

Table X2_1. Cif file corresponding to the $Si_{47}Al_1O_{96}H_1$ unit cell, with proton attached to O1.

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_audit_creation_date         'Tue Aug 19 00:00:00 2008'
_audit_creation_method       'generated by GS'

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_cell_length_b             17.4298
_cell_length_c             17.4298
_cell_angle_alpha          60.33
_cell_angle_beta           60.33
_cell_angle_gamma          60.33

_symmetry_space_group_name_H-M   'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.7218    0.2777    0.5069
 O    0.6798    0.6822    0.1766
 O    0.9642    0.6780    0.1791
 O    0.1799    0.9620    0.6796
 O    0.6799    0.9638    0.6806
 O    0.6792    0.6795    0.9603
 O    0.6798    0.1762    0.6842
 O    0.9610    0.1792    0.6806
 O    0.1809    0.6793    0.9600
 O    0.1798    0.6789    0.6784
 O    0.6786    0.1817    0.9624
 O    0.9635    0.6787    0.6782
 O    0.6804    0.9596    0.1794
 O    0.3205    0.3206    0.8217
 O    0.0381    0.3201    0.8211
 O    0.8186    0.0288    0.3231
 O    0.3228    0.0354    0.3217
 O    0.3195    0.3206    0.0391
 O    0.3195    0.8228    0.3200
 O    0.0402    0.8186    0.3202
 O    0.8210    0.3199    0.0390
 O    0.8153    0.3305    0.3196
 O    0.3212    0.8204    0.0375
 O    0.0374    0.3202    0.3200
 O    0.3203    0.0385    0.8211
 O    0.6148    0.8116    0.0354
 O    0.0379    0.6162    0.0358
 O    0.0379    0.0367    0.6161
 O    0.6161    0.0349    0.8144
 O    0.8106    0.6214    0.0320
 O    0.8121    0.0391    0.6089
 O    0.0362    0.0362    0.8110
 O    0.0384    0.8095    0.0362
 O    0.0365    0.6163    0.8102
 O    0.6163    0.0382    0.0371
 O    0.0371    0.8106    0.6162
 O    0.8099    0.0351    0.0342
 O    0.3849    0.1890    0.9642
 O    0.9633    0.3839    0.9630
```

O	0.9614	0.9615	0.3834
O	0.3846	0.9639	0.1882
O	0.1888	0.3838	0.9637
O	0.1886	0.9657	0.3832
O	0.9649	0.9622	0.1885
O	0.9636	0.1887	0.9647
O	0.9629	0.3859	0.1869
O	0.3848	0.9628	0.9631
O	0.9675	0.1818	0.3916
O	0.1896	0.9631	0.9639
O	0.6317	0.8620	0.1445
O	0.8610	0.6371	0.1427
O	0.1465	0.8596	0.6345
O	0.6317	0.8598	0.8596
O	0.8601	0.6331	0.8579
O	0.8629	0.1469	0.6299
O	0.8595	0.1479	0.8604
O	0.1473	0.8602	0.8598
O	0.1470	0.6330	0.8593
O	0.6308	0.1484	0.8625
O	0.8611	0.8597	0.6351
O	0.8617	0.8587	0.1443
O	0.3658	0.1399	0.8551
O	0.1400	0.3668	0.8532
O	0.8441	0.1356	0.3695
O	0.3670	0.1397	0.1410
O	0.1389	0.3685	0.1398
O	0.1386	0.8546	0.3679
O	0.1408	0.8513	0.1396
O	0.8539	0.1383	0.1419
O	0.8527	0.3694	0.1388
O	0.3670	0.8535	0.1394
O	0.1445	0.1417	0.3680
O	0.1398	0.1397	0.8545
O	0.4995	0.7864	0.2135
O	0.9984	0.5004	0.2139
O	0.2158	0.9975	0.5008
O	0.4998	0.0026	0.7855
O	0.7865	0.5007	0.9990
O	0.7755	0.2203	0.5063
O	0.0004	0.2129	0.7872
O	0.2157	0.7856	0.9986
O	0.2138	0.4998	0.7859
O	0.4989	0.2153	0.0021
O	0.0001	0.7856	0.5002
O	0.7880	0.9991	0.2099
O	0.4995	0.2130	0.7868
O	0.0008	0.4996	0.7854
O	0.7852	0.9917	0.5018
O	0.5004	0.0002	0.2141
O	0.2149	0.5000	0.9986
O	0.2141	0.7881	0.4995
O	1.0000	0.7855	0.2140
O	0.7867	0.2114	0.0027
O	0.7864	0.5055	0.2085
O	0.4996	0.7850	1.0000
O	0.0038	0.2155	0.5003
O	0.2134	0.0007	0.7866
Al	0.8600	0.2156	0.3840
Si	0.6060	0.7855	0.1428
Si	0.9653	0.6073	0.1432

Si	0.1454	0.9638	0.6075
Si	0.6065	0.9649	0.7852
Si	0.7843	0.6080	0.9627
Si	0.7842	0.1402	0.6134
Si	0.9644	0.1439	0.7850
Si	0.1456	0.7834	0.9638
Si	0.1443	0.6071	0.7834
Si	0.6059	0.1461	0.9668
Si	0.9655	0.7837	0.6069
Si	0.7853	0.9629	0.1419
Si	0.3920	0.2158	0.8573
Si	0.0354	0.3928	0.8557
Si	0.8525	0.0314	0.3934
Si	0.3935	0.0349	0.2164
Si	0.2151	0.3933	0.0357
Si	0.2149	0.8580	0.3926
Si	0.0363	0.8545	0.2159
Si	0.8561	0.2146	0.0376
Si	0.8537	0.3970	0.2149
Si	0.3931	0.8553	0.0353
Si	0.0374	0.2147	0.3937
Si	0.2157	0.0354	0.8565
Si	0.6065	0.7835	0.9641
Si	0.1452	0.6070	0.9635
Si	0.9678	0.1449	0.6056
Si	0.6051	0.1426	0.7888
Si	0.7849	0.6115	0.1397
Si	0.7846	0.9627	0.6060
Si	0.1443	0.9648	0.7843
Si	0.9660	0.7830	0.1436
Si	0.9652	0.6067	0.7832
Si	0.6070	0.9649	0.1442
Si	0.1446	0.7843	0.6069
Si	0.7839	0.1442	0.9652
Si	0.3923	0.2162	0.0369
Si	0.8556	0.3934	0.0353
Si	0.0351	0.8552	0.3928
Si	0.3925	0.8565	0.2155
Si	0.2154	0.3930	0.8562
Si	0.2172	0.0356	0.3934
Si	0.8564	0.0327	0.2158
Si	0.0352	0.2154	0.8570
Si	0.0340	0.3931	0.2159
Si	0.3925	0.0358	0.8562
Si	0.2166	0.8550	0.0350

Table X2_2. Cif file corresponding to the $Si_{47}Al_1O_{96}H_1$ unit cell, with proton attached to O2.

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_audit_creation_method       'generated by GS'

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_cell_length_b             17.4298
_cell_length_c             17.4298
_cell_angle_alpha          60.33
_cell_angle_beta           60.33
_cell_angle_gamma          60.33

_symmetry_space_group_name_H-M   'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.8325    0.1820    0.2963
 O    0.6803    0.6812    0.1757
 O    0.9632    0.6782    0.1797
 O    0.1793    0.9612    0.6806
 O    0.6787    0.9630    0.6799
 O    0.6795    0.6799    0.9600
 O    0.6805    0.1752    0.6864
 O    0.9634    0.1790    0.6796
 O    0.1807    0.6790    0.9603
 O    0.1784    0.6794    0.6784
 O    0.6783    0.1810    0.9634
 O    0.9639    0.6790    0.6769
 O    0.6802    0.9587    0.1810
 O    0.3205    0.3200    0.8223
 O    0.0395    0.3201    0.8190
 O    0.8173    0.0327    0.3225
 O    0.3234    0.0345    0.3229
 O    0.3193    0.3204    0.0397
 O    0.3199    0.8227    0.3206
 O    0.0392    0.8214    0.3197
 O    0.8198    0.3211    0.0382
 O    0.8143    0.3271    0.3151
 O    0.3207    0.8196    0.0391
 O    0.0395    0.3209    0.3206
 O    0.3200    0.0386    0.8212
 O    0.6151    0.8118    0.0350
 O    0.0378    0.6161    0.0363
 O    0.0377    0.0370    0.6159
 O    0.6143    0.0347    0.8149
 O    0.8120    0.6218    0.0304
 O    0.8122    0.0297    0.6274
 O    0.0360    0.0361    0.8120
 O    0.0382    0.8090    0.0371
 O    0.0366    0.6161    0.8096
 O    0.6162    0.0374    0.0388
 O    0.0355    0.8119    0.6158
 O    0.8099    0.0342    0.0343
 O    0.3833    0.1890    0.9657
 O    0.9634    0.3844    0.9601
```

O	0.9618	0.9637	0.3831
O	0.3847	0.9636	0.1889
O	0.1887	0.3837	0.9637
O	0.1888	0.9660	0.3837
O	0.9639	0.9635	0.1896
O	0.9639	0.1900	0.9649
O	0.9629	0.3845	0.1893
O	0.3838	0.9625	0.9636
O	0.9709	0.1850	0.3830
O	0.1900	0.9625	0.9637
O	0.6316	0.8610	0.1457
O	0.8610	0.6360	0.1431
O	0.1457	0.8599	0.6343
O	0.6313	0.8598	0.8592
O	0.8605	0.6330	0.8566
O	0.8613	0.1464	0.6342
O	0.8596	0.1477	0.8604
O	0.1469	0.8601	0.8609
O	0.1463	0.6331	0.8594
O	0.6298	0.1461	0.8649
O	0.8596	0.8591	0.6303
O	0.8616	0.8590	0.1460
O	0.3660	0.1393	0.8560
O	0.1403	0.3676	0.8520
O	0.8496	0.1431	0.3531
O	0.3667	0.1394	0.1421
O	0.1386	0.3690	0.1395
O	0.1391	0.8570	0.3661
O	0.1399	0.8528	0.1392
O	0.8538	0.1407	0.1432
O	0.8563	0.3675	0.1361
O	0.3668	0.8535	0.1400
O	0.1455	0.1417	0.3687
O	0.1394	0.1391	0.8548
O	0.4998	0.7857	0.2134
O	0.9984	0.5006	0.2144
O	0.2164	0.9968	0.5017
O	0.4990	0.0014	0.7858
O	0.7867	0.5014	0.9984
O	0.7802	0.2045	0.5084
O	0.9993	0.2132	0.7879
O	0.2154	0.7848	0.9997
O	0.2141	0.5000	0.7859
O	0.4985	0.2145	0.0037
O	0.0013	0.7864	0.4986
O	0.7871	0.0013	0.2093
O	0.4994	0.2125	0.7885
O	0.0017	0.5000	0.7829
O	0.7861	0.0068	0.5013
O	0.5004	0.9992	0.2155
O	0.2150	0.5000	0.9982
O	0.2127	0.7881	0.4996
O	0.9994	0.7863	0.2145
O	0.7875	0.2091	0.0041
O	0.7874	0.5042	0.2061
O	0.4995	0.7849	0.0007
O	0.0017	0.2147	0.5002
O	0.2135	0.0002	0.7865
Al	0.8548	0.2220	0.3951
Si	0.6064	0.7849	0.1426
Si	0.9651	0.6071	0.1436

Si	0.1446	0.9641	0.6079
Si	0.6058	0.9651	0.7849
Si	0.7848	0.6088	0.9616
Si	0.7841	0.1407	0.6123
Si	0.9645	0.1440	0.7846
Si	0.1455	0.7830	0.9644
Si	0.1442	0.6070	0.7833
Si	0.6054	0.1453	0.9677
Si	0.9651	0.7841	0.6060
Si	0.7847	0.9629	0.1422
Si	0.3924	0.2153	0.8581
Si	0.0366	0.3932	0.8532
Si	0.8538	0.0300	0.3934
Si	0.3935	0.0345	0.2173
Si	0.2151	0.3932	0.0355
Si	0.2155	0.8586	0.3927
Si	0.0360	0.8554	0.2155
Si	0.8563	0.2156	0.0368
Si	0.8549	0.3957	0.2134
Si	0.3929	0.8551	0.0359
Si	0.0382	0.2151	0.3928
Si	0.2158	0.0351	0.8562
Si	0.6065	0.7839	0.9638
Si	0.1450	0.6069	0.9635
Si	0.9657	0.1449	0.6065
Si	0.6059	0.1423	0.7884
Si	0.7855	0.6107	0.1389
Si	0.7843	0.9647	0.6108
Si	0.1439	0.9645	0.7848
Si	0.9657	0.7827	0.1443
Si	0.9657	0.6068	0.7818
Si	0.6068	0.9639	0.1454
Si	0.1434	0.7849	0.6071
Si	0.7839	0.1433	0.9650
Si	0.3919	0.2158	0.0378
Si	0.8563	0.3942	0.0329
Si	0.0367	0.8559	0.3921
Si	0.3928	0.8562	0.2158
Si	0.2159	0.3930	0.8559
Si	0.2176	0.0356	0.3944
Si	0.8560	0.0341	0.2145
Si	0.0355	0.2156	0.8564
Si	0.0344	0.3930	0.2168
Si	0.3923	0.0356	0.8565
Si	0.2167	0.8548	0.0350

Table X2_3. Cif file corresponding to the $Si_{47}Al_1O_{96}H_1$ unit cell, with proton attached to O3.

```
data_fau_O3H
_audit_creation_date         'Tue Aug 19 00:00:00 2008'
_audit_creation_method       'generated by GS'

_cell_length_a             17.4298
_cell_length_b             17.4298
_cell_length_c             17.4298
_cell_angle_alpha          60.33
_cell_angle_beta           60.33
_cell_angle_gamma          60.33

_symmetry_space_group_name_H-M   'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.0090    0.1249    0.3574
 O    0.6803    0.6828    0.1752
 O    0.9637    0.6785    0.1794
 O    0.1800    0.9615    0.6800
 O    0.6791    0.9624    0.6807
 O    0.6789    0.6798    0.9605
 O    0.6792    0.1747    0.6856
 O    0.9646    0.1794    0.6780
 O    0.1810    0.6794    0.9598
 O    0.1788    0.6789    0.6787
 O    0.6787    0.1820    0.9617
 O    0.9647    0.6783    0.6775
 O    0.6804    0.9594    0.1808
 O    0.3200    0.3201    0.8233
 O    0.0397    0.3203    0.8192
 O    0.8197    0.0302    0.3231
 O    0.3223    0.0354    0.3217
 O    0.3198    0.3207    0.0398
 O    0.3196    0.8240    0.3203
 O    0.0399    0.8192    0.3202
 O    0.8194    0.3211    0.0385
 O    0.8189    0.3328    0.3174
 O    0.3206    0.8196    0.0388
 O    0.0344    0.3203    0.3199
 O    0.3199    0.0389    0.8212
 O    0.6143    0.8126    0.0350
 O    0.0385    0.6156    0.0364
 O    0.0400    0.0379    0.6125
 O    0.6137    0.0343    0.8159
 O    0.8116    0.6241    0.0291
 O    0.8112    0.0344    0.6181
 O    0.0362    0.0364    0.8105
 O    0.0381    0.8093    0.0362
 O    0.0362    0.6161    0.8108
 O    0.6159    0.0386    0.0387
 O    0.0365    0.8114    0.6152
 O    0.8092    0.0356    0.0346
 O    0.3831    0.1890    0.9660
 O    0.9627    0.3837    0.9618
```

O	0.9629	0.9621	0.3839
O	0.3845	0.9644	0.1880
O	0.1883	0.3837	0.9652
O	0.1861	0.9666	0.3836
O	0.9650	0.9631	0.1888
O	0.9636	0.1906	0.9643
O	0.9651	0.3870	0.1828
O	0.3837	0.9624	0.9635
O	0.9740	0.1797	0.3775
O	0.1897	0.9628	0.9638
O	0.6312	0.8624	0.1449
O	0.8611	0.6381	0.1416
O	0.1457	0.8595	0.6349
O	0.6306	0.8596	0.8597
O	0.8600	0.6331	0.8566
O	0.8601	0.1386	0.6434
O	0.8600	0.1477	0.8595
O	0.1470	0.8605	0.8602
O	0.1468	0.6330	0.8595
O	0.6300	0.1465	0.8641
O	0.8603	0.8587	0.6333
O	0.8617	0.8596	0.1445
O	0.3656	0.1393	0.8565
O	0.1394	0.3670	0.8544
O	0.8519	0.1365	0.3639
O	0.3666	0.1402	0.1420
O	0.1401	0.3687	0.1412
O	0.1390	0.8544	0.3676
O	0.1405	0.8519	0.1396
O	0.8540	0.1392	0.1413
O	0.8538	0.3682	0.1379
O	0.3661	0.8539	0.1400
O	0.1430	0.1395	0.3708
O	0.1393	0.1394	0.8546
O	0.4995	0.7867	0.2132
O	0.9972	0.5010	0.2146
O	0.2179	0.9953	0.5012
O	0.4990	0.0018	0.7856
O	0.7865	0.5015	0.9993
O	0.7867	0.2149	0.5090
O	0.9999	0.2135	0.7871
O	0.2153	0.7853	0.9991
O	0.2137	0.4996	0.7869
O	0.4987	0.2153	0.0028
O	0.0010	0.7847	0.4998
O	0.7881	0.9999	0.2105
O	0.4990	0.2126	0.7888
O	0.0015	0.4996	0.7845
O	0.7859	0.9967	0.5016
O	0.5002	0.9998	0.2155
O	0.2155	0.5002	0.9986
O	0.2141	0.7886	0.4997
O	1.0000	0.7862	0.2137
O	0.7875	0.2114	0.0016
O	0.7882	0.5064	0.2043
O	0.4991	0.7845	0.0012
O	0.9916	0.2145	0.5005
O	0.2134	0.0007	0.7865
Al	0.8425	0.2213	0.3940
Si	0.6061	0.7861	0.1422
Si	0.9649	0.6082	0.1431

Si	0.1457	0.9631	0.6080
Si	0.6059	0.9649	0.7849
Si	0.7843	0.6090	0.9617
Si	0.7838	0.1417	0.6122
Si	0.9647	0.1444	0.7840
Si	0.1455	0.7835	0.9639
Si	0.1439	0.6068	0.7839
Si	0.6058	0.1461	0.9668
Si	0.9649	0.7838	0.6065
Si	0.7850	0.9637	0.1425
Si	0.3920	0.2153	0.8584
Si	0.0358	0.3928	0.8549
Si	0.8537	0.0331	0.3933
Si	0.3940	0.0350	0.2161
Si	0.2158	0.3935	0.0360
Si	0.2149	0.8575	0.3930
Si	0.0360	0.8552	0.2158
Si	0.8559	0.2156	0.0369
Si	0.8553	0.3977	0.2121
Si	0.3926	0.8551	0.0358
Si	0.0389	0.2157	0.3932
Si	0.2156	0.0354	0.8565
Si	0.6060	0.7839	0.9641
Si	0.1455	0.6071	0.9634
Si	0.9630	0.1426	0.6096
Si	0.6055	0.1419	0.7885
Si	0.7856	0.6129	0.1374
Si	0.7841	0.9637	0.6079
Si	0.1441	0.9649	0.7846
Si	0.9657	0.7836	0.1437
Si	0.9654	0.6067	0.7827
Si	0.6071	0.9649	0.1452
Si	0.1438	0.7842	0.6073
Si	0.7840	0.1443	0.9644
Si	0.3924	0.2163	0.0373
Si	0.8552	0.3937	0.0345
Si	0.0352	0.8550	0.3930
Si	0.3927	0.8568	0.2153
Si	0.2153	0.3927	0.8573
Si	0.2185	0.0330	0.3948
Si	0.8565	0.0339	0.2160
Si	0.0353	0.2160	0.8564
Si	0.0337	0.3949	0.2139
Si	0.3924	0.0357	0.8564
Si	0.2164	0.8549	0.0353

Table X2_4. Cif file corresponding to the $Si_{47}Al_1O_{96}H_1$ unit cell, with proton attached to O4.

```
data_fau_O4H
_audit_creation_date          'Tue Aug 19 00:00:00 2008'
_audit_creation_method        'generated by GS'

_cell_length_a              17.4298
_cell_length_b              17.4298
_cell_length_c              17.4298
_cell_angle_alpha           60.33
_cell_angle_beta            60.33
_cell_angle_gamma           60.33

_symmetry_space_group_name_H-M   'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.7488    0.3657    0.3564
 O    0.6790    0.6813    0.1774
 O    0.9641    0.6783    0.1789
 O    0.1794    0.9617    0.6800
 O    0.6793    0.9625    0.6802
 O    0.6791    0.6790    0.9615
 O    0.6790    0.1775    0.6835
 O    0.9633    0.1786    0.6791
 O    0.1805    0.6793    0.9600
 O    0.1794    0.6788    0.6782
 O    0.6784    0.1808    0.9628
 O    0.9617    0.6798    0.6789
 O    0.6805    0.9593    0.1793
 O    0.3204    0.3199    0.8219
 O    0.0385    0.3202    0.8202
 O    0.8181    0.0290    0.3235
 O    0.3230    0.0346    0.3223
 O    0.3196    0.3203    0.0395
 O    0.3191    0.8230    0.3203
 O    0.0401    0.8188    0.3204
 O    0.8206    0.3191    0.0405
 O    0.8099    0.3323    0.3204
 O    0.3210    0.8198    0.0380
 O    0.0435    0.3224    0.3217
 O    0.3201    0.0385    0.8213
 O    0.6155    0.8109    0.0356
 O    0.0378    0.6158    0.0355
 O    0.0379    0.0364    0.6155
 O    0.6150    0.0352    0.8139
 O    0.8112    0.6187    0.0336
 O    0.8099    0.0377    0.6157
 O    0.0360    0.0364    0.8115
 O    0.0380    0.8093    0.0363
 O    0.0366    0.6158    0.8102
 O    0.6163    0.0373    0.0373
 O    0.0364    0.8107    0.6164
 O    0.8102    0.0348    0.0339
 O    0.3827    0.1892    0.9653
 O    0.9633    0.3841    0.9621
```

O	0.9610	0.9619	0.3837
O	0.3845	0.9639	0.1884
O	0.1890	0.3841	0.9633
O	0.1881	0.9661	0.3834
O	0.9645	0.9621	0.1890
O	0.9635	0.1898	0.9646
O	0.9631	0.3797	0.1963
O	0.3839	0.9627	0.9635
O	0.9727	0.1933	0.3731
O	0.1896	0.9628	0.9638
O	0.6314	0.8611	0.1456
O	0.8608	0.6368	0.1433
O	0.1462	0.8592	0.6350
O	0.6319	0.8596	0.8598
O	0.8604	0.6314	0.8593
O	0.8605	0.1441	0.6361
O	0.8595	0.1479	0.8598
O	0.1470	0.8603	0.8602
O	0.1471	0.6323	0.8592
O	0.6309	0.1469	0.8627
O	0.8602	0.8609	0.6326
O	0.8617	0.8587	0.1448
O	0.3664	0.1393	0.8552
O	0.1397	0.3674	0.8531
O	0.8489	0.1386	0.3607
O	0.3666	0.1396	0.1416
O	0.1385	0.3692	0.1389
O	0.1383	0.8551	0.3679
O	0.1406	0.8516	0.1396
O	0.8539	0.1379	0.1420
O	0.8559	0.3681	0.1382
O	0.3665	0.8536	0.1397
O	0.1453	0.1417	0.3692
O	0.1393	0.1394	0.8543
O	0.4990	0.7860	0.2136
O	0.9975	0.5011	0.2136
O	0.2165	0.9963	0.5014
O	0.4996	0.0007	0.7861
O	0.7858	0.4998	0.0014
O	0.7824	0.2176	0.5045
O	0.9993	0.2135	0.7874
O	0.2152	0.7852	0.9991
O	0.2142	0.4997	0.7854
O	0.4989	0.2143	0.0022
O	0.0007	0.7852	0.5001
O	0.7877	0.9992	0.2100
O	0.4993	0.2129	0.7881
O	0.0007	0.4998	0.7846
O	0.7847	0.9983	0.5008
O	0.5004	0.9999	0.2143
O	0.2151	0.5000	0.9987
O	0.2136	0.7882	0.4996
O	0.0004	0.7853	0.2140
O	0.7870	0.2109	0.0024
O	0.7870	0.5047	0.2101
O	0.4995	0.7849	0.0006
O	0.9992	0.2139	0.5002
O	0.2135	0.0003	0.7865
Al	0.8595	0.2075	0.3957
Si	0.6052	0.7856	0.1431
Si	0.9655	0.6081	0.1426

Si	0.1448	0.9637	0.6078
Si	0.6067	0.9648	0.7845
Si	0.7840	0.6075	0.9633
Si	0.7830	0.1454	0.6083
Si	0.9644	0.1442	0.7841
Si	0.1453	0.7836	0.9638
Si	0.1445	0.6069	0.7830
Si	0.6061	0.1452	0.9661
Si	0.9643	0.7848	0.6067
Si	0.7852	0.9630	0.1418
Si	0.3924	0.2152	0.8576
Si	0.0359	0.3929	0.8544
Si	0.8528	0.0338	0.3921
Si	0.3933	0.0348	0.2167
Si	0.2159	0.3933	0.0350
Si	0.2144	0.8584	0.3929
Si	0.0363	0.8546	0.2161
Si	0.8562	0.2138	0.0376
Si	0.8576	0.3996	0.2095
Si	0.3926	0.8553	0.0355
Si	0.0388	0.2165	0.3918
Si	0.2157	0.0352	0.8563
Si	0.6063	0.7839	0.9640
Si	0.1454	0.6069	0.9631
Si	0.9647	0.1438	0.6070
Si	0.6063	0.1429	0.7867
Si	0.7844	0.6127	0.1398
Si	0.7838	0.9656	0.6066
Si	0.1439	0.9649	0.7844
Si	0.9660	0.7834	0.1437
Si	0.9651	0.6069	0.7828
Si	0.6069	0.9646	0.1444
Si	0.1440	0.7845	0.6070
Si	0.7839	0.1438	0.9646
Si	0.3922	0.2156	0.0371
Si	0.8563	0.3926	0.0341
Si	0.0347	0.8556	0.3931
Si	0.3918	0.8567	0.2157
Si	0.2160	0.3929	0.8557
Si	0.2174	0.0353	0.3941
Si	0.8560	0.0324	0.2164
Si	0.0351	0.2155	0.8566
Si	0.0368	0.3926	0.2185
Si	0.3928	0.0353	0.8561
Si	0.2164	0.8549	0.0351

Table X3_a. Cif file corresponding to the $Si_{34}Al_{14}O_{96}H_{14}$ unit cell with Al distribution-a.

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data_Si34_Al14_H14_a
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_audit_creation_method            'generated by GS'

_cell_length_a                    17.7073
_cell_length_b                    17.7073
_cell_length_c                    17.7073
_cell_angle_alpha                 61.34
_cell_angle_beta                  61.34
_cell_angle_gamma                 61.34

_symmetry_space_group_name_H-M    'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.0062    0.3600    0.1228
 H    0.1048    0.0089    0.0045
 H    0.4969    0.7237    0.0113
 H    0.8186    0.1654    0.8196
 H    0.1853    0.8358    0.2914
 H    0.9989    0.7229    0.2755
 H    0.2381    0.5132    0.0428
 H    0.8813    0.6317    0.9965
 H    0.6292    0.9995    0.8876
 H    0.3730    0.3606    0.0015
 H    0.2622    0.0159    0.5031
 H    0.5031    0.0243    0.2547
 H    0.2681    0.5079    0.7153
 H    0.7264    0.0026    0.5030
 O    0.6789    0.6729    0.1701
 O    0.9639    0.6777    0.1752
 O    0.1815    0.9611    0.6822
 O    0.6931    0.9620    0.6760
 O    0.6697    0.6747    0.9750
 O    0.6834    0.1636    0.6771
 O    0.9537    0.1749    0.6819
 O    0.1671    0.6847    0.9768
 O    0.1794    0.6731    0.6776
 O    0.6790    0.1784    0.9643
 O    0.9645    0.6761    0.6761
 O    0.6708    0.9796    0.1744
 O    0.3338    0.3242    0.8075
 O    0.0253    0.3252    0.8302
 O    0.8259    0.0343    0.3145
 O    0.3166    0.0378    0.3231
 O    0.3275    0.3293    0.0353
 O    0.3319    0.8149    0.3229
 O    0.0319    0.8223    0.3229
 O    0.8255    0.3127    0.0407
 O    0.8281    0.3256    0.3217
 O    0.3086    0.8394    0.0352
 O    0.0365    0.3136    0.3299
 O    0.3274    0.0276    0.8338
 O    0.6093    0.8122    0.0376
```

O	0.0211	0.6102	0.0412
O	0.0284	0.0348	0.6145
O	0.6259	0.0310	0.8252
O	0.8242	0.6168	0.0326
O	0.8255	0.0367	0.5984
O	0.0436	0.0277	0.8182
O	0.0372	0.8295	0.0334
O	0.0372	0.6114	0.8083
O	0.6121	0.0418	0.0213
O	0.0333	0.8033	0.6277
O	0.8101	0.0395	0.0382
O	0.3805	0.1934	0.9544
O	0.9601	0.3851	0.9697
O	0.9722	0.9582	0.3882
O	0.3964	0.9541	0.1946
O	0.1966	0.3978	0.9585
O	0.1852	0.9621	0.3937
O	0.9591	0.9587	0.1856
O	0.9680	0.1844	0.9663
O	0.9699	0.3771	0.1785
O	0.4065	0.9742	0.9542
O	0.9639	0.1868	0.3866
O	0.1678	0.9726	0.9771
O	0.6352	0.8517	0.1457
O	0.8504	0.6368	0.1557
O	0.1540	0.8490	0.6286
O	0.6333	0.8536	0.8651
O	0.8624	0.6352	0.8551
O	0.8547	0.1466	0.6347
O	0.8511	0.1464	0.8605
O	0.1541	0.8540	0.8581
O	0.1472	0.6257	0.8582
O	0.6412	0.1583	0.8495
O	0.8703	0.8590	0.6184
O	0.8461	0.8672	0.1520
O	0.3680	0.1493	0.8398
O	0.1312	0.3688	0.8603
O	0.8513	0.1508	0.3630
O	0.3641	0.1355	0.1443
O	0.1493	0.3656	0.1394
O	0.1489	0.8470	0.3503
O	0.1340	0.8502	0.1458
O	0.8564	0.1346	0.1354
O	0.8548	0.3566	0.1447
O	0.3652	0.8558	0.1469
O	0.1369	0.1379	0.3749
O	0.1375	0.1500	0.8510
O	0.5044	0.7780	0.2140
O	0.9873	0.5033	0.2192
O	0.2191	0.0007	0.4990
O	0.5022	0.0167	0.7739
O	0.7828	0.4896	0.0133
O	0.7867	0.2162	0.4988
O	0.9933	0.2208	0.7918
O	0.2120	0.7934	0.9992
O	0.2170	0.5038	0.7733
O	0.5049	0.2198	0.9913
O	0.0159	0.7803	0.4978
O	0.7796	0.0051	0.2139
O	0.5076	0.2066	0.7850
O	0.9957	0.4985	0.7902

O	0.7850	0.9981	0.4993
O	0.4953	0.0030	0.2190
O	0.2178	0.5040	0.0072
O	0.2021	0.7713	0.5057
O	0.9948	0.7814	0.2250
O	0.7926	0.2134	0.9944
O	0.7941	0.4974	0.2048
O	0.4986	0.7822	0.0005
O	0.9945	0.2099	0.5054
O	0.2207	0.9896	0.7892
Al	0.1357	0.9567	0.6202
Al	0.6093	0.9605	0.7829
Al	0.7821	0.6017	0.9609
Al	0.9763	0.1403	0.7803
Al	0.8655	0.0413	0.3807
Al	0.2237	0.8493	0.3973
Al	0.3848	0.8742	0.0346
Al	0.2192	0.0436	0.8474
Al	0.1276	0.6220	0.9646
Al	0.9561	0.7909	0.1347
Al	0.6137	0.9630	0.1316
Al	0.3994	0.2058	0.0319
Al	0.2206	0.3849	0.8558
Al	0.0404	0.3913	0.2225
Si	0.6073	0.7803	0.1429
Si	0.9589	0.6066	0.1483
Si	0.7884	0.1415	0.6018
Si	0.1406	0.7912	0.9655
Si	0.1392	0.6108	0.7818
Si	0.6075	0.1485	0.9595
Si	0.9716	0.7783	0.6061
Si	0.7760	0.9700	0.1460
Si	0.3961	0.2182	0.8474
Si	0.0305	0.3933	0.8616
Si	0.3857	0.0353	0.2191
Si	0.2158	0.3966	0.0369
Si	0.0306	0.8577	0.2190
Si	0.8617	0.2116	0.0330
Si	0.8547	0.3892	0.2148
Si	0.0322	0.2131	0.4000
Si	0.6098	0.7806	0.9656
Si	0.9610	0.1390	0.6107
Si	0.6125	0.1470	0.7824
Si	0.7848	0.6062	0.1474
Si	0.7937	0.9609	0.6065
Si	0.1499	0.9604	0.7857
Si	0.9633	0.6054	0.7821
Si	0.1436	0.7781	0.6076
Si	0.7801	0.1440	0.9703
Si	0.8548	0.3873	0.0392
Si	0.0351	0.8541	0.3937
Si	0.3985	0.8494	0.2195
Si	0.2118	0.0359	0.3929
Si	0.8527	0.0348	0.2137
Si	0.0342	0.2193	0.8558
Si	0.4002	0.0407	0.8505
Si	0.8579	0.2180	0.3931
Si	0.2092	0.8588	0.0395

Table X3_b. Cif file corresponding to the $Si_{34}Al_{14}O_{96}H_{14}$ unit cell with Al distribution-b.

```
data_Si34_Al14_H14_b
_audit_creation_date              'Wed Aug 13 00:00:00 2008'
_audit_creation_method            'generated by GS'

_cell_length_a                    17.6726
_cell_length_b                    17.6726
_cell_length_c                    17.6726
_cell_angle_alpha                 61.21
_cell_angle_beta                  61.21
_cell_angle_gamma                 61.21

_symmetry_space_group_name_H-M    'P1'
_symmetry_Int_Tables_number       1

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 H    0.9943    0.6338    0.6448
 H    0.9998    0.6390    0.9794
 H    0.0994    0.3772    0.0050
 H    0.2734    0.0012    0.7282
 H    0.3447    0.9976    0.1508
 H    0.2532    0.7281    0.5021
 H    0.4134    0.0900    0.9747
 H    0.5078    0.2819    0.7305
 H    0.7264    0.5035    0.9937
 H    0.3203    0.1824    0.8066
 H    0.9708    0.2824    0.7338
 H    0.9846    0.7315    0.2811
 H    0.7180    0.0134    0.4924
 H    0.1875    0.1786    0.2855
 O    0.6845    0.6766    0.1798
 O    0.9646    0.6847    0.1639
 O    0.1808    0.9743    0.6721
 O    0.6775    0.9668    0.6867
 O    0.6732    0.6796    0.9723
 O    0.6897    0.1652    0.6725
 O    0.9499    0.1771    0.6882
 O    0.1750    0.6758    0.9880
 O    0.1779    0.6772    0.6764
 O    0.6760    0.1716    0.9745
 O    0.9750    0.6778    0.6738
 O    0.6815    0.9562    0.1817
 O    0.3245    0.3172    0.8346
 O    0.0189    0.3338    0.8195
 O    0.8201    0.0381    0.3191
 O    0.3278    0.0265    0.3266
 O    0.3072    0.3108    0.0232
 O    0.3139    0.8157    0.3332
 O    0.0365    0.8220    0.3257
 O    0.8195    0.3190    0.0359
 O    0.8255    0.3184    0.3208
 O    0.3259    0.8413    0.0178
 O    0.0371    0.3338    0.3191
 O    0.3133    0.0460    0.8212
 O    0.6180    0.8084    0.0416
```

O 0.0287 0.6262 0.0214
O 0.0327 0.0361 0.6248
O 0.5844 0.0372 0.8257
O 0.8091 0.6047 0.0448
O 0.8322 0.0353 0.5982
O 0.0303 0.0439 0.8202
O 0.0422 0.8193 0.0429
O 0.0394 0.6229 0.8271
O 0.6143 0.0318 0.0434
O 0.0187 0.8244 0.6243
O 0.8095 0.0342 0.0421
O 0.4008 0.1565 0.9568
O 0.9740 0.3928 0.9559
O 0.9519 0.9588 0.3977
O 0.3811 0.9612 0.1921
O 0.1603 0.3845 0.9747
O 0.1903 0.9641 0.3894
O 0.9564 0.9682 0.1849
O 0.9536 0.1793 0.9726
O 0.9608 0.3919 0.1910
O 0.3866 0.9755 0.9732
O 0.9665 0.1873 0.3810
O 0.1827 0.9696 0.9609
O 0.6399 0.8542 0.1482
O 0.8624 0.6292 0.1432
O 0.1567 0.8718 0.6206
O 0.6418 0.8557 0.8643
O 0.8544 0.6392 0.8662
O 0.8624 0.1523 0.6239
O 0.8514 0.1459 0.8683
O 0.1463 0.8515 0.8675
O 0.1660 0.6433 0.8458
O 0.6448 0.1335 0.8663
O 0.8582 0.8486 0.6211
O 0.8616 0.8605 0.1496
O 0.3760 0.1511 0.8242
O 0.1462 0.3555 0.8397
O 0.8559 0.1396 0.3639
O 0.3640 0.1293 0.1486
O 0.1379 0.3562 0.1450
O 0.1306 0.8731 0.3627
O 0.1507 0.8539 0.1338
O 0.8381 0.1431 0.1461
O 0.8539 0.3732 0.1419
O 0.3628 0.8504 0.1418
O 0.1557 0.1454 0.3485
O 0.1370 0.1429 0.8434
O 0.5095 0.7782 0.2206
O 0.0135 0.5066 0.1951
O 0.2024 0.0217 0.4970
O 0.5075 0.9704 0.7881
O 0.7788 0.5056 0.9962
O 0.7892 0.2132 0.4947
O 0.9819 0.2240 0.7834
O 0.2218 0.7918 0.9948
O 0.2153 0.5054 0.7881
O 0.5051 0.2077 0.9950
O 0.0161 0.7808 0.4991
O 0.7812 0.9980 0.2191
O 0.5040 0.2238 0.7806
O 0.0103 0.5033 0.7796

O	0.7736	0.0110	0.4931
O	0.5037	0.9869	0.2178
O	0.2078	0.4891	0.0057
O	0.2026	0.7868	0.4993
O	0.9995	0.7766	0.2197
O	0.7773	0.2126	0.0071
O	0.7853	0.4981	0.2233
O	0.4996	0.7968	0.9985
O	0.0106	0.2081	0.5072
O	0.2216	0.9966	0.7858
Al	0.0414	0.8639	0.2120
Al	0.0299	0.2254	0.3955
Al	0.1607	0.6078	0.9565
Al	0.6249	0.1258	0.7858
Al	0.7870	0.9613	0.6119
Al	0.1368	0.9609	0.7883
Al	0.9703	0.6061	0.7980
Al	0.1301	0.7918	0.6208
Al	0.3950	0.2084	0.0388
Al	0.8664	0.3854	0.0342
Al	0.3967	0.8348	0.2251
Al	0.2104	0.3966	0.8479
Al	0.0258	0.2203	0.8631
Al	0.4011	0.0198	0.8552
Si	0.6111	0.7796	0.1478
Si	0.9643	0.6101	0.1357
Si	0.1426	0.9736	0.6071
Si	0.6043	0.9575	0.7894
Si	0.7800	0.6143	0.9655
Si	0.7931	0.1397	0.5988
Si	0.9531	0.1399	0.7911
Si	0.1495	0.7833	0.9695
Si	0.1505	0.6117	0.7841
Si	0.6103	0.1374	0.9675
Si	0.9654	0.7907	0.6027
Si	0.7830	0.9638	0.1478
Si	0.3974	0.2182	0.8479
Si	0.0370	0.3961	0.8476
Si	0.8554	0.0399	0.3864
Si	0.3978	0.0299	0.2214
Si	0.2069	0.3878	0.0392
Si	0.2103	0.8629	0.3899
Si	0.8490	0.2153	0.0392
Si	0.8561	0.3930	0.2189
Si	0.3930	0.8658	0.0344
Si	0.2115	0.0424	0.8580
Si	0.6067	0.7873	0.9682
Si	0.9642	0.1438	0.6086
Si	0.7837	0.6008	0.1489
Si	0.9652	0.7869	0.1382
Si	0.6118	0.9575	0.1459
Si	0.7792	0.1417	0.9731
Si	0.0331	0.8576	0.3949
Si	0.2212	0.0335	0.3945
Si	0.8521	0.0370	0.2140
Si	0.0351	0.3965	0.2160
Si	0.8612	0.2140	0.3907
Si	0.2198	0.8630	0.0293