Electronic Supplementary Material (ESI) for Nanoscale.


# Supplementary Information for:

# Properties of hydrated $TiO_2$ and $SiO_2$ nanoclusters: dependence on size, temperature and water vapour pressure

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*Ti-O and Si-O distance distributions*

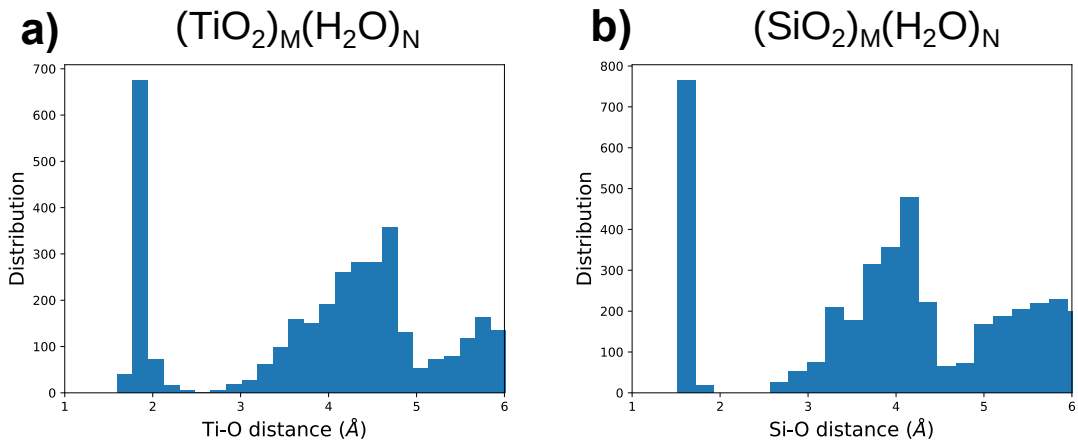


**Figure S1.** a) Ti-O distance distribution over all $(TiO_2)_M(H_2O)_N$ global minima candidates. b) Si-O distance distribution over all $(SiO_2)_M(H_2O)_N$ global minima candidates.

In figure S1 we report the Ti-O (Fig S1 a) and Si-O (Fig S1 b) distance distribution over the whole set of global minima candidates. The histogram shows that the M-O distance is spread in a three-modal distribution with minima in 2.5 and 5 for Ti-O and 2.1 and 4.75 for Si-O. Therefore, in order to calculate the average coordination number of Si and Ti cations we consider the number of first O atom neighbours inside the cut-off radius distance of 2.5 Å for $(TiO_2)_M(H_2O)_N$ and 2.1 for $(SiO_2)_M(H_2O)_N$ systems.

*Total and hydration energies of nanoclusters*

**Table S1.** Total energy, hydration energy at 0K and hydration free energy at 300K of global minima candidate $(TiO_2)_M(H_2O)_N$ nanoclusters. All values are in eV and are the result of calculations using the PBE0 functional with a tier-1/tight numerical basis set. Hydration energies are normalized by the number of oxide units of the nanocluster (i.e. M).

| Structure | Total energy | $\Delta E_{hyd}$/M (0K) | $\Delta G_{hyd}$/M (300K) |
|---|---|---|---|
| $(TiO_2)_4(H_2O)_0$ | -109591.526385000 | 0.000 | 0.000 |
| $(TiO_2)_4(H_2O)_1$ | -111675.264275576 | -0.728 | -0.540 |
| $(TiO_2)_4(H_2O)_2$ | -113759.247100736 | -1.517 | -1.163 |
| $(TiO_2)_4(H_2O)_3$ | -115840.533332674 | -1.633 | -1.093 |
| $(TiO_2)_4(H_2O)_4$ | -117921.782115139 | -1.739 | -0.981 |
| $(TiO_2)_8(H_2O)_0$ | -219189.847545000 | 0.000 | 0.000 |
| $(TiO_2)_8(H_2O)_1$ | -221272.915420889 | -0.280 | -0.196 |
| $(TiO_2)_8(H_2O)_2$ | -223356.299783769 | -0.600 | -0.452 |
| $(TiO_2)_8(H_2O)_3$ | -225439.226319991 | -0.863 | -0.609 |
| $(TiO_2)_8(H_2O)_4$ | -227520.835847176 | -0.961 | -0.644 |
| $(TiO_2)_8(H_2O)_5$ | -229602.136873834 | -1.020 | -0.576 |
| $(TiO_2)_{12}(H_2O)_0$ | -328788.617829000 | 0.000 | 0.000 |
| $(TiO_2)_{12}(H_2O)_1$ | -330871.745529406 | -0.191 | -0.136 |
| $(TiO_2)_{12}(H_2O)_2$ | -332954.718314729 | -0.370 | -0.249 |
| $(TiO_2)_{12}(H_2O)_3$ | -335037.247621494 | -0.512 | -0.343 |
| $(TiO_2)_{12}(H_2O)_4$ | -337119.289873198 | -0.614 | -0.401 |
| $(TiO_2)_{12}(H_2O)_5$ | -339200.683946106 | -0.661 | -0.369 |
| $(TiO_2)_{12}(H_2O)_6$ | -341282.207339540 | -0.720 | -0.326 |
| $(TiO_2)_{16}(H_2O)_0$ | -438387.315807000 | 0.000 | 0.000 |
| $(TiO_2)_{16}(H_2O)_1$ | -440470.305785652 | -0.135 | -0.080 |
| $(TiO_2)_{16}(H_2O)_2$ | -442553.214281150 | -0.265 | -0.187 |
| $(TiO_2)_{16}(H_2O)_3$ | -444635.299203332 | -0.344 | -0.216 |
| $(TiO_2)_{16}(H_2O)_4$ | -446717.771656194 | -0.447 | -0.293 |
| $(TiO_2)_{16}(H_2O)_5$ | -448799.271203031 | -0.489 | -0.277 |
| $(TiO_2)_{16}(H_2O)_6$ | -450880.708071367 | -0.527 | -0.265 |
| $(TiO_2)_{16}(H_2O)_7$ | -452962.039211837 | -0.559 | -0.237 |
| $(TiO_2)_{16}(H_2O)_8$ | -455043.707090292 | -0.612 | -0.216 |
| $(SiO_2)_4(H_2O)_0$ | -48002.6390278000 | 0.000 | 0.000 |
| $(SiO_2)_4(H_2O)_1$ | -50087.3335856515 | -0.967 | -0.744 |
| $(SiO_2)_4(H_2O)_2$ | -52173.3910310210 | -2.275 | -1.825 |
| $(SiO_2)_4(H_2O)_3$ | -54255.1869114091 | -2.518 | -1.867 |
| $(SiO_2)_4(H_2O)_4$ | -56336.5647800218 | -2.656 | -1.810 |
| $(SiO_2)_8(H_2O)_0$ | -96011.4043516000 | 0.000 | 0.000 |
| $(SiO_2)_8(H_2O)_1$ | -98097.0278750840 | -0.599 | -0.477 |
| $(SiO_2)_8(H_2O)_2$ | -100182.535852963 | -1.185 | -0.947 |
| $(SiO_2)_8(H_2O)_3$ | -102267.338674625 | -1.682 | -1.342 |
| $(SiO_2)_8(H_2O)_4$ | -104349.476285513 | -1.846 | -1.430 |
| $(SiO_2)_8(H_2O)_5$ | -106430.686231327 | -1.894 | -1.381 |
| $(SiO_2)_{12}(H_2O)_0$ | -144022.253806000 | 0.000 | 0.000 |
| $(SiO_2)_{12}(H_2O)_1$ | -146108.262282385 | -0.431 | -0.358 |
| $(SiO_2)_{12}(H_2O)_2$ | -148193.837840203 | -0.827 | -0.683 |
| $(SiO_2)_{12}(H_2O)_3$ | -150277.983224293 | -1.104 | -0.902 |
| $(SiO_2)_{12}(H_2O)_4$ | -152361.599422819 | -1.337 | -1.074 |

| | | | |
|---|---|---|---|
| $(SiO_2)_{12}(H_2O)_5$ | -154443.495096819 | -1.426 | -1.116 |
| $(SiO_2)_{12}(H_2O)_6$ | -156524.598700983 | -1.449 | -1.069 |
| $(SiO_2)_{16}(H_2O)_0$ | -192035.449962000 | 0.000 | 0.000 |
| $(SiO_2)_{16}(H_2O)_1$ | -194120.574716013 | -0.268 | -0.214 |
| $(SiO_2)_{16}(H_2O)_2$ | -196206.349746144 | -0.578 | -0.471 |
| $(SiO_2)_{16}(H_2O)_3$ | -198290.633880571 | -0.794 | -0.640 |
| $(SiO_2)_{16}(H_2O)_4$ | -200373.732834230 | -0.936 | -0.740 |
| $(SiO_2)_{16}(H_2O)_5$ | -202456.332524720 | -1.047 | -0.813 |
| $(SiO_2)_{16}(H_2O)_6$ | -204537.676764259 | -1.079 | -0.797 |
| $(SiO_2)_{16}(H_2O)_7$ | -206618.763454576 | -1.096 | -0.774 |
| $(SiO_2)_{16}(H_2O)_8$ | -208699.966734881 | -1.119 | -0.736 |

**Table S2**. Parameters for the FFSiOH*, FFSiOH*-mod and FFSiOH IPs used in the Monte Carlo basin hopping global optimization searches of hydrated titania clusters. [a] O-O parameters of FFSiOH*-mod. [b] and [c] Morse potential acting between atoms pairs with different cutoff distances: 0.0 - 1.2 Å for the interaction in [b] and 1.2 - 2.5 Å for the interaction in [c]. [d] Morse potential acting only between bonded all pairs of atoms within a cutoff distance of 4.00 Å expect on bonded species. [e] hydrogen bond three-body interaction parameters according the formula: if $\theta > 90°$, $E_{H-bond} = A_{2,3}/r_{2,3}^{12} - B_{2,3}/r_{2,3}^{10} \times (\cos\theta_{1,2,3})^4$; if $\theta < 90°$, $E_{H-bond} = 0$. Cut-offs are: 1,2 = 1.00 Å, 1,3 = 2.00 Å and 2,3 = 2.71 Å.

| FFTiOH* | | | |
|---|---|---|---|
| Buckingham | Aij | Bij | Cij |
| Ti-O | 22054.2 | 0.190000 | 0.00 |
| H-O | 1054.2 | 0.145000 | 0.00 |
| O-O | 15039.9 (16039.9)[a] | 0.227708 (0.232708)[a] | 0.0 |
| Charges Q(Ti) = 2.7226, Q(O) = 1.3613 and Q(H)=0.68065 | | | |

| FFTiOH | | | |
|---|---|---|---|
| Buckingham | Aij | Bij | Cij |
| $O1_{shel}$-$O1_{shel}$ | 15039.909 | 0.227708 | 0.0 |
| $O1_{shel}$-$O2_{shel}$ | 6768.7644 | 0.245932 | 0.0 |
| $O2_{shel}$-$O2_{shel}$ | 1688.1482 | 0.292545 | 0.0 |
| $Ti_{core}$-$O1_{shel}$ | 22054.2000 | 0.190000 | 0.0 |
| Morse | $D_e$ | a | $r_e$ |
| $Ti_{core}$-$O2_{shel}$ | 0.045897 | 2.6598 | 2.33921 |
| ($H_{core}$-$O2_{shel}$)[b] | 0.009359 | 3.2461 | 1.76617 |
| ($H_{core}$-$O2_{shel}$)[c] | 0.11097337 | 1.6830 | 2.48921 |
| Morse X12[d] | | | |
| $H_{core}$-$O1_{shel}$ | 0.006439 | 1.8794 | 3.17953 |
| hydrogen-bond[e] | A | B | |
| $H_{core}$-$O2_{shel}$-$O2_{shel}$ | 3653.26 | 0.00 | |
| Spring K($O1_{core}$- $O1_{shel}$)= 256.71027, K($O2_{core}$- $O2_{shel}$)= 130.84247 | | | |
| Charges: $Ti_{core}$= 2.7226, $O1_{core}$= 1.919810, $O1_{shel}$=-3.281110, $O2_{core}$= 1.429114, $O2_{shel}$=-2.767837, $H_{core}$= 0.658073 | | | |

*XYZ coordinates of most energetically stable isomers considered in Table S1:*

12
(SiO2)4(H2O)0 Energy = -48002.639027816

| | | | |
|---|---|---|---|
| Si | -1.16824736 | 0.00006205 | 0.00002247 |
| Si | -3.52005046 | -0.00004121 | -0.00002324 |
| O | -2.34204567 | 1.17534434 | -0.00019840 |
| O | -2.34194418 | -1.17532157 | 0.00021535 |
| O | 0.00000497 | -0.00014702 | -1.17741477 |
| O | -0.00000397 | 0.00033021 | 1.17747324 |
| Si | 1.16824836 | 0.00006632 | 0.00003404 |
| O | 2.34205693 | 1.17533271 | -0.00019533 |
| O | 2.34193491 | -1.17533320 | 0.00023633 |
| Si | 3.52005147 | -0.00006885 | -0.00001905 |
| O | -5.02758507 | -0.00011763 | -0.00007595 |
| O | 5.02758608 | -0.00012915 | -0.00008669 |

15
(SiO2)4(H2O)1 Energy = -50087.3335856515

| | | | |
|---|---|---|---|
| H | -3.33710111 | -2.61340590 | -0.00001556 |
| O | -0.02161851 | -1.34111190 | -0.00000874 |
| O | -0.02161680 | 1.34111132 | -0.00001125 |
| Si | 0.91254339 | -0.00000089 | -0.00000587 |
| O | 2.10187700 | -0.00000281 | -1.17651054 |
| Si | -1.65791496 | 1.14612995 | -0.00000012 |
| O | -1.98459363 | 0.00000041 | -1.17786381 |
| O | 4.77720370 | -0.00000265 | 0.00001058 |
| Si | -1.65791643 | -1.14612843 | 0.00000077 |
| O | -2.37913368 | -2.57731042 | 0.00000512 |
| O | -2.37913043 | 2.57731286 | 0.00000399 |
| O | -1.98457542 | 0.00000152 | 1.17786937 |
| Si | 3.26697606 | -0.00000206 | 0.00000502 |
| O | 2.10186666 | -0.00000031 | 1.17650987 |
| H | -3.33709783 | 2.61340930 | 0.00000216 |

18
(SiO2)4(H2O)2 Energy=-52173.391031021

| | | | |
|---|---|---|---|
| H | -2.87412400 | 0.24357800 | 2.63830400 |
| O | -2.28835800 | 0.91426500 | 2.27286500 |
| Si | -1.18335200 | 0.44170900 | 1.18308300 |
| O | -1.71409900 | -0.77751700 | 0.17498800 |
| O | -0.75810600 | 1.71635500 | 0.20706100 |
| O | 0.23620500 | -0.13041700 | 1.84612600 |
| Si | -0.64598200 | -1.24948100 | -1.00759300 |
| Si | 0.39737800 | 1.38902900 | -0.95127000 |
| Si | 1.43345100 | -0.58132200 | 0.77504200 |
| O | 0.75643400 | -1.71476800 | -0.23262700 |
| O | -1.30475900 | -2.41703700 | -1.92136100 |
| O | -0.23511800 | 0.13160300 | -1.84853800 |
| O | 0.82742000 | 2.68539500 | -1.82613500 |
| O | 1.71843900 | 0.77660900 | -0.15158400 |
| O | 2.76691800 | -1.18485800 | 1.47431900 |

H 3.36011700 -0.56769200 1.91472600
H 0.12978700 3.27576800 -2.12817000
H -0.71329300 -2.95184500 -2.46066500

21
(SiO2)4(H2O)3 Energy=-54255.1869114091
O 1.01140356 0.68487309 1.31708574
O -1.26023121 -0.90833889 -1.27535569
O 0.91961966 -1.58912786 0.00948838
O 0.90549707 0.67729211 -1.31351724
Si -2.15060816 -0.60886309 0.06917727
O -1.19116101 -0.84141360 1.36879983
Si 1.01337998 1.67029144 -0.00394098
Si 0.37660031 -0.86856388 -1.36556032
O 0.93514632 -1.60477946 2.73981516
O 0.82632353 -1.62306183 -2.72127474
Si 0.44758410 -0.84680110 1.39998935
O -0.21927145 2.72572545 0.05402177
O 2.39985778 2.50923723 -0.08271743
O -2.61123634 0.96505932 0.12901346
O -3.50300411 -1.50562698 0.07100960
H -3.41176423 1.18504108 -0.35111837
H 1.78616525 -1.34998818 3.09794914
H -1.10125065 2.33823937 0.13476619
H -3.42960747 -2.41501598 -0.22191007
H 2.31423135 3.45689052 0.02961889
H 1.68115772 -1.39022676 -3.08546095

24
(SiO2)4(H2O)4 Energy=-56336.5647800218
H 4.52075437 -1.12286186 0.29894523
H 1.32814864 -1.90322794 -1.18605768
O -0.80620073 -1.28417812 0.91967163
O 2.22966939 1.06901638 -1.08831037
O -0.09154467 -0.06820838 3.18165648
O -0.32007221 2.29636431 -1.48738469
O 4.10796063 -0.26200605 0.21382477
Si -1.38112588 1.61122074 -0.47092003
O -2.92671746 -2.27481455 -0.48653260
Si 0.01523571 -0.02348120 1.56633011
O 2.24485605 -1.66591583 -0.97730505
O -0.66410968 1.33391320 0.97990381
Si 2.52901542 -0.28079776 -0.18302123
O 1.58136675 -0.10956234 1.13031833
Si -1.58205675 -1.36484105 -0.50872164
O -2.68888360 2.56403141 -0.33789968
O -1.92415309 0.15104239 -0.99503791
O -0.51696145 -2.10861189 -1.51619012
H -2.53074170 3.50277527 -0.44559187
H -0.86687720 -2.43979873 -2.34477951
H -3.73756604 -1.84202967 -0.21489398
H 0.59315347 1.98416986 -1.38864912

H 0.73686199 -0.08380058 3.66123433
H 2.85381405 1.21169939 -1.80292222

24
(SiO2)8(H2O)0 Energy = -96011.404351640
O -1.83871565 4.26116128 -2.49533138
Si 1.83599377 -0.72968906 0.00044217
O 2.27699411 -1.92559720 -1.01339908
O -1.92560832 -2.27699114 1.01339296
Si 3.15730580 1.36206057 1.58516485
O 4.26113611 1.83872233 2.49537347
O 0.16209454 2.97701207 -1.01461671
Si -1.83599457 0.72969159 0.00042675
O -4.26116495 -1.83873679 2.49531302
O 0.57356921 -1.33076764 0.85173061
Si -0.72969080 -1.83599332 -0.00043819
O 2.97700096 -0.16209151 1.01465062
O 1.92559637 2.27698659 1.01342998
Si -1.36205654 3.15732193 -1.58513234
O 1.83874276 -4.26114065 -2.49534128
O -2.27698329 1.92560679 -1.01341122
Si 1.36207350 -3.15730802 -1.58513939
O -1.33076139 -0.57357023 -0.85173454
O -0.57357945 1.33076424 0.85173340
Si -3.15732420 -1.36206904 1.58512019
O -0.16208385 -2.97700223 -1.01463932
O 1.33076983 0.57357852 -0.85171584
Si 0.72969002 1.83599585 -0.00041740
O -2.97701299 0.16208707 1.01461868

27
(SiO2)8(H2O)1 Energy = -98097.027875084
O -1.60072111 4.93416100 -1.46849810
O 0.91564083 -0.57636664 1.83837562
O -4.35862376 -0.89724095 2.28019998
O -3.22767615 0.05569585 -0.09056104
Si 1.46669840 0.97145911 2.02968601
O -0.64510599 0.76889240 0.17603766
O -1.41134411 3.27640577 0.77216481
Si -3.14065374 -0.33187689 1.58084251
O -2.20569751 2.20692498 -1.47549931
Si -1.21709110 1.96484763 1.61874579
O 0.09333395 -1.68459927 -0.49073439
Si -0.32624610 -0.93683082 0.87495952
O 0.15475046 1.85868167 2.47545951
Si -1.29769930 3.55621000 -0.92000834
O 0.53771748 -1.84231172 -3.17642481
Si -2.16234635 0.69040654 -1.05957147
O 1.89159531 1.46791174 0.51860474
O -2.43453720 1.12492988 2.15632569
Si 0.05799742 -0.92705469 -1.96071675
O 0.28312404 2.90197637 -1.16704541

O 1.07128728 0.36126044 -1.80610957
O 2.72131288 1.09965168 3.00707950
Si 0.83944174 1.51223733 -0.70170938
O -1.70523066 -1.29396641 1.53190494
O -1.46524339 -0.32434131 -2.11395518
H -0.03323721 -2.52448179 -3.53390583
H 2.61401288 1.03099208 3.95729327

30
(SiO2)8(H2O)2 Energy = -100182.535852963
Si 4.91960386 10.30557707 2.24396409
Si 5.82117424 10.59679260 4.92876358
Si 7.79700430 10.64100168 2.87716777
Si 6.93978697 8.58352844 0.92281119
Si 6.27262169 7.51826418 4.58386670
Si 8.87764103 8.00594288 2.92923983
Si 6.75235712 11.43871564 0.24719228
Si 4.52917412 7.49756832 1.98368694
O 5.43089114 11.30933009 6.31523271
O 6.50887249 9.50563785 2.38908962
O 3.94551135 9.04295701 1.98574234
O 10.25870186 7.21794802 3.15296925
O 5.17118385 7.15215231 3.42970685
O 5.71434091 7.53408941 0.83429269
O 5.22418701 11.30698582 1.05570452
O 4.71438403 10.88694284 3.73720620
O 3.38866040 6.41231669 1.66162337
O 7.78661817 7.45401844 3.98913682
O 7.79413738 11.60842045 1.62314115
O 5.94146070 9.00292533 5.18836414
O 6.22703037 6.41703168 5.76267677
O 8.29414389 7.83998751 1.39261353
H 2.91170732 6.47916455 0.83289858
H 11.00802511 7.43381980 2.59576750
H 5.40675588 6.30020417 6.24294007
H 5.33203285 12.26260835 6.33013209
O 6.88147548 12.45139901 -0.87523436
O 7.02802033 9.76773732 -0.12522481
O 7.23202459 11.17434220 4.29386953
O 9.04447157 9.64039034 3.10185906

33
(SiO2)8(H2O)3 Energy = -102267.338674625
Si 7.56192640 9.60430489 4.21300337
Si 7.76845047 8.84419376 0.55440064
Si 9.92521726 8.92938155 2.78376007
Si 5.71726601 10.27456630 2.18065003
Si 6.17344291 7.58544554 2.43975930
Si 7.53800129 7.73383543 6.34091300
Si 6.58922465 5.65390603 4.45518936
Si 9.47459446 6.39905392 4.52766821
O 7.31644429 8.18272074 3.44522973

O 8.09922790 8.85813737 -1.02739166
O 5.74833831 6.18500723 3.12107153
O 7.35702339 7.73055663 7.94661225
O 6.83292874 10.12763832 0.99559414
O 6.47863744 10.65779063 3.59810218
O 10.04217603 7.42918888 3.39716287
O 8.16942185 5.53595742 4.04873864
O 6.90874844 7.49632464 0.98499808
O 11.44805798 9.46029577 2.61704202
O 9.19511946 8.91572019 1.32122916
O 10.65217536 5.34145435 4.87605176
O 7.33552316 9.28342167 5.78769900
O 6.44663380 6.69196211 5.71026729
O 4.63869353 11.40355089 1.78001601
H 5.73375731 3.60894946 4.23028634
H 7.35878841 8.80741250 -1.63286617
H 11.58270607 10.22852981 2.06128713
H 4.18781884 11.86125164 2.49053641
H 7.66665096 8.50092425 8.42382296
H 11.54313934 5.61572754 4.65613467
O 5.04465579 8.77061893 2.36127426
O 9.01847973 7.24729405 5.85310497
O 9.09999954 9.93806539 3.80619152
O 5.95183087 4.24141220 4.91546097

36
(SiO2)8(H2O)4 Energy = -104349.476285513
Si 5.48172935 8.24225432 4.63902219
Si 9.56127371 9.42999534 5.61181580
Si 6.89522158 10.94688372 5.17670125
Si 10.20142593 9.76155638 2.59963406
Si 8.15312056 6.74332389 5.02954322
Si 8.79037221 7.07430059 2.01486195
Si 7.51595879 11.24411518 2.16274257
Si 6.09274706 8.55363943 1.62018229
O 6.33793646 12.18302732 6.06677728
O 5.43027748 8.08431461 3.02231959
O 4.08988649 7.73496516 5.29758591
O 9.03212564 10.69334932 1.96069338
O 8.20027042 10.27960243 5.88016446
O 6.65224845 7.31965018 5.27217968
O 8.39073032 6.44037867 3.45615658
O 10.60972847 9.63318532 6.83136380
O 7.28952657 11.57763479 3.73731513
O 11.66103181 10.23640617 2.07765828
O 8.35836057 5.33104954 5.79566970
O 6.44682395 10.13979914 1.65047092
O 7.26216155 12.56488338 1.25752263
O 5.75170341 9.80457353 5.00384518
O 9.22163457 7.84734504 5.56016109
O 7.45771968 7.71715678 1.34092396
H 6.05608796 11.98405775 6.96002085

H 11.12522786 10.44006819 6.83118174
H 3.28024638 8.02032226 4.87322072
H 8.98964929 5.08786937 1.03060019
H 7.69707816 13.37236669 1.53270734
H 5.14265915 8.62079990 -0.39190840
H 11.90750444 9.98437782 1.18735812
H 8.24153797 5.32522429 6.74602516
O 9.42885894 5.93859519 1.05075221
O 10.21736123 9.92998969 4.21118119
O 9.92966887 8.21519251 2.18113030
O 4.98400475 8.25024611 0.47671965

39
(SiO2)8(H2O)5 Energy = -106430.686231327
H 2.84069832 6.89361091 1.09192272
H 3.82808133 6.61635067 2.23364937
O 3.70707258 6.52422337 1.27775309
Si 5.80897548 7.78495836 4.17649764
Si 9.34290465 9.67093864 5.76912644
Si 6.52752915 10.63182302 4.85773008
Si 10.44050685 10.07980334 2.92348549
Si 8.52457442 6.74578503 5.01524386
Si 9.60644464 7.18037849 2.11588431
Si 7.64063421 11.03299128 1.91181247
Si 6.89173026 8.19258862 1.17513342
O 5.67874299 11.83805595 5.53099669
O 6.24636547 7.89642590 2.64045796
O 4.37175633 7.00092819 4.15976689
O 9.23809685 10.86899102 2.17261606
O 7.86830991 10.34164558 5.73009469
O 6.90040276 6.94032171 5.03324054
O 9.02554249 6.53753052 3.49429677
O 10.01732515 10.11569490 7.17603337
O 6.89108301 11.09248767 3.35496904
O 11.87213906 10.77016384 2.60277999
O 8.93007633 5.41063825 5.84121805
O 7.08432824 9.80131058 1.02347642
O 7.33794142 12.37817499 1.06074299
O 5.63524804 9.26448267 4.82296590
O 9.21222058 8.05186202 5.69433991
O 8.36327330 7.49433271 1.11994908
H 5.61687707 11.84402240 6.48649392
H 10.97353208 10.16611188 7.19373617
H 4.06924477 6.60598958 4.97794905
H 10.27997153 5.41861508 0.93780820
H 7.51627958 13.21499754 1.49038150
H 5.11176556 7.19891423 0.36424632
H 12.21503153 10.66613063 1.71466751
H 8.94037971 5.47709653 6.79619709
O 10.65251112 6.17053424 1.39929117
O 10.25468565 10.19220837 4.53240937
O 10.44281556 8.52516672 2.45945235

O 5.93408996 7.60531343 0.02758316

36
(SiO2)12(H2O)0 Energy = -144022.253805869
O 1.57100421 0.18699227 2.73844267
Si 0.04670764 0.04107870 2.13428217
Si 2.66146904 0.08585461 1.51706564
O 0.20670815 -1.36770770 1.36733845
Si -2.59244925 -0.02516154 1.63422538
O 3.39941713 -1.28119599 1.27620925
O 1.83628184 0.34050942 -0.04670453
O 3.30255259 1.61981133 1.28899776
Si 2.48211759 1.96905311 -0.09222252
O -1.44957431 -0.08010278 2.80975731
O -0.14794276 1.41944571 1.32141505
Si -0.27561407 2.28867113 -0.03798196
O 1.25470551 3.02062053 -0.08556543
Si 2.59249390 0.02515012 -1.63413671
Si 0.27565877 -2.28868256 0.03807065
O -1.83623715 -0.34052079 0.04679322
Si 3.32850934 -2.44491594 -0.02562206
O 3.24164140 1.56620542 -1.49353058
O -3.34131687 1.33224975 1.37328171
Si -2.48207291 -1.96906452 0.09231121
O -3.24159673 -1.56621684 1.49361924
Si -0.04666294 -0.04109009 -2.13419349
Si -2.66142440 -0.08586603 -1.51697694
O 4.41520940 -3.50222395 -0.02895979
O 3.34136142 -1.33226124 -1.37319302
Si -3.32846474 2.44490447 0.02571076
O -1.70149786 2.99437424 -0.02049952
O -0.20666325 1.36769637 -1.36724983
O 1.70154248 -2.99438585 0.02058820
O 0.14798760 -1.41945703 -1.32132631
O 1.44961900 0.08009134 -2.80966869
O -1.25466081 -3.02063190 0.08565413
O -3.30250790 -1.61982275 -1.28890907
O -3.39937259 1.28118452 -1.27612057
O -4.41516474 3.50221253 0.02904849
O -1.57095952 -0.18700366 -2.73835392

39
(SiO2)12(H2O)1 Energy = -146108.262282385
O -0.74175429 -3.40628232 0.05275989
Si -1.11331808 4.65610061 -1.16033996
Si -0.34568603 2.17459715 -2.09529848
O 2.48425777 -0.57727026 -2.04329549
Si 3.19755333 -1.23998883 -0.70554685
O -0.35502095 -1.24434484 3.88334984
O -1.90779305 -2.98291594 2.67339972
O -2.97122048 1.44321619 1.07231264
Si 0.92652221 -0.16933677 -1.77002394

O 1.67430281 0.17234084 2.37580324
O -1.52272861 1.55255852 -1.14022983
Si -1.92231805 2.37671979 0.22422523
O 0.29012084 4.70663664 -0.24568338
Si 0.80611079 3.19099993 0.18699608
Si -1.47634404 -2.50271833 1.23620755
O -2.31655355 3.88981955 -0.29579056
Si 0.50869252 -2.33711227 -0.20202294
O 0.94106714 0.31814567 -0.18029570
O -0.87351624 0.49728598 2.04547324
Si 2.07276216 0.81363745 0.91132204
O -0.50177146 2.66003040 0.99315133
Si 0.22524805 -0.52057650 2.59481267
Si -2.41644500 0.05367795 1.77926481
O 2.13003565 -2.42260994 -0.17856147
O -2.91394794 -0.57149249 3.17241416
Si -2.01239563 -1.80722981 3.97372042
O 2.08067065 2.46814389 0.97319171
O -2.35533323 -1.23241686 0.70508272
O 0.21807324 0.82677646 -2.86335442
O -1.48298017 6.16348546 -1.57071907
O -2.49753184 -2.30247409 5.32385601
O 0.13529681 -1.75395441 1.38108973
O 4.59428592 -1.97060838 -1.00600145
O 1.03037643 2.57029772 -1.30685298
O 0.07843949 -1.55868157 -1.56414438
O -0.89223010 3.66447356 -2.51108979
H -2.31209902 6.32340448 -2.02428504
H 5.40619808 -1.48115852 -0.86532745
O 3.39326283 -0.00850410 0.38965116

42
(SiO2)12(H2O)2 Energy = -148193.837840203
O -0.66709155 0.06474241 -5.64157616
Si 1.97182954 2.90823135 -0.86580810
Si -0.96441925 -1.93768889 1.71850036
O -0.91421012 -3.44650426 -1.45375150
Si -0.43992750 1.74990473 -1.79489465
O 0.76567866 0.60940582 -1.62088219
O -0.61291674 -1.33391283 -3.46304249
O 1.17440345 -2.01216509 -1.76552067
Si -0.18195646 0.12506704 -4.10308262
O -1.68771155 1.49245840 -0.74732340
O -1.29539456 -0.95859671 -1.02818829
Si 1.61752089 -3.03897427 0.94765262
O 0.00124258 0.72228057 0.92111843
Si 1.35788117 -1.41621886 3.25599851
Si -1.29989079 0.16045037 0.13913599
O 1.78940687 0.04318650 2.61718760
Si 2.14069863 0.64922174 -2.56538121
O 2.75025620 2.08618765 -2.09142753
O 2.86514441 -2.78125139 -0.09849657

Si 1.60040765 0.66094597 1.10213638
O 2.63737117 4.37360770 -0.73251499
Si 2.47602710 -1.44993976 -0.98780987
Si -0.79683720 -4.19587357 0.01058070
O 3.17586339 -0.58158609 -2.19893163
O 2.47359416 -0.33231305 0.18300416
Si -0.42549427 -1.95386346 -1.95003980
O 0.77893148 -4.38060641 0.54631282
O -1.57252509 -3.37769950 1.24862530
O 1.46302822 0.42700732 -4.03329810
O -1.99867326 -0.70709048 1.35317414
O -0.28710088 -1.71886895 3.18833951
O 2.09291604 2.15809302 0.61248718
O 2.06625718 -2.72274400 2.48574778
O 0.41200989 -1.89895883 0.77741264
O 1.84379709 -1.35419226 4.79482091
O -0.88980331 1.43066856 -3.33084485
H 2.98891518 4.60603450 0.12750446
H 1.67653350 -2.12446742 5.33920787
H -1.50545089 -6.23357536 0.54891078
H -0.49957925 0.83598761 -6.18469679
O 0.39763538 3.08951734 -1.38863554
O -1.47870614 -5.64331013 -0.20502618

45
(SiO2)12(H2O)3 Energy = -150277.983224293
O -2.55546139 0.34468848 2.40923522
Si 1.89780105 -2.76121970 0.93270006
Si 2.09715521 -0.65104138 -0.88748802
O 2.98234961 -0.86247140 -2.23548380
Si 2.59431035 -2.06128443 -3.30131968
O -0.73130763 -1.50856178 2.81803515
O 1.88440607 -2.73888859 2.60320451
O 3.44163258 -1.78581791 -4.64363018
Si -4.03264623 1.18105376 -1.07668376
O -0.41617220 2.71997688 -0.32147393
O -0.91579125 0.41602634 -1.38161245
Si -1.99351017 3.19319548 -0.18457233
O -0.20702852 0.51225807 1.17294209
Si 0.04356173 1.16304663 -0.30040512
Si 0.20349000 -2.82889413 2.59575024
O 0.77401806 -1.57821344 -1.08023155
Si -3.47577021 1.56699980 1.82581978
O 2.64969295 -1.35821973 0.47607830
O -4.46865683 2.08139793 2.99414625
Si 2.04866727 -4.38628921 -1.52775769
O -4.32732906 1.05664504 0.52858238
Si 0.08646352 -2.48593902 -2.24033378
Si -1.95703753 -0.82576855 -1.20171606
O 0.95544043 -2.08189198 -3.57574244
O 1.61464348 0.89405254 -0.68488856
Si -1.36751264 -0.50880981 1.70015139

O -5.37640821 1.41226324 -1.94394228
O -2.51660917 2.78560968 1.30978961
O -2.07788610 4.78421359 -0.45969013
O -0.36834377 -3.95388248 3.60351189
O -3.40748938 -0.23352160 -1.62292873
O -1.48520550 -2.06951221 -2.18048680
O -1.97750845 -1.25773354 0.37510506
O 2.93196300 -3.50392092 -2.59710129
O 2.49015442 -3.95228331 -0.00932408
O 0.24854992 -3.04696993 0.96227334
H 2.03901782 -6.42139901 -2.43172213
H 3.26281485 -2.32993214 -5.41112155
H -1.28270683 5.29629616 -0.30921288
H -5.85226041 2.23246198 -1.80949789
H 0.20168649 -4.70803327 3.76428143
H -4.42508080 1.61684697 3.83036174
O -2.97557733 2.42743208 -1.24246619
O 2.33638442 -5.97129773 -1.64046605
O 0.46559638 -4.03336747 -1.87536911

48
(SiO2)12(H2O)4 Energy = -152361.599422819
O -1.29284708 -1.10787224 -2.54854041
Si 1.30635239 -0.66299891 -0.24078729
Si -1.74891841 1.48326408 2.31026830
O 1.10708479 -1.61599133 -1.53824199
Si 1.53965820 3.18871306 -1.85694004
O -5.74384196 0.55404485 3.14929938
O 0.89038777 -0.14543826 -3.74978504
O 0.45760211 0.70409179 -0.46601219
Si 2.08732171 0.94806671 -3.73803982
O 0.72040170 -1.44119842 1.07108987
O 2.68410102 0.98021905 -5.24143973
Si 3.44729087 1.03021746 -1.08747107
O 1.50477884 2.40809328 -3.29018060
Si -0.85287659 -1.21997611 1.45382036
Si -2.15297534 -0.39303987 -1.37988565
O 5.00482089 1.25907268 -0.71834669
Si 0.27216149 -1.39530752 -2.93001579
O -3.70635259 -0.84128327 -1.48557224
O -1.68197985 -0.88115435 0.09779379
Si -4.48220844 0.06477226 2.26072101
O -1.91712977 1.22788067 -1.41817537
Si -4.64172208 -1.45961171 -0.28276122
Si -0.69380434 1.84968262 -0.52478923
O -3.34833391 1.23468578 2.24337977
O -4.99934764 -0.24524165 0.74810854
Si -3.24290348 -2.64141651 2.08054210
O -0.96113942 0.05738435 2.45134269
O 0.03370087 3.13172353 -1.19723545
O -3.84137158 -1.32292865 2.84231817
O -1.60362998 -2.51948808 2.06564748

O 2.84270951 -0.15272645 -0.10555116
O -3.89488565 -2.63763627 0.57351695
O 0.37805948 -2.70001472 -3.87965400
O -1.22693637 2.23437605 0.95490999
O 3.22601217 0.54281476 -2.63269477
O 2.66942432 2.45879828 -0.92432512
H 3.34801423 1.64222007 -5.43670844
H -0.09527710 -3.48673027 -3.60767224
H -6.31012754 -1.69695016 -1.73673869
H -0.60189623 2.78020940 3.71730656
H 1.24061473 5.37885531 -2.08139475
H -4.45551941 -4.35614013 2.81239264
H 5.48132554 0.50871398 -0.36157192
H -5.57898760 1.25258579 3.78336721
O -5.96472641 -2.11486103 -0.94719442
O -3.55771400 -4.02504759 2.85397219
O -1.48316293 2.42350230 3.60171442
O 1.95559303 4.74396538 -2.02818608

51
(SiO2)12(H2O)5 Energy = -154443.495096819
O -2.36586684 -0.07315504 4.52513978
Si 0.43737557 0.57690388 -1.80551243
Si -0.67276856 -2.02261848 -0.45852985
O -2.97514907 3.11566194 -1.67446791
Si 3.26704950 -1.05080588 1.13515774
O -0.19889583 -2.52968194 1.00109063
O 0.90844876 0.14228039 -3.29278628
O 2.20263439 -0.93521060 -5.34298084
Si 2.17425189 1.73663000 0.36987011
O -0.48847441 -3.21199323 -1.54103114
O 2.94855233 3.16609046 0.44295310
Si 0.52688803 -2.02406411 2.36948896
O 0.26016777 -0.74246563 -0.86018200
Si 1.74660637 -1.16569732 -3.80808469
Si -1.71693505 0.03843945 3.04370374
O -0.38335475 -0.87361521 3.06348337
Si 3.33015847 -2.54990885 -1.69705901
O 4.78281279 -3.18124690 -2.03987641
O 3.01304819 -1.38933347 -2.79797236
Si -3.19162591 -0.54879708 0.36740156
O 0.81718774 -2.50015692 -3.74744569
Si -2.04288502 2.04854580 -0.88891444
Si -0.45981916 2.53295726 1.73953798
O -1.22767332 2.76291493 0.32219927
O 3.32359619 -1.95772842 -0.19417224
Si 0.70881967 -3.63202265 -2.57302095
O 3.18125467 0.52638053 0.74185650
O -2.76199784 -0.51310313 1.92617763
O 1.99295108 -1.42672528 2.05899718
O 0.96891795 1.80749239 1.45027325
O -4.73533067 -1.03709377 0.32300993

O -0.96381319 1.38087859 -1.91806083
O 0.74365682 -3.27153711 3.38332858
O 4.65043009 -1.34443817 1.93523587
O 2.14208523 -3.66734005 -1.80214361
O -0.26251258 3.94710650 2.50737217
H 4.68264046 -1.07987452 2.85511395
H -0.50975174 -5.42162522 -3.06102998
H -3.12993368 0.47334258 4.71157750
H -5.20763940 -0.91850382 -0.50152952
H 3.75009016 3.26170245 -0.07248831
H -0.03074127 -3.60790353 3.83529033
H -2.54046085 3.86645316 -2.07936220
H 5.28625947 -3.52956475 -1.30318915
H 0.51618312 4.45521464 2.27548983
H 2.41497473 -0.04036604 -5.60843153
O -1.35097392 1.58353873 2.69878929
O 0.37851111 -5.08942953 -3.19160220
O -3.05007203 0.91917622 -0.31470749
O 1.57589471 1.51321044 -1.13024677
O -2.23315217 -1.59373369 -0.44009043

54
(SiO2)12(H2O)6 Energy = -156524.598700983
O 1.70420328 2.07653383 -0.94904479
Si -0.64501273 2.67421163 2.28496502
Si -2.83618688 -1.57473735 3.33910474
O 2.82458795 0.46260820 0.86267421
Si 2.59297026 -0.98188411 1.58392711
O -4.29417827 4.43412707 1.66257950
O -3.10060374 -2.93861865 2.46356903
O -2.11369287 -1.30154886 -1.40993693
Si 0.32140023 2.84613006 -0.63722173
O 2.45810461 -0.40033789 -1.59942183
O -2.22780735 2.91177076 2.07788199
Si -0.25933364 -0.45415241 2.25946971
O -0.36825232 1.11234094 2.62412236
Si 2.80547611 0.92145457 -0.70929277
Si -3.52112412 -0.49983502 -1.37767237
O 4.21461486 1.58971032 -1.15749043
Si -3.55068137 3.08058952 1.16858177
O -3.62915790 -0.29044232 2.73473796
O -2.49088486 3.25998838 -2.98433521
Si -2.46861738 2.37681783 -1.62507526
O -6.09114747 -0.31112193 1.89891706
Si -0.94843706 -1.84315471 -0.41799258
Si -4.58988200 0.18233398 1.51453826
O 3.89105951 -1.30172118 2.50053323
O -3.29460030 1.01598337 -1.91579339
Si 1.97929489 -1.89717494 -1.16520006
O 0.20230624 3.09845143 0.96174006
O 0.26598382 4.25976830 -1.45415703
O 0.37350942 -2.07439576 -1.33211786

O -1.31256900 -3.25600400 0.27692277
O -0.94610630 1.99226461 -1.17777358
O 2.74767936 -2.95788441 -2.11930863
O -4.63987812 -1.23523755 -2.29750032
O -3.31404383 -1.86212201 4.86355366
O -4.10824168 -0.51372355 0.13290727
O -3.17433442 3.19859378 -0.40827506
H 4.98435623 1.01996183 -1.16798555
H -3.58646877 -1.10561869 5.38477523
H -6.75980433 -0.24500126 1.21616561
H 2.27865671 -3.76872248 -2.31873976
H -5.02957405 4.74522731 1.13440038
H -1.81905343 3.94525459 -3.02789710
H -4.47165297 -1.27049932 -3.23979472
H 0.95653923 4.90161033 -1.28649160
H -3.93913116 -3.38296950 2.60092857
H 0.70035038 3.51600647 3.84481639
H 3.76740209 -1.90450291 3.23441299
H -1.97239081 -3.26010994 0.98588520
O 2.38766096 -2.09431039 0.40769348
O -4.52662104 1.79408540 1.38154913
O -1.24069312 -1.30559099 3.23251213
O -0.66148549 -0.67304289 0.69898193
O 1.26359016 -0.95100678 2.52701587
O -0.20426954 3.59953032 3.54212796

48
(SiO2)16(H2O)0 Energy = -192035.449961704
Si -3.95197770 -0.66551395 -1.54741799
O -1.31534619 0.13091669 -1.51689864
Si -2.28333159 1.43395546 -1.47493567
O -1.37393359 -2.10609652 0.00010157
Si 1.39340818 -1.49072582 1.50707746
O 2.89148344 -1.77160934 2.17018379
Si -2.28330215 1.43406538 1.47489271
O -3.66465230 0.83189056 2.18410699
O -2.89312932 -1.76944961 -2.17001990
O -0.00094242 -2.00595535 -2.22172082
Si 1.39337785 -1.49083808 -1.50697598
Si -3.95194686 -0.66539886 1.54756468
O -2.89308590 -1.76928783 2.17022802
O -0.00089776 -2.00578965 2.22188884
Si 0.00100126 2.91765618 1.19954489
O -3.66469588 0.83172798 -2.18407758
Si -1.39482144 -1.48962404 -1.50699345
O 1.31514477 0.12976375 -1.51673050
Si -1.39479116 -1.48951159 1.50715104
O -1.31531580 0.13102982 1.51693352
O -3.50136132 -0.53334309 0.00006395
O -5.51281860 -1.12857356 -1.38023615
Si -6.37352406 -1.38188623 0.00012402
O -5.51279105 -1.12847098 1.38044826

O -7.82220425 -1.80929836 0.00015460
O 1.37210943 -2.10743080 0.00007394
Si 2.28409804 1.43208457 -1.47495675
Si 2.28412789 1.43219431 1.47482229
O 1.31517535 0.12987671 1.51671280
O 2.72430380 1.96442905 -0.00009148
O 3.66500542 0.82896665 2.18404866
O 3.66496124 0.82880421 -2.18416603
O 2.89143970 -1.77177087 -2.17009165
Si 0.00097718 2.91756726 -1.19974411
O -1.36683118 2.67352709 -2.08339107
O 1.36858311 2.67249002 2.08323106
O 1.36854127 2.67233516 -2.08343943
O -1.36678942 2.67368212 2.08323748
O -2.72307693 1.96658650 -0.00003693
O 0.00150368 4.10499360 -0.00014365
O 0.00051263 1.78165812 -0.00005742
Si 3.95114354 -0.66864667 -1.54750553
Si 3.95117495 -0.66853177 1.54749408
O 3.50069116 -0.53615122 -0.00000610
O 5.51167724 -1.13275331 1.38035089
Si 6.37219903 -1.38673774 -0.00000385
O 5.51164936 -1.13285557 -1.38035986
O 7.82059032 -1.81513039 -0.00000199

51
(SiO2)16(H2O)1 Energy = -194120.574716013
Si 4.28823508 2.39513009 0.23217266
O 5.24244046 -3.63841698 0.25614109
O -5.80850872 -0.07021340 3.35216450
H 6.19395672 -3.52963893 0.22845797
H 5.00021450 4.48848323 -0.03128963
O 2.76544000 -2.86140008 0.25503385
Si -4.13157269 1.54815083 -0.21130590
O -1.47757497 1.56045432 -1.78244247
O 1.20975962 1.58379826 1.54330550
Si -1.28156801 0.08014527 -2.40710061
O 4.62192511 -1.33749383 1.53613257
O -4.71785699 1.41658340 -1.78858668
Si -4.08709483 -1.60799008 -0.23976413
O -4.81545568 -1.39441834 1.13783418
O 2.73849252 2.91940248 -0.07356839
Si -4.01031620 -0.02393876 -2.12414675
O 2.98067500 0.20466432 -2.57719960
O -3.15690231 0.19652602 2.59137790
Si -1.43814569 2.16129626 -0.26457715
O 4.79888680 1.43766242 -1.03347578
O 0.90591386 -1.08001648 1.02440580
Si 1.27285420 2.21446616 0.05920248
O -5.03002200 1.25974754 1.04690840
O 5.25263156 3.67354903 0.40404905
Si 3.95839816 0.06032782 -1.26249953

O 2.55446408 -0.15530971 2.77636402
O -2.76644616 -0.15015433 -3.15781876
Si -4.80312588 -0.01384255 2.21652782
O -1.69070495 -1.54275586 1.34487436
O 1.46363170 -1.55754437 -1.56720369
Si 4.32519198 -2.31537914 0.22082209
O 3.04078757 0.03236820 0.11751085
O -2.93322164 -2.74285254 -0.44853395
Si -1.41083449 -2.17539254 -0.11214766
O -0.34402964 0.00862536 3.00083697
O -1.14504812 -1.08331731 -1.29608532
Si 3.71776907 0.01690660 1.63578910
O -0.11597691 3.11872622 -0.10719545
O -3.34956399 -0.01489355 -0.51058128
Si 1.32095348 -2.18819465 -0.07909159
O -2.99274395 2.70504272 -0.09744399
O 4.68288916 -1.39645504 -1.13068887
Si 1.05115810 0.08410188 2.14757940
O -0.06430182 -3.11161231 -0.11199024
O 4.43228117 1.48508438 1.61490105
Si 1.41162854 -0.05850412 -2.17434086
O -1.31418034 1.01311349 0.85707405
O 0.13814639 0.01393663 -3.23347131
Si -1.68745755 -0.06549595 2.02841458
O -4.82168531 -1.39489004 -1.74310739
O 1.04866398 1.11224696 -1.11393330

54
(SiO2)16(H2O)2 Energy = -196206.349746144
O 2.94774724 -0.29877475 0.11375818
Si 3.98758008 0.01480817 -1.15164741
Si 3.50412879 -0.93025694 1.54475465
O 4.04554013 -2.38397460 1.04502144
O 4.58042596 -1.48659500 -1.40084362
O 4.93290877 1.15775214 -0.47279856
O 5.83278532 2.55718960 1.57374380
O 4.57436324 0.21404094 1.99370462
O 4.45884671 -4.14574725 -0.95793460
Si 4.61615203 1.61318457 1.09348892
H 5.61954847 3.27995931 2.16486104
H 5.39997439 -4.26318010 -0.82271985
Si 3.81926071 -2.71616831 -0.57361157
O -4.29022954 -0.46045063 -2.15957270
O -1.93554258 -2.12332299 0.98791123
Si -1.93298461 -0.89606054 2.05001425
O 3.16022658 0.51302652 -2.47394847
O 2.22486609 -2.81858033 -0.95430019
Si 1.58870020 0.81924040 -2.07575241
O -0.68395407 1.53551698 -0.70400817
Si -1.91751109 -2.13826278 -0.63996134
O -0.51379601 -0.89448809 2.88966662
O -2.13323377 3.10893798 0.86812099

O 0.57812379 3.40978867 0.73117219
O 0.97256208 1.04211541 1.71159996
Si 0.81719071 -0.55178128 1.99038487
O 2.26225461 -1.04604857 2.59480828
O 0.54843566 1.65281527 -3.05087036
Si -2.96701152 1.67941318 0.84536757
Si -0.82775095 2.07919552 -2.26363802
O -0.51026984 -2.79504161 -1.17535077
O -6.05292359 -0.47065408 2.67286780
Si -0.79751067 3.07343774 -0.08959842
O 3.19056005 2.43623689 1.27366983
Si -4.63739322 -0.25661257 1.93163441
O -0.95093078 3.64523396 -1.66748885
O -3.38081302 -2.72574347 -1.08644350
Si -4.63319848 -1.63790771 -1.03293614
O 1.85129278 1.81810974 -0.82345685
O 0.61100952 -1.39105489 0.63271151
Si 1.66614901 2.15262563 0.74634666
O -6.04650988 -2.34995065 -1.34189456
H -6.13463650 -2.82758566 -2.16774672
O -3.38810452 -0.93027000 2.79607437
O -4.27872847 1.36163512 1.77141894
Si -2.97739168 0.44904761 -1.80680258
O -1.90451889 0.54587524 1.31023966
H -6.16242068 -0.09251272 3.54629538
O -4.72269863 -0.96113787 0.45666709
O 0.93694313 -0.65596080 -1.88058344
O -3.47648438 1.50678345 -0.68332295
O -2.15854271 1.37149144 -2.91298666
O -1.90822695 -0.63767171 -1.25670053
Si 0.86117702 -1.92678357 -0.86729102

57
(SiO2)16(H2O)3 Energy = -198290.633880571
O 1.07782598 3.86703091 3.42803342
O -5.58596587 2.38626659 -1.95802396
Si 1.80034313 -1.35099652 -1.96509855
Si -1.38395855 0.82395556 1.89607150
Si 0.92814391 2.57854846 2.46255177
Si 1.81066086 -2.20024694 0.85513248
Si -0.91982681 -1.04696876 -1.96871682
Si -0.93518384 -2.01921126 1.07603137
Si -3.60077010 -1.26065125 -1.39806256
Si 0.86237105 3.51668583 -0.64604648
Si -3.92772685 -2.69293472 0.97248939
Si 4.53396688 -1.65772620 1.15267217
Si -1.48907567 1.76148907 -1.11231348
Si 2.79763640 1.36631549 -1.15857394
Si 2.83830217 0.50814742 1.66326575
Si -4.54426001 1.37264625 -1.25881979
O 4.17543497 -0.33522121 2.07968245
O 2.08581458 2.78477645 -1.47797215

O -4.56932006 -0.10874880 -2.02823916
O -0.55296344 3.06925139 -1.35480994
O -0.65786295 -1.52767877 -0.44347335
O -4.96857148 1.07672396 0.32532747
O -3.07636618 2.09537514 -1.32389661
O 3.27060632 -2.70354100 1.39035331
O 4.12345498 0.90772399 -2.00061291
O 2.16222625 1.51874024 2.73518089
O 4.62403839 -1.22269227 -0.42105062
O 0.93797981 3.12077850 0.93183974
O -1.07566526 0.56137325 -2.12930902
O 1.72936591 -0.61285483 1.24643546
O -4.49508796 -1.31905147 1.71074828
O -2.30504801 -2.90286839 1.19060863
O 3.24289114 1.41755151 0.39232654
O -2.37764832 -1.67891621 -2.39103460
O 0.43261134 -2.86120139 1.45028722
O -1.11060557 1.32576790 0.39310219
O -1.03022051 -0.75035702 2.08699232
O -0.46675295 1.77664214 2.82672851
O 0.39814824 -1.56050742 -2.79876693
O 1.85391124 -2.42454638 -0.75260770
O 1.70424597 0.18166812 -1.40590829
O -3.00566317 0.92605508 2.17264437
O -4.26152413 -2.55111267 -0.65356765
O -2.97401371 -0.44061900 -0.10195155
O 3.24162995 -1.46064081 -2.72136736
Si 4.50776746 -0.70082541 -1.96572127
Si -3.94087742 0.10181063 1.13058356
O 5.91108433 -1.00117304 -2.70090342
O 5.94436960 -2.32203092 1.56544621
O 1.01596287 5.12488917 -0.73760700
O -4.72526226 -3.94444486 1.60413465
H 1.07217182 3.71498615 4.37363646
H -6.49725568 2.10217073 -2.03924578
H 6.00800996 -0.71317242 -3.60952064
H 6.03875954 -2.64319988 2.46311379
H 0.77014406 5.54154868 -1.56418686
H -4.25473133 -4.77552679 1.67646250

60
(SiO2)16(H2O)4 Energy = -200373.732834230
H 5.73430805 2.49713176 2.38995016
H 5.42186012 1.61161504 -3.35391793
H 4.85738473 -3.85045424 -2.34911756
O 4.51713314 1.44896370 -0.00087380
O 4.81390491 -2.90092938 -2.46649855
Si 3.76882103 -2.08150072 -1.54102132
O 4.07142855 -0.49800571 1.76352421
O 4.79055745 -3.00516037 2.41168883
Si 3.76053763 -2.07902676 1.57481096
O 3.92916774 -2.50283399 0.02065079

O 4.07633969 -0.50823932 -1.74398123
O 5.42885589 1.59641590 2.50236081
Si 4.21100975 1.10059148 1.55680804
H 4.80182506 -2.90274738 3.36381826
O 5.45623247 1.69966013 -2.40099055
Si 4.21456851 1.09905274 -1.55304163
O -4.32743860 0.15157691 -2.13192394
O -1.86174395 -2.49262372 0.03503590
Si -1.87568701 -1.81459968 1.50299500
O 2.81416872 1.79679284 -2.03843310
O 2.22894962 -2.40046580 -2.01405480
Si 1.29436363 1.39848306 -1.62129855
O -1.20382016 3.19887486 -0.03913198
Si -1.87368030 -1.85294967 -1.45010454
O -0.47587743 -2.23004678 2.22893288
O -2.40646861 2.26303855 2.18313378
O 0.23438531 2.54295195 2.11496284
O 0.97689007 -0.02228972 2.22020979
Si 0.89368067 -1.53681296 1.64564873
O 2.22299522 -2.35529340 2.08130585
O 0.23172545 2.48675430 -2.17641722
Si -3.03079719 0.94935250 1.46900346
O -1.33092339 4.65245419 -2.20749815
Si -1.17558640 3.13869868 -1.65945646
O -0.47318110 -2.28750520 -2.16370342
O -6.00291894 -1.91691722 2.26261044
Si -1.17384519 3.18032424 1.58219703
O 2.81702438 1.84006225 1.99650760
Si -4.62532573 -1.34601285 1.64963165
O -1.32877225 4.70770212 2.09135086
O -3.30929014 -2.26594250 -2.10827697
Si -4.62370573 -1.38963776 -1.61020208
O 1.19230284 1.34377751 -0.01491247
O 0.82635101 -1.49963450 0.02235206
Si 1.29606770 1.43877568 1.58996859
O -6.00032937 -1.97762735 -2.20908909
H -6.08644517 -2.02721772 -3.16199620
O -3.31166847 -2.20985510 2.17096207
O -4.32835676 0.20807576 2.13140396
Si -3.03057761 0.91045764 -1.48858369
O -1.85790644 -0.18301372 1.40265167
H -6.09216973 -1.93621262 3.21631861
O -4.72970687 -1.41743505 0.02033327
O 0.97766460 -0.07844418 -2.21363430
O -3.47476942 1.40271504 -0.01601391
O -2.40793179 2.20593989 -2.23654123
H -1.33787726 4.86307301 3.03625627
H -1.34008902 4.78398439 -3.15599476
O -1.85686653 -0.21915952 -1.39269271
Si 0.89622863 -1.57799022 -1.59982319

(SiO2)16(H2O)5 Energy = -202456.332524720
Si -3.77853787 -2.21729117 -1.58426889
O -4.63224246 -3.25723003 -2.48507876
O 2.79962874 -2.53258727 1.32540187
H -5.83478594 1.36484413 3.29158892
O -2.26973117 -2.36628464 1.93922514
Si -3.84156948 -2.24686063 1.51242394
O -4.74934030 -3.20115209 2.45494740
O -4.29449208 -0.69335426 -1.79237649
H 0.99399767 4.89620512 -3.04796736
O 2.47251130 -2.60378794 3.89275087
Si -0.91468738 -1.53862401 1.61635937
O 4.18017567 1.00855409 -1.18866615
O -0.64309322 2.69658740 -2.00165207
H 1.96308308 -2.46445100 4.69170380
O 1.99124817 2.40811449 -1.84401888
Si 1.98710665 -1.77315353 -2.50834803
O -1.05024052 -0.02592621 2.20058104
O 0.41833882 -2.16333674 -2.29780988
O 1.92073221 0.57289364 0.07959369
Si 2.56267568 0.96822117 -1.38380592
O -3.17690420 1.58067394 2.14775427
O 2.49450475 -2.25158909 -3.97047046
H 4.94359539 -4.24668572 0.76413725
O -2.19780138 -2.29164067 -1.98493625
Si 4.91634415 0.36555183 0.13096198
O 2.16044168 -0.15710077 -2.46867862
O 4.13791809 0.95329456 1.44383937
Si 3.74941355 -2.52836618 0.01072922
O -1.59416957 1.37842521 0.07047871
O 6.46755281 0.80415469 0.23343589
Si 1.92051329 -1.91629657 2.53196407
O -0.97597660 0.06484048 -2.10039862
O 0.66685681 3.58700580 0.15945135
Si 2.51454045 0.89552410 1.58084265
O -0.71813343 2.60562133 2.23192249
O -4.73932826 1.24032020 -0.00599187
Si 0.67713604 3.29496428 1.75719158
O 2.08137167 -0.29280963 2.58474045
O 2.85426161 -2.47415866 -1.33211431
Si -4.52836520 0.86906449 1.55658291
O 0.33885685 -2.26206411 2.34149748
O 4.76654831 -1.25514536 0.07033334
Si 0.73497758 3.37335888 -1.44161191
O 0.79497810 4.66918007 2.60182236
O -5.83179804 1.42934841 2.33607217
Si -1.63518680 1.39550783 1.67967358
O -4.36561883 -0.73499004 1.73611544
O -3.10287489 1.66386581 -2.05354133
Si -4.46830101 0.89831248 -1.57181375
O -5.71970707 1.36792717 -2.48580616
O -0.65830080 -1.49885541 0.02088637

Si -1.57913008 1.46157021 -1.53718463
O 0.93876758 4.84156265 -2.09335537
O -3.98790864 -2.67806788 -0.04660554
Si -0.85726478 -1.47334956 -1.58411256
O 4.59788323 -3.90918163 -0.06285943
O 1.93281376 2.30805743 2.10425378
H 7.09821275 0.33464727 -0.31315893
H 1.53426152 5.24602280 2.40784624
H -6.06996216 2.24621953 -2.33396220
H -4.64885060 -3.10966445 -3.43105348
H -4.66625101 -4.14718288 2.33160440
H 2.44083582 -3.18626339 -4.17176550

66
(SiO2)16(H2O)6 Energy = -204537.676764259
Si -1.53224923 0.34354885 3.15498367
O 4.71604871 0.14999218 -0.72619004
O -1.47566748 1.53180990 2.04384438
H -3.99639630 -4.58067690 -1.35556773
O -1.23468275 0.89108441 -0.49783385
Si 0.74471443 3.83636144 0.06501325
O 2.35276318 1.88405430 3.44468081
O 4.16316941 -3.41792096 2.65199479
O 1.26910371 3.41306502 -1.41361579
Si -4.55496240 1.44266834 0.01539201
O -4.50759290 0.77279014 -1.46472941
O 2.41315233 1.03749137 -1.67035140
H -4.71480349 0.23652764 -4.41672061
O 0.76038129 5.44911263 0.21510218
Si 4.84458465 0.41131033 0.87102880
O 1.15623054 -3.14581776 -1.28046656
O -1.43809032 0.98097573 4.64623358
H -5.03894138 -2.71419543 2.84820553
H -2.22578657 1.40457556 4.98911231
O 2.23595022 2.70037880 -3.76602794
Si -3.96410117 -1.02861069 1.86790771
O 0.05348852 1.51616633 -2.77398387
O 4.28756804 0.47203082 -3.35993641
O 3.51682926 -4.07828861 -2.10073250
Si 2.33317654 1.80362151 1.82169440
O -3.25738393 2.39063182 0.27542930
O -0.19362292 -0.99396381 -1.95637685
H 1.53354013 2.09848454 3.89468453
H -6.70414837 2.02236913 0.02555077
O -3.60137112 -1.72000603 -1.77364512
Si 3.64152364 0.01790373 -1.92914439
O -1.47791643 -3.05788150 -0.90239706
O 2.05304206 -1.81382139 2.39652713
Si -0.91193002 0.45663842 -2.03317318
O 1.70020236 3.15071526 1.18773891
O 3.12501969 -1.51445901 -2.01991122
Si -3.76171964 -0.26507512 -2.46829550

O 3.28676371 -2.87623501 0.27087577
O -3.92006093 -4.06882137 -0.54958473
Si 2.77140031 -2.90581233 -1.26648946
O -5.19470553 -1.80760929 2.58117487
O 3.87572843 1.62962184 1.34996672
Si 0.85611220 -0.87407336 1.83309476
O 6.39541952 0.80476021 1.13095385
O -4.64774440 -0.49758793 -3.80529775
Si -0.09888752 -2.20318840 -0.87706109
O -2.30154284 0.35039272 -2.86198882
O -0.21534666 -0.59770483 3.01515949
Si 3.48868853 -2.25237758 1.75052040
O 4.44475978 -0.94122538 1.68163338
O -4.61189312 0.24663385 1.11451241
Si -3.04362567 -2.70506171 -0.61014187
O -2.89640976 -0.51636592 2.98489462
O 1.46884515 0.52617189 1.28122760
Si -1.68963443 2.06461563 0.52898375
O -5.84127427 2.41643616 0.15619904
O -3.15824266 -1.99192756 0.83829832
Si 1.50840296 2.16796939 -2.42273586
O -0.80378631 3.39253824 0.29831297
O 0.11098086 -1.62362165 0.61638742
H 6.60736830 1.18947941 1.98181474
H 1.52660544 5.90916282 -0.12848759
H 2.98895198 2.16963014 -4.04595937
H 4.93922153 -0.10441449 -3.76064506
H 3.43259539 -4.97373350 -1.77157999
H 4.22003971 -3.26231797 3.59518485

69
(SiO2)16(H2O)7 Energy = -206618.763454576
Si 2.86163987 2.53453363 -1.59565982
Si -4.40803738 -0.18824486 1.70144597
O -0.97161725 -2.18553812 2.25023921
Si -0.06916118 -1.24348471 -3.02794698
O 1.24638617 2.53611670 -1.78829265
Si 2.93768199 2.47864092 1.49482017
Si 2.29823676 -2.36927689 -1.33361258
Si 2.59635457 -2.30226276 1.66091908
O -0.00046429 1.00226579 -0.00274143
Si 4.64505571 -0.14273838 1.40941680
Si -2.86544082 2.53888662 1.58093396
Si -4.64518400 -0.15755820 -1.40933442
O 0.06014154 0.29572890 -2.53590975
Si 0.07112856 -1.22573269 3.03480412
Si -2.94139740 2.46577814 -1.50917849
Si -2.29471006 -2.36491735 1.34669906
Si 4.40829912 -0.19109707 -1.70099550
Si -0.01777584 1.55505391 -1.53373719
Si -2.59304092 -2.31541873 -1.64814104
O 0.31169718 -1.35853812 -4.60240688

O -1.58509426 -1.76717193 -2.78910427
Si 0.01566876 1.56417394 1.52494895
O -0.06017180 0.31066166 2.53455658
O -0.30952126 -1.33284648 4.60987861
O 1.34643322 2.44273233 1.79526650
O -2.01719418 -1.88164603 -0.17633513
O -2.68365595 -3.95132492 1.23254172
O -2.73212760 -3.92517455 -1.76730409
O -1.25017811 2.54460853 1.77349222
O -1.35006438 2.42969938 -1.80904884
O -3.44299986 1.08403438 1.98659035
O -3.56452403 0.99039843 -1.77334784
O -3.52904288 -1.52909704 1.98814795
O -4.04203960 -1.59808800 -1.85805161
H -2.81650498 -4.43927137 2.04580656
H -2.82766762 -4.37329533 -0.92002764
O -3.22116283 2.89284055 0.03505178
O -3.55465793 3.61809784 2.57721734
O -3.56523162 3.56877133 -2.52114548
O -4.96907013 -0.17788888 0.18341664
O -6.00000222 0.18965408 -2.23606401
O -5.71551979 -0.16514288 2.66138850
O 4.96948745 -0.17156517 -0.18309019
O 5.71562994 -0.17211834 -2.66123899
O 3.21652156 2.89779550 -0.05173610
O 3.56098668 3.58740655 2.50077086
O 3.54895498 3.60948904 -2.59783548
O 1.58774792 -1.74873642 2.79874847
O 0.97476769 -2.19772144 -2.23815523
O 2.69040574 -3.95421509 -1.21049938
O 2.73760121 -3.91110488 1.78958970
O 2.01976364 -1.87795890 0.18665855
O 4.04444713 -1.58176122 1.86631788
O 3.53073834 -1.53450552 -1.97990360
O 3.44207838 1.07862615 -1.99334135
O 3.56196154 1.00510076 1.76649549
O 5.99899759 0.21189069 2.23445775
H 2.83447700 -4.36401641 0.94502023
H 2.82412118 -4.44648274 -2.02101386
H -0.29377906 -0.95667882 -5.22617498
H 0.29551541 -0.92698519 5.23147684
H -4.51381009 3.54766743 -2.65277918
H 4.50948493 3.56699891 2.63310007
H -6.76860594 -0.35633000 -2.06693161
H 6.76904354 -0.33281320 2.06777646
H -5.57296152 0.06376134 3.58041378
H -3.24645963 4.52326264 2.52333199
H 5.57281145 0.05215042 -3.58136548
H 3.23975766 4.51456213 -2.54833908

72
(SiO2)16(H2O)8 Energy = -208699.966734881

H -5.29354790 -1.44313401 2.88334072
H -5.19671416 1.51826859 -3.03214164
H 5.02252452 -0.29311108 2.93587009
H 5.09547971 0.19480011 -2.83796261
O 3.67330295 -1.83286035 -0.78513777
H 5.34025945 -3.00708222 1.20741990
O 4.75357886 -2.35437432 1.59117380
O 2.78497699 -0.66909875 1.45725143
H -0.25563041 -0.99979488 5.25550603
O -0.48078737 -1.80920527 4.78324404
O -0.03112495 -0.18970318 2.69588928
H 0.55909579 1.78572492 5.49304217
O 0.03508409 0.17772406 -2.71675508
H 5.41887989 2.90395098 -1.10122258
H 0.41549599 -5.54649804 1.79675515
H -0.30541219 -5.39605874 -1.04346789
H 0.65995248 -1.80588425 -5.50065909
H -5.17032801 -1.45426566 -2.32962831
H -5.19862647 1.52939052 2.18808758
H 0.55397528 5.52693506 -1.80682979
H -0.11754301 0.99077250 -5.28019375
H -0.23830642 5.38853506 1.01470516
O 0.46799545 5.02805469 -0.99394852
O 4.62459722 -0.63388208 -2.96218490
O -4.73478184 -0.68555261 2.70588582
O -4.65595386 0.75150044 -2.83905402
O -4.86579170 -2.18341227 -1.78056610
O -4.86709136 2.25477301 1.64979222
O -0.48115387 -4.88474602 -1.84041412
O -0.34145699 1.80372937 -4.81345516
O -0.44183068 4.88046683 1.80710360
O 0.37540274 1.02200206 4.94506191
O 0.35869173 -5.04682967 0.98180168
O 0.47463231 -1.03980163 -4.95653554
O 4.56330944 0.54363559 3.04927930
O 4.83031115 2.26155050 -1.49921805
O -3.67441830 -1.87796001 0.57592150
O -2.80805000 -0.49049632 -1.51907698
O -2.83433472 0.52568506 1.43258124
O -3.63216359 1.92524437 -0.68121986
Si -3.44983583 -1.91003994 -1.03753638
Si -3.35552463 -0.94528162 1.86247527
Si -3.29484272 0.98885650 -1.96033370
Si -3.44104463 1.95566010 0.93662137
O -2.40598208 -3.09930474 -1.37965139
O -2.14030986 1.69565854 -2.84451066
O -2.23521154 -1.66885770 2.77660712
O -2.38445656 3.12724935 1.29975692
Si -0.81044569 -3.32131310 -1.57233712
Si -0.56120004 1.60765224 -3.21989428
Si -0.79062218 3.32265595 1.53098702
Si -0.66307536 -1.60898001 3.18549294

O -0.34239622 2.46837194 2.83684600
O 0.01386019 2.76295553 0.21626135
O 0.09659068 -2.83715127 2.44176482
O -0.02872359 -2.77473122 -0.23849742
O -0.31669134 -2.47473814 -2.86677819
O 0.20404902 2.82258687 -2.46024392
Si 0.52441176 1.19439059 3.32234440
O 2.07448068 1.42494542 2.90469209
Si 0.67538454 -3.44146303 1.06089669
Si 0.75970573 3.41761532 -1.06586863
Si 0.58232869 -1.21515840 -3.33086444
Si 3.28677787 0.75348523 2.06914174
O 2.36245612 3.16552926 -0.96708701
O 2.28398421 -3.21612138 1.00030200
O 3.68499703 1.75881333 0.85054756
Si 3.41668088 1.95714893 -0.73637052
Si 3.36393167 -2.02604945 0.79489383
O 2.11805920 -1.47156258 -2.87685139
O 2.83041277 0.61027337 -1.41276774
Si 3.32167294 -0.82107825 -2.01264920

12
(TiO2)4(H2O)0 Energy = -109591.526384618
Ti -1.62305486 0.66663062 0.92298670
Ti 2.28712019 -0.25922034 0.60065038
O 0.32005662 0.19031191 0.65454957
O -2.15366123 1.00618488 2.39205721
O 3.13382892 -0.24565509 1.95633688
O 1.48127522 -1.91162516 -0.02137934
Ti 0.47088247 1.37323640 -0.91366923
O 0.03888326 -0.12349441 -1.85552287
Ti -0.13663591 -1.33388760 -0.50714215
O -1.74527060 -1.14758394 0.24457058
O -1.01745447 2.09553607 -0.24241093
O 2.20912340 1.33157365 -0.50838480

15
(TiO2)4(H2O)1 Energy = -111675.264275576
Ti 0.00426869 0.18808305 2.09587818
O -0.00646809 1.72282228 1.33002175
O 1.40388922 -0.66169610 1.46843289
O -1.38962581 -0.67710140 1.47679362
O 1.49549967 0.70216305 -1.02439410
Ti 1.60213727 -0.92300797 -0.40583769
O 3.06303573 -1.84864996 -0.91744492
H 3.81001630 -1.59305770 -1.46046178
O -0.02293387 3.29325898 -1.30467552
Ti -0.01296776 1.83169201 -0.64335914
O -1.51117956 0.68560579 -1.01539183
O 0.00602192 -1.70120667 -0.80055042
Ti -1.59618613 -0.94062321 -0.39626645
O -3.04979491 -1.88235339 -0.89919096

H -3.80270369 -1.63510676 -1.43786262

18
(TiO2)4(H2O)2 Energy = -113759.247100736
O -0.03896240 1.23967463 3.29476178
O 2.93756690 -2.03007946 5.97140505
O 1.98370910 3.50399507 3.56598944
O 2.39721156 0.66691295 4.65833703
Ti 2.18166943 -0.76314751 1.46247076
O 0.38764600 -1.32479371 4.41768258
O 2.38161583 1.02282928 1.84111691
Ti 2.20233733 -1.11624641 4.60864132
Ti 1.70567095 1.74209947 3.33973326
O 2.82648264 -1.55957195 2.96184605
Ti -0.51454022 -0.50242398 3.10245550
O 0.40861743 -1.00470991 1.59628326
O 2.93991188 -1.30842169 -0.07390994
H 2.43238541 4.19067506 3.07257302
H 3.41981782 -1.79702755 6.76477007
H 2.62340869 -1.70580359 -0.88521044
O -2.28605423 -0.80529584 3.04970041
H -2.90191212 -1.32988787 3.56138392

21
(TiO2)4(H2O)3 Energy = -115840.533332674
O 2.26419010 0.62946389 4.63789670
O 5.06316137 0.42585397 3.52454680
O 0.19385769 0.62118065 -0.06062713
O 2.56121723 0.42966145 1.81393204
Ti 0.46102511 0.77692468 4.72533909
O 0.58754316 -3.13375692 4.33488307
O -0.22075458 -0.67625624 5.48652564
Ti 3.34506076 -0.08171481 3.36978743
Ti 0.80831235 0.05799463 1.53431724
O 2.12838985 -4.38601488 2.09038768
Ti 1.63804619 -2.84291644 2.86076362
O -0.01636848 0.76797185 2.94062853
O 3.07729997 -1.86639210 3.39286524
H -0.50284257 1.22740644 -0.31388306
H 5.90645752 0.02208121 3.31979815
H 0.41254416 -3.98185279 4.74708650
O -0.09510543 2.25074723 5.59473378
H 0.29194385 3.12538777 5.64989153
H -0.03151314 -1.59158790 5.21255557
H 1.98502533 -4.74890297 1.21532736
O 0.73700658 -1.76997277 1.75896220

24
(TiO2)4(H2O)4 Energy = -117921.782115139
O 1.68710810 -0.55379585 -0.55048729
H 1.14554441 -0.00218859 -1.12861221
H 2.57471746 -0.18053202 -0.56473880

O 2.44989119 0.63123199 4.64807962
O 5.14761116 0.21481961 3.33753566
O -0.25275817 0.87599549 0.29634938
O 2.56260993 0.42000884 1.80786166
Ti 0.62750614 0.73937583 4.80225776
O 0.52010176 -3.15568357 4.41788949
O 0.00870528 -0.68679402 5.66052466
Ti 3.37913032 -0.14375776 3.32622126
Ti 0.79944641 -0.01065080 1.52568048
O 1.98564585 -4.43563712 2.13352716
Ti 1.53477608 -2.87907599 2.91053747
O 0.11168436 0.64881740 3.05911426
O 2.98714861 -1.92030365 3.39923700
H -0.99821467 1.39180497 0.61212073
H 5.73583087 0.56365407 4.00742667
H 0.29354524 -4.00630222 4.79761921
O 0.08122854 2.24288416 5.63476579
H 0.27595125 3.16081826 5.44288077
H 0.10021366 -1.60905388 5.35724271
H 1.80565880 -4.77675029 1.25647605
O 0.61347035 -1.81580202 1.81246959

24
(TiO2)8(H2O)0 Energy = -219189.847545120
O 0.41909717 1.15133900 0.14430470
Ti -3.19235737 0.24890534 0.00910442
O -0.01808009 -0.18525292 2.62273378
O 0.15106603 2.83885069 1.90368149
Ti 0.70087769 -2.67409671 -0.16558249
O -0.36762354 -1.09731474 -0.05377494
O -2.62800974 -0.96203371 1.43243903
Ti 3.24383089 -0.19488097 0.08142494
O 2.67948322 1.01605834 -1.34190950
O 4.81787245 -0.45130216 0.08707529
Ti -0.91748423 -1.12733687 -1.86210452
O 0.06955378 0.23927715 -2.53220410
O -4.76639891 0.50532676 0.00345369
Ti 1.02957716 1.47545698 -1.61509408
O 0.20563403 3.10475133 -1.32331475
O -0.09959247 -2.78482652 -1.81315176
Ti 0.96895794 1.18136100 1.95263407
O 2.24722513 -1.87888529 -0.07421397
O 2.62837877 0.76807232 1.66396706
Ti -0.97810369 -1.42143257 1.70562376
O -0.15416049 -3.05072689 1.41384465
O -2.57690503 -0.71404826 -1.57343752
Ti -0.64940417 2.72812110 0.25611231
O -2.19575155 1.93290958 0.16474345

27
(TiO2)8(H2O)1 Energy = -221272.915420889
H -4.09696953 3.00901719 4.43467089

O 5.00870283 -2.62610977 0.11140930
H 5.33432677 -3.42358462 -0.30809727
O -0.42747475 2.13273228 -0.85337401
Ti 0.75836776 2.00063398 -2.41950843
O 2.49747376 2.15059034 -1.54293179
O 2.17519271 -2.19925677 0.92455748
Ti -0.23740771 1.80534095 0.82972386
O 3.01344313 -1.73506429 -1.87697119
O 0.13138169 -2.16838174 -1.14529353
Ti 1.31099518 -1.10123734 -2.06938440
O -0.45270835 -0.07449313 1.16369440
O -0.72368014 -2.43553416 1.77553963
Ti 2.61789287 1.29829681 -0.04471475
O -1.53582837 2.45945947 1.99446208
O 1.50559443 2.04477175 1.22057525
Ti -2.54726751 1.44210530 3.06029981
O 3.99332617 0.13647799 0.26053578
O -3.75828466 2.15097879 4.17831288
Ti 3.57799054 -1.59445086 -0.14263941
O -1.36272137 0.19440843 3.75593140
O -3.08104702 0.02157285 2.00427997
Ti 0.48218246 -1.73231337 0.56963426
O 0.80744181 0.19443651 -3.12547923
O 1.44964896 -0.11922230 -0.48239732
Ti -1.58399489 -0.91795771 2.36490287
O 0.48332325 3.13109340 -3.51403248

30
(TiO2)8(H2O)2 Energy = -223356.299783769
H 2.83337740 5.37578865 2.60928958
O 0.37111914 -0.52693066 3.13523229
H 5.63326352 0.16301803 -0.64038089
H 1.13984996 -3.93113841 3.59026698
O -0.28816933 -0.82367687 -1.88221826
H 0.85013464 0.01935064 -5.09132104
O -0.04388027 0.82692774 0.54673304
Ti -2.95724150 1.38723928 0.90651464
O -1.99470860 2.64758280 -0.22328992
O -1.89457353 1.37639475 2.53942285
Ti -0.30043369 2.45645977 -0.52433083
O 1.34345624 0.06825033 -4.27182057
O 0.19277661 1.92485925 -2.17952187
Ti 0.94957159 0.31949044 -2.54517871
O 0.81606704 3.63305463 0.26590109
O 2.99078693 1.83289311 0.88563899
Ti -0.88004676 -0.79870276 -0.17325073
O 3.00090542 4.55237622 2.14963904
O 0.91812506 2.45286531 2.81033082
Ti 3.21882827 0.18918448 0.14816218
O -4.51511840 1.68590195 1.09947456
O 4.95693486 -0.16819765 -0.04795819
Ti 2.00683879 3.18627380 1.56095356

O -0.20969212 -2.09792802 0.88437955
O 2.39410454 0.19056728 -1.46341336
Ti 1.10048611 -1.83371330 2.11164516
O 1.57519933 -3.30251503 3.01360844
O -2.52483697 -0.33102767 0.09568984
Ti -0.19259549 1.06331873 2.49217128
O 2.47113818 -1.06654184 1.22178348

33
(TiO2)8(H2O)3 Energy = -225439.226319991
H -4.64941489 2.42436519 0.08590107
O 1.46371349 -2.63727348 -0.86802648
H -0.09756820 -3.19199129 -4.24051054
H 4.17568494 -4.16914312 0.07142055
O -4.10974745 -2.91232666 0.42804972
H -4.34078395 -3.77074814 0.07089928
H -0.16137903 3.00483188 -3.97146599
O 0.19018410 2.14995439 -3.71966051
H -0.52947937 3.45700001 4.53224242
O 3.03835047 -0.58528604 0.51290561
Ti 0.08818773 1.21373322 -2.19273663
O -0.02094228 -0.13402827 3.44012805
O 1.58027361 1.76719588 1.89630855
Ti 2.49572172 -2.33144907 0.57232561
O 3.89069789 -3.45165192 0.63847032
O 0.05805492 -0.57873978 -2.52820888
Ti -2.58548111 -1.96718924 0.38665869
O 0.00660160 -3.38393994 -3.30706228
O 0.27582476 -0.36728895 0.68919864
Ti 0.01546077 -2.25633833 -1.91383762
O 1.43814828 -2.48648981 2.05760315
O -3.72245753 2.62286164 0.22865528
Ti 1.76147007 0.68706942 0.46426502
O -1.53585051 -2.45475611 -0.97638684
O -2.92994338 -0.17702797 0.33106564
Ti -2.32420790 1.50404716 0.30460895
O -1.34423175 1.90021682 1.79423751
O -1.58891643 -2.22333818 1.87942009
Ti -0.00679168 -1.41421109 2.17021515
O -1.32184877 1.69907560 -1.20602837
O 0.05061419 2.73789400 4.27938273
Ti 0.05159355 1.60916563 2.88971495
O 1.53473917 1.48493650 -1.13399482

36
(TiO2)8(H2O)4 Energy = -227520.835847176
H 0.73201104 -2.96795361 5.04244585
O -1.00006986 0.78249704 0.32607294
H -4.06734813 1.05231126 -1.74758396
H 1.16452415 -6.50309266 -2.65518207
O 0.54242866 -5.77469869 -2.65603868
H 5.66007042 -3.54401558 0.24885411

H 0.59694516 2.84019988 3.01189265
O 1.89836718 1.00523819 -0.00370458
H 4.34674637 2.12243444 -1.76256625
H -3.97536532 -4.25941927 1.35928002
O 0.30789907 -2.81986927 -2.93057203
H -0.10418810 -1.33272795 -5.74497350
O -0.08404514 -0.73993936 -4.99277673
Ti 2.79436288 0.17641669 -1.30472414
O 0.52702605 2.63526639 2.07877237
O 1.61763818 -0.24843132 -2.60517364
Ti 0.14340104 -1.07032840 -3.24092407
O 4.12495432 1.20667561 -1.93505110
O 1.18850795 -2.38814636 4.43171094
Ti 3.19832675 -2.96950217 0.14661374
O -1.28204646 -0.46255904 -2.27942321
O 2.11349777 -3.95757559 -0.93623724
Ti 0.54399899 1.05861531 1.21635466
O 2.31547939 -2.69494485 1.69522822
O 4.75885284 -3.81590839 0.42628373
Ti -2.10803003 -0.18015023 -0.72364378
O -3.02450922 -4.37544714 1.36272207
O -3.67785204 0.66045788 -0.96508533
Ti -1.70809227 -3.31456585 0.75325314
O 3.45436609 -1.38497302 -0.63312839
O -2.36175087 -1.79446835 0.08521852
Ti 0.55948888 -4.20820800 -1.77568176
O -0.55188551 -2.88459619 2.09646122
O 0.77713102 -0.29648653 2.35373836
Ti 0.93188053 -2.08386361 2.67932661
O -0.75571878 -4.13111226 -0.54258069

39
(TiO2)8(H2O)5 Energy = -229602.136873834
H 1.88926230 -2.50644478 -2.32518018
O 0.28350854 -1.32058483 0.26328779
H -2.15927971 -3.11504988 2.93878365
H 1.23212627 4.79255669 3.83090735
O -1.20533781 2.72054147 -3.39157909
H -2.66830634 -2.50459431 -0.49968456
H 3.90417278 -3.09792848 0.50783378
O 1.08302904 2.14958069 -1.62590990
H -4.30792157 2.47479503 2.00513760
H 2.47949235 -1.16239085 5.68034830
O -3.46269092 2.81436468 1.70892314
H -0.74301847 3.34086124 -3.95678107
H -1.26467371 -2.85791824 -3.57776994
O -2.05767486 0.21693734 1.61281823
H 4.82246652 2.51905590 -1.53678363
O 2.13876466 -1.55934007 4.87815527
Ti 2.23558562 -1.38755593 0.11802592
O -0.90302430 -2.95396060 -2.69433973
O 2.89483918 0.23078560 -0.38937124

Ti -1.94667456 1.96058032 1.25764695
O -1.59230698 2.13690689 -0.51134501
O -0.14981007 -1.34862829 2.96644617
Ti -0.45417878 -1.60532475 -1.57523290
O -0.53226522 2.63767576 2.17537941
O -0.74779530 -0.03227780 -2.30635348
Ti 1.20196982 2.57225296 2.61725051
O 2.46852995 -1.33310980 1.91400587
O -2.24993036 -2.81090764 2.03188051
Ti 1.52476010 -0.80573547 3.35876770
O 1.46940877 -1.84677604 -1.76988641
O 1.64530145 3.93857376 3.69873697
Ti 2.55830246 1.97291728 -0.55422264
O 3.96518890 2.84337645 -1.25848174
O 3.34202377 -2.79648620 -0.21071256
Ti -1.22738382 -1.39748422 1.50923274
O -1.97780650 -1.84892812 -0.38516401
O 2.13647238 2.62536517 1.06866898
Ti -0.61919802 1.77956344 -1.97765599
O 1.54567051 0.99150159 3.43305929

36
(TiO2)12(H2O)0 Energy = -328788.617828857
Ti -0.64842705 0.43725026 3.16656738
Ti 2.51483792 -1.61524434 -1.85482960
Ti 2.37968065 0.68919627 2.45043816
Ti -1.31293169 1.28987852 -0.21366960
Ti -3.57921506 -2.94816349 2.24063976
Ti -3.70802510 -2.12768270 -0.40713168
Ti -0.45803278 -2.89121833 2.25972259
Ti 1.99454776 -1.94508067 1.37476747
Ti -4.57179783 1.15141994 -0.22356474
Ti 1.83664330 1.27549628 -0.20695203
Ti -0.65422871 -1.94220045 -1.15424643
Ti -3.29342831 -0.10594772 2.53220650
O -2.23721770 0.60819526 3.93122483
O 2.95133595 1.81754337 1.16255860
O 1.25154416 -3.31513103 2.44890670
O -4.43343854 0.86862331 1.71405511
O -4.08298222 -1.61503515 3.31102468
O -2.29990072 -2.73512066 -1.36412356
O 2.84976780 -2.32354735 -0.05497186
O 0.99649600 1.20436538 3.51273119
O 0.70933956 -2.21828981 -2.19100779
O 3.03562280 -0.96279566 2.58249169
O -2.02105290 -3.82971756 2.56013539
O -5.83643660 2.00314434 -0.69637102
O 1.29591258 -0.04513543 1.08305366
O 2.42443054 0.29204223 -1.50798980
O -4.50394560 -3.33705240 0.73991097
O 3.57929413 -2.04796627 -2.96297001
O 0.28435192 2.18414902 -0.38688125

O -4.52105293 -0.67270307 -0.88405031
O -2.86079882 1.95238021 -0.63270427
O -1.04671394 -0.19478815 -1.17960786
O -2.80077536 -1.57438667 1.19647074
O -0.00257248 -2.28076949 0.57957245
O -1.51994541 0.69797005 1.56175229
O -0.49189033 -1.35531607 3.19706266

39
(TiO2)12(H2O)1 Energy = -330871.745529406
H -6.58209655 -2.75697502 3.73554700
O -1.60803249 3.44521759 4.70794071
H -1.16445257 4.29065860 4.62330529
Ti 0.58404804 -3.85170542 -1.22900653
Ti 0.76786199 -2.45083301 2.85637448
Ti -1.86423227 -3.39745002 0.68485518
Ti 2.65520320 -3.21709405 0.51080126
Ti -1.59346254 -1.10330091 4.08917077
Ti -1.57950834 -0.33256433 -0.89721754
Ti -3.17862092 0.43003182 1.65583624
Ti 0.45810036 -1.18325356 -3.29861561
Ti 1.99682315 -0.59384026 -0.45694511
Ti -4.25454715 -2.44419928 2.74929782
Ti 0.66556711 0.73925666 1.57969612
Ti -1.58550016 1.95489216 3.73523622
O 2.21769093 -3.43446968 2.26319017
O -3.10815833 1.88450607 2.70714019
O 1.18523658 -0.77133622 2.41269820
O -1.66718351 -0.34859089 2.37219980
O -4.45943449 -0.82619404 1.95931762
O 1.86301556 -0.43261379 -2.15600653
O -2.09981014 -1.97102542 -0.35052488
O -1.14115211 -0.36495461 -2.58081518
O 2.15232427 0.95022348 0.63628144
O -5.80234625 -3.12570163 3.31817087
O -0.08111758 -2.07519187 4.42158795
O 0.42477079 -3.04877824 -2.75665343
O -3.11774183 -2.05827441 4.13223208
O 2.21521489 -4.51680207 -0.67934689
O -0.92126374 -4.50478254 -0.42626601
O -0.12673164 2.00347871 2.64180076
O 3.43980692 -1.69136610 0.02263389
O -1.58710749 0.50666839 4.87985005
O -3.42991226 -3.58895512 1.59192654
O -0.69443377 -3.01603972 2.00010815
O 0.66887690 -0.95145429 -4.86508075
O -0.00097339 -0.01928924 0.00707527
O 1.07355470 -2.39512795 -0.09670328
O -2.79075987 0.77556021 -0.07114038

42
(TiO2)12(H2O)2 Energy = -332954.718314729

H 1.29444167 -5.41332104 -2.46586518
O 1.73198776 -1.68826052 -2.43392028
H -6.57287173 1.99230637 3.39832231
H 3.86309605 -0.39153253 -4.53798324
O -0.97046719 -3.03192108 2.03417963
H -0.87140348 -4.82085723 4.99255326
Ti -1.47248677 -0.03040781 3.51223200
Ti -0.42164389 1.86583807 -1.81753765
Ti -4.19796849 1.37296573 2.65651155
Ti -2.17612899 0.59550256 0.18118289
Ti 1.57839723 -3.16908874 -1.35391092
Ti 2.44493012 -2.00697505 1.44008049
Ti -0.75114535 -1.97076551 0.56329069
Ti 0.23024752 2.99652175 0.68709046
Ti 0.01459945 -2.91761449 3.54153616
Ti 2.00311457 0.58979463 0.39301561
Ti 2.05643858 0.02693658 -2.81253955
Ti -1.53397010 3.02241008 2.81643072
O 1.81548596 2.22968827 1.14165523
O -2.02950019 -1.15448068 -0.38166108
O -1.46304931 2.22695328 1.19429685
O -3.77738509 0.86239435 0.95330612
O 1.85246687 -4.64688894 -2.32413871
O -0.13535346 -4.36903995 4.57860822
O -0.24397005 4.09961880 2.10679394
O 2.76717308 -3.11444026 0.05902833
O 2.71392427 0.68566321 -1.23209384
O 0.02123095 3.48338456 -1.04648424
O 3.22948717 0.21469750 -4.15154245
O -2.12443122 1.45276565 -1.47060820
O -3.36952656 2.95562283 2.98269498
O 1.01431904 -1.14475560 0.64927829
O -0.63987594 -1.41606686 4.33496355
O 0.55989948 1.03064035 -3.10342956
O -3.26524174 0.17466420 3.66717856
O 1.73338619 -2.66202334 2.97864344
O 0.10526795 1.05119863 -0.28866684
O -0.87028319 1.68681634 3.81114584
O 3.22795466 -0.39886808 1.38623697
O -1.20524158 -0.30089929 1.76830646
O -0.05309932 -3.18202339 -0.64568681
O -5.95616093 1.37979664 2.99694197

45
(TiO2)12(H2O)3 Energy = -335037.247621494
H -3.26834585 3.89783336 -3.11876170
O -1.20554604 2.89226657 -0.83033672
H 5.29181383 0.89024313 0.64082257
H -3.09673646 -5.99729932 -1.30367922
O -3.63076888 -5.41246362 -0.76448903
H 2.51813517 1.63857749 6.25342092
H 2.17346967 -5.33287471 3.34091805

O -0.31362146 -1.51953183 -0.79423616
H -6.98160369 -3.51460790 3.19138530
Ti -2.70838060 2.09904211 -1.41755448
Ti -0.00080194 2.54685304 0.52716746
Ti -3.80300975 0.50223243 1.25689913
Ti -3.40401553 -3.72551502 -0.21004274
Ti 1.14386366 -3.03021637 3.24216887
Ti -1.76309851 -2.57899283 2.43361032
Ti 2.80789631 1.22534898 1.06311322
Ti 0.62639916 -1.11492588 0.67344913
Ti -2.05308518 -1.12086700 -1.13842892
Ti -0.95501775 0.94574771 2.62416362
Ti -5.03447822 -2.18816120 2.23185628
Ti 1.67775899 0.22628221 4.31133819
O -3.42006049 -2.28513953 3.08677759
O 1.80637421 2.63183547 0.44295873
O -0.62149606 -3.46365485 3.49545251
O 2.19673986 -4.42297436 3.64081956
O 2.45736179 0.78312908 5.82666568
O -5.25368361 -0.42761066 1.78329158
O -2.00474882 -3.56390701 0.92392294
O -6.37341068 -2.77783162 3.26116866
O 1.68323456 -1.57227561 4.17928983
O 2.42682043 0.92916769 2.81704111
O -0.70618118 -1.06363343 2.20959235
O 1.23839273 -2.63402403 1.47839943
O -3.50789095 3.07936289 -2.68230828
O 2.20086860 -0.27680503 0.28799280
O -0.18924547 0.76470028 0.81051104
O -2.96783514 -2.61305809 -1.58924871
O -0.63839890 2.74262746 2.16248196
O -3.82794878 1.80360888 -0.00181392
O -0.04325580 0.78045729 4.16586821
O -2.75207015 0.93412973 2.66084535
O 4.55511475 1.48907883 0.76921451
O -4.86163046 -3.16237544 0.72801541
O -2.28614720 0.42447844 -2.03508753
O -2.83011923 -0.81026072 0.47135911

48
(TiO2)12(H2O)4 Energy = -337119.289873198
H 2.90640416 -3.41750496 -4.69474411
O -3.11321489 -3.05835767 0.74382286
H -5.80756286 1.07709592 4.90229328
H 1.08720552 -5.66129799 4.86738255
O 2.78316737 -2.74865448 -4.01950688
H -1.71770869 -1.70153613 7.23744483
H 0.95542759 1.91877937 -4.46396124
O -1.85115826 -4.98080396 -1.22424299
H -4.84666034 -0.22890525 -4.60775190
H -0.05846012 3.62267692 4.61061528
O -2.99611503 -1.41823828 4.29285004

H -2.80053371 -5.82932038 -4.43849558
Ti 1.48409386 -2.55784573 -2.79721301
Ti -1.54850792 -4.27951620 -2.87080978
Ti 1.22999117 -2.42014448 0.40431425
Ti 0.29299758 -4.27091464 2.88733504
Ti -0.29231622 0.47611034 0.65495244
Ti -3.39581329 -1.27884578 0.57644544
Ti -1.27050500 -1.60081512 4.74715148
Ti -1.67571937 -4.06576317 0.32712326
Ti -0.30173294 0.54448492 -2.74796275
Ti -3.31372386 -1.16270532 -2.82120431
Ti -1.11455399 1.54743669 3.60806413
Ti -4.00722206 -0.09342888 3.54913479
O 0.74462041 -0.89274785 -2.91401437
O -2.00941834 0.02702151 -3.09865961
O 1.08380362 -0.67479910 0.85492285
O 0.19534440 -3.77425365 -3.05287961
O -5.45274786 0.25881174 4.55303706
O -0.52412549 -0.00688198 4.32114284
O -1.96319612 -5.46293812 -4.15126259
O -2.92206896 1.33289632 3.44779032
O -0.73708370 2.94862283 4.66430325
O -3.90624849 -0.95006927 -1.11813510
O -4.64913533 -0.94265026 -4.00009971
O 2.16459726 -2.69663111 -1.11650752
O 1.55014958 -3.49032087 1.82133493
O -0.46752923 -2.96230665 3.84145046
O -0.97886978 -4.92160444 1.75545293
O -0.34343944 1.70929958 1.99101853
O -0.24051628 1.11679897 -1.02464234
O -4.46589768 -0.64003751 1.88007161
O 0.99223040 -5.55788825 3.92003760
O -1.81688680 -0.45162957 0.87163434
O 0.20592716 1.84736185 -3.87159318
O -0.44284671 -2.83089643 -0.12838242
O -1.13042516 -1.90923727 6.50967157
O -2.59165618 -2.82274726 -2.97338802

51
(TiO2)12(H2O)5 Energy = -339200.683946106
H -7.15430972 0.94588782 2.88482968
O -1.82328567 0.73071229 -1.26798042
H -2.11536913 -7.45664462 1.52987979
H -4.45285124 3.51016183 -2.52181447
O -0.63869355 -0.19816004 1.18457359
H 2.44074335 0.24854736 -0.18303541
H -4.46237240 -0.43146132 -2.92051215
O -4.98695088 -1.56174181 1.37498571
H -2.82348952 3.27258304 5.37581588
H -1.28114709 -5.90918230 -4.51081159
O -1.75170488 -4.97962381 -1.44664391
H -1.09262014 5.78582592 0.15391251

H 3.08969876 -2.48829669 -3.05898953
O -0.27172386 -1.04977215 -1.60868718
H 3.00149715 -4.96700385 2.14827711
Ti -1.03126261 -4.05123237 -2.80781012
Ti -1.96803911 -5.22203913 0.33987874
Ti -3.51825868 1.62614450 -1.25698278
Ti 0.93591338 -3.57699495 1.69667292
Ti -0.15354098 0.53964858 -0.35447136
Ti -5.12782566 0.25550026 1.52942439
Ti 1.33899980 -2.06448599 -1.41361078
Ti -1.36079253 3.32738691 0.74004972
Ti -2.15861763 -1.16753395 -1.89431040
Ti -0.91047562 -1.10252845 2.72254779
Ti -3.48753707 -2.53143097 1.12636795
Ti -2.46572609 1.56047307 3.55734874
O -2.38709787 -2.08666213 2.46871515
O 2.13019433 -4.69464037 2.43840658
O 1.65954670 -0.05823539 -0.64827179
O -4.71399897 0.98135418 -0.07422437
O 1.60675807 -2.78995996 0.24300742
O -2.09182552 -6.97509021 0.70213667
O -6.78614573 0.72900630 2.02756892
O -2.97153490 2.37436785 5.07682405
O -2.72509470 -1.93167053 -0.39579612
O 2.84604902 -1.84778157 -2.38604684
O -4.24923361 2.57623156 -2.60997409
O -1.71793944 2.72774603 2.43238601
O -0.91541014 5.06944869 0.76397527
O -3.90498589 0.81682763 2.71671899
O -0.56665730 -4.46991436 1.17985618
O -2.78220515 3.01763752 -0.28278869
O -1.29358687 0.20509506 3.90826684
O -3.44465688 -4.33033678 0.92492867
O -0.93569254 -5.03932810 -4.30688413
O -0.03161283 2.29985872 0.02708953
O 0.60179956 -3.47186724 -2.29827203
O -3.65497382 -0.10556842 -2.51684318
O 0.45320157 -2.27530422 2.88348270
O -2.01948146 -2.53368644 -3.06145418

54
(TiO2)12(H2O)6 Energy = -341282.207339540
H 1.69238106 -5.04932106 -3.32586486
O -2.77418492 -2.76863028 -0.06022647
H -3.80244991 -1.73625077 6.41209521
H 2.81290194 3.69785349 -0.46689810
O -0.46170196 -2.68660866 1.94511859
H -4.11678250 0.94936585 4.13914397
H 3.01057630 -4.73705204 0.64921541
O 1.14659239 -1.43662651 -2.10968961
H -0.45719285 0.59278701 -2.81510425
H -4.31137477 -3.82259345 -3.31492715

O -2.91115772 -0.57141957 -1.92124638
H -3.62916268 5.62154358 0.46578594
H 1.85209718 3.56671184 5.40124098
O -3.15908466 -2.25218758 2.69660842
H 2.48616266 -2.44187475 3.48731559
H -3.98966245 -0.01520196 0.84705286
O 1.58820447 -2.61899117 3.19526339
H -0.33624185 4.90253847 -0.16624279
Ti 0.49081894 -3.12646495 -2.14794802
Ti -2.73530981 -1.28195162 4.11359804
Ti -2.04548291 0.57490952 -0.87234229
Ti 0.80523831 1.85411473 3.85544443
Ti 0.85232576 -0.41538605 -0.62684416
Ti -2.81542309 -2.41291630 -1.83503937
Ti -2.00116885 -1.86010747 1.29324414
Ti -2.04732757 1.41939120 2.39880577
Ti -2.42398732 3.34670156 0.30006943
Ti 0.87288699 2.67447276 0.59361946
Ti 1.28099291 -3.06956228 1.13941645
Ti 0.08891355 -1.42864185 3.51435331
O -3.23425169 4.91689562 -0.04681469
O -1.08395593 -1.85222149 4.77749712
O -3.02723819 -0.00605766 0.87262036
O -0.83575295 -0.80729617 -0.01586229
O 1.46954771 2.69438335 5.29929702
O -0.58641213 4.04986697 0.19993030
O -3.35570474 0.54181002 3.72114737
O -0.98121040 2.11967586 3.65651251
O -3.14124180 2.77275114 1.86912352
O -1.04876051 1.77667533 0.82250283
O -1.33371271 -0.45645979 2.69803499
O -1.29313425 -2.99500048 -2.55609358
O 1.41513600 2.53975484 2.32003128
O -3.86951416 -1.62923897 5.46327341
O 0.64779022 -3.73006048 -0.47442401
O 1.54036735 1.22942302 -0.19299088
O 1.37330753 -4.14714126 -3.33969261
O 2.66094474 -4.23434178 1.38829800
O 1.95493912 3.95333513 -0.11880843
O -2.89326655 2.18636436 -0.99179817
O -4.24236162 -3.16297567 -2.62376318
O -0.44713529 0.85283406 -1.88957351
O 1.03130406 0.05192191 3.96517268
O 1.76998151 -1.44763052 0.59959497

48
(TiO2)16(H2O)0 Energy = -438387.315807357
Ti -4.81955805 -0.59044955 -1.02022986
Ti 2.35408253 -2.17931532 0.25148733
Ti 1.47832991 -0.62868571 3.24667112
Ti -0.04928390 -3.74433622 0.16346660
Ti -3.61676016 1.81738592 -1.69044552

Ti -1.89862203 2.22518997 0.75292106
Ti 4.47093989 -0.01996841 4.62584705
Ti -3.35362916 -0.59659904 1.58560582
Ti -2.15179933 -1.91743866 -1.26221119
Ti 4.59077308 -0.94495705 1.53660525
Ti -0.76515308 0.89312549 -2.16128098
Ti 2.24642454 1.01179386 -1.27179435
Ti -1.12576968 -2.30430686 2.24147215
Ti 4.12975693 2.48301595 2.47822004
Ti 5.08242911 1.45168591 0.07596962
Ti 1.06918063 2.46060093 1.68584365
O 2.15667632 -0.73355858 -0.85453771
O -2.71364164 1.07281088 1.88439014
O -5.02016838 -0.81038388 0.75552575
O -0.97047026 -4.02652883 1.75382537
O -2.11270323 -1.55122878 0.58705778
O 0.95208546 1.25570112 -2.56804941
O 3.83990935 0.92596305 1.40989748
O 0.27407488 -2.10166203 0.79017815
O 5.15141863 -0.29735443 6.04606259
O 4.12915240 -2.32799914 0.38178768
O -2.78105729 -1.62482154 2.90468805
O -0.62047927 3.20906771 1.54412182
O 1.69370371 2.09899949 0.03817033
O 5.87815361 -0.07331236 0.43684251
O 5.33749515 2.89933992 1.15340117
O -3.21444058 0.25885472 -0.76421358
O 0.81998183 0.92517450 2.55130590
O -3.92970952 -2.00047195 -1.74378616
O 4.01175927 1.47115574 -1.40295912
O -2.25107410 1.76592280 -2.85896101
O -1.11283197 -0.87156724 -2.29083519
O 2.48204351 3.27219939 2.48390459
O -3.20984871 2.94487237 -0.34948745
O 4.67315730 1.79824851 3.96899936
O 1.69936709 -3.87402585 -0.21012377
O 2.56345070 -0.33595971 4.56686224
O -5.23705583 0.95947934 -1.92548806
O 5.14558795 -1.11684316 3.16038274
O 2.58830571 -1.31718623 1.94563902
O 0.05845459 -1.77626183 3.47016696
O -1.27744831 -3.47575445 -1.18743721
O -0.86682666 1.30108730 -0.41147125

51
(TiO2)16(H2O)1 Energy = -440470.305785652
H 1.06810230 8.59994091 0.26850070
O 1.70236161 -3.04169131 -1.79927710
H 3.58139774 -4.66296386 1.06085110
O 3.17249883 -1.06819137 0.00884070
O 1.09131751 -0.73080621 -3.60416960
O 2.59217408 1.02774648 -1.84822127

Ti 1.50841494 0.98408583 -3.24320117
O -2.91783214 3.42094192 2.20097474
O -2.13024005 2.73579328 -2.24830173
O -1.35442658 0.33236018 0.47865734
Ti -0.64151613 2.70235465 -3.89456834
O -0.02317636 1.62964935 -2.45640628
O 0.99883186 -2.72329501 0.99425994
Ti -2.83042958 -0.61035851 1.06875516
O -0.61190433 6.12509733 -1.17898757
Ti 2.40645323 -2.73968633 -0.09518463
O 2.89273508 1.93977616 0.91079936
O -2.05768618 0.31926969 -1.99222174
Ti -4.02851622 3.16191888 -1.35739987
Ti -1.12025018 1.68902498 -0.81915552
O 0.64771881 1.86328129 -0.14777387
Ti -1.26224587 4.03566343 1.68073779
O -5.13532352 3.14252229 0.13016750
O -2.03916144 1.76269714 -4.64651004
Ti -2.74792960 -1.34969652 -2.12803863
O -3.04153959 2.00967907 -0.16995635
O -1.11296210 3.66573524 -0.15963898
Ti 0.50027506 -1.83426409 -2.28345653
O -3.41144893 -1.47995229 -0.44484847
O -3.69565882 -0.60320420 -3.49512157
Ti 0.41133421 6.14296822 0.29609749
O -0.76504417 4.46118331 -3.45007672
O -3.35129494 4.85627326 -1.62869476
O -0.81724362 5.75722915 1.62475691
O 1.23518989 7.70436908 0.56599328
O -4.56953618 2.13065010 -2.73494872
Ti 0.01789500 -1.14402089 1.07555381
O -1.26791721 -2.33785491 -2.44148476
O 1.17990548 -0.04540048 1.63225373
Ti 1.47521993 3.03464403 0.95319037
Ti -1.56043625 4.70168774 -1.81849905
O 0.99603639 2.22752140 -4.53921604
Ti -4.03377716 2.30333811 1.32145409
O -4.02002227 0.57246291 1.87497385
O 1.58516344 4.74166332 0.31915975
Ti -3.13832711 1.15081970 -3.34568847
O 0.17965120 3.17324167 2.27508581
O 3.57412091 -4.01950729 0.35095171
Ti 2.24634775 0.47562898 -0.04183655
O 0.59006844 -0.78207157 -0.80043047
O -1.67526220 -1.60126523 1.93501567

54
(TiO2)16(H2O)2 Energy = -442553.214281150
H 1.11013990 6.59643546 -4.71735257
O -0.99166812 0.81841637 0.19275337
H -6.11879822 4.91906107 -0.79265091
O -5.53585296 4.29254795 -0.36133388

O -1.56434245 -1.92286330 -3.75009545
O 1.15714130 5.63975576 -4.68698418
Ti -2.72232219 0.48062014 -0.16407300
O -0.06180796 3.43890487 0.65495870
O 3.93233757 -2.61047647 -1.82368886
O 2.68574744 0.05742874 -2.92597000
Ti 1.53781010 -1.10350664 1.39556941
O -1.36355899 4.09164270 -4.30304339
O -1.89002471 -4.03444255 0.60796639
Ti 0.52021366 1.71467695 0.51934024
O 1.48782065 1.82467278 -0.98653615
Ti -1.52734227 -2.24992114 0.61503741
O -0.94380304 -4.57821255 -2.11128275
O -2.43858806 -6.67829696 -0.63185352
Ti 1.97547631 -5.33710838 0.66153479
Ti -2.35347930 2.85604980 -3.45215991
O 1.21242909 -2.54954286 -2.78930380
Ti 2.49142511 -1.51578519 -2.02235604
O -2.91076860 -1.07375117 0.77896048
O 0.30790003 -5.90621785 0.22803450
Ti -0.54413615 -2.86389797 -2.55970656
O -0.08677170 -1.86993931 1.62546501
O -1.34746610 2.73778752 -1.92382548
Ti -3.97851794 3.56773636 -0.85262353
O -2.57886460 4.67738346 -0.42797854
O -3.73602397 1.98187169 0.01548608
Ti -0.91017683 4.11804589 -0.79838751
O 1.35169619 0.66659752 1.76222552
O -2.32643765 1.24975644 -4.29761654
O 4.72799178 -3.47504350 1.06442388
O -0.07635534 0.32505661 -2.88251864
O 3.42726090 -5.61093362 -0.40689604
Ti 3.87416948 -3.83107061 -0.46608326
O -3.91121812 3.36436334 -2.66037430
O 1.27243525 2.87217577 -3.67266040
Ti 0.32749454 4.42862840 -3.66885000
Ti -1.74844207 -0.16193077 -3.29679846
O 2.71487840 -1.95482299 2.49090466
Ti 3.60181610 -3.52403581 2.52705871
O -0.92387017 -1.96535225 -1.05254483
O 0.09528528 5.06666322 -1.97810509
Ti -1.26697674 -5.33458925 -0.48496259
O 2.56440448 -5.04159482 2.34844432
O 1.99079200 -1.00667092 -0.36431379
O 2.17349967 -3.59522126 0.17066275
H -3.16444351 -6.98154894 -0.08528243
H 4.84412060 -2.95981396 4.64538229
Ti 1.40401092 1.33191565 -2.70634489
O 4.55668880 -3.63729935 4.03089007
O -2.85007380 0.02159688 -1.88766629

(TiO2)16(H2O)3 Energy = -444635.299203332

| | | | |
|---|---|---|---|
| H | -2.95487599 | 5.50652288 | -5.95304227 |
| O | 1.02256244 | -2.39218754 | -0.49481911 |
| H | 5.32567501 | 5.89088500 | -2.47415376 |
| O | -4.78171301 | 2.80034683 | -0.21701270 |
| O | -0.04232486 | 4.11976028 | -1.54806277 |
| O | 1.48292797 | -0.75245679 | 1.69082983 |
| Ti | -0.44222015 | 1.81488045 | -0.47709701 |
| O | -3.19798238 | 2.34604964 | -4.21326208 |
| O | -1.24549664 | 1.81996388 | -2.24388467 |
| O | 1.07859419 | -1.42426232 | -3.22648899 |
| Ti | 3.00587193 | 1.33825126 | -0.80818036 |
| O | 2.98441902 | -0.36929549 | -1.36129945 |
| O | 0.80285082 | 1.42676481 | -3.77432638 |
| Ti | -2.57163346 | 4.03952883 | -3.93569211 |
| O | -0.74093775 | 0.76406829 | 1.04308240 |
| Ti | 2.45097819 | 0.55674382 | 2.41589365 |
| O | -1.35669789 | 3.44578156 | 2.89425606 |
| O | -2.95985535 | 5.08745234 | 0.79936985 |
| Ti | -3.43882417 | 3.95857160 | -0.52118384 |
| Ti | 0.16219329 | -1.14024996 | 0.48918486 |
| O | -2.00410582 | 2.95465931 | 0.02291725 |
| Ti | -1.36669044 | 4.31824087 | 1.33093533 |
| O | -3.88599189 | 0.58261226 | -1.83079814 |
| O | 0.24642944 | 3.01424863 | 0.94884577 |
| Ti | -0.00766374 | 0.01678298 | -3.04496242 |
| O | -0.77777655 | 3.91944347 | -4.15825845 |
| O | 3.26534584 | -3.23485872 | -2.28202251 |
| Ti | -0.49323597 | 1.82441375 | 2.65832073 |
| O | -0.01769666 | 5.47438968 | 0.84564684 |
| O | 2.11261257 | 3.92619866 | -3.36692637 |
| Ti | -2.70048028 | 1.04294802 | -3.08849213 |
| O | -3.27770453 | 5.18654216 | -5.10884973 |
| O | -3.59719364 | 0.35581818 | 1.05980855 |
| O | -0.05536606 | -0.04039328 | -1.11316967 |
| O | 3.17926765 | 1.42301335 | 0.97992872 |
| O | -1.66335078 | -0.28456627 | -3.73934843 |
| Ti | -2.39879648 | -0.51596975 | 2.14708936 |
| O | 3.70441193 | -0.03260531 | 3.54710253 |
| O | 2.71830634 | 4.79294865 | -0.68547282 |
| Ti | 2.12994242 | -1.91949562 | -1.85462753 |
| Ti | 3.48499402 | 4.13724878 | -2.18233537 |
| O | 1.35815847 | 2.14329131 | -1.12809625 |
| Ti | -4.66977741 | 0.97425566 | -0.22103270 |
| O | -3.43015522 | -1.59921370 | 3.12637176 |
| O | 4.07375201 | 2.47545139 | -1.69929116 |
| Ti | 1.00795278 | 4.38106878 | -0.16512227 |
| O | 4.79016159 | 5.17758217 | -2.82275567 |
| O | 1.18761797 | 1.58667749 | 3.23955297 |
| O | -1.30739723 | -1.74746317 | 1.30408378 |
| H | -6.64320458 | -0.42446554 | 0.48955657 |
| H | 3.59252515 | -3.58291727 | -3.11240536 |

O -1.59200154 0.59531355 3.37198631
H -3.29689285 -2.52515707 3.33704138
H 3.78033729 -0.77212815 4.15083843
O -6.29731169 0.24345834 -0.10509765
O -3.14651236 4.42708779 -2.24473620
Ti 0.50776905 3.14972525 -3.14127858

60
(TiO2)16(H2O)4 Energy = -446717.771656194
H 2.24150481 -1.68188336 7.14038691
O -0.69045325 1.88050703 -0.34880209
H 2.00929666 -2.30699810 -7.65781233
O 4.44303507 3.99165380 -1.23312732
O -2.21817663 -2.28438618 -3.48463409
O -2.04423282 -0.45310037 -1.31206709
Ti 1.33605293 -1.15313979 -5.49150485
O 1.53334380 0.22977147 0.82685573
O 1.70514967 0.58804650 -5.10677728
O -2.81897336 2.13591255 -2.37887236
Ti 3.26940560 2.63964788 -1.20846641
O 1.83188041 -0.97720199 6.63828757
O -5.58526824 0.80843521 2.50597394
Ti 4.27834400 -0.69481198 -0.50715283
O -3.27442530 -2.02211848 -6.23982361
Ti 1.04566928 -0.83606759 5.03480423
O 0.88710674 0.11063806 -2.46132234
O -4.47717995 -4.17714827 1.58731073
Ti -1.75129616 -2.16073222 -1.74582632
Ti -0.26905300 -2.38905867 2.73418260
O 2.23485987 -1.71966007 -6.93577144
Ti -2.19973086 2.05596883 -4.06093985
O -0.40960120 2.27182139 -3.94317710
O -2.95836528 3.30185981 -5.10412351
Ti 1.44842051 -1.59535682 -2.30327394
O 4.09442347 1.08116692 -0.86131952
O 3.96396096 -1.10590953 1.23488582
Ti -0.93712940 0.88257431 3.35379859
O 1.28352620 -2.50328341 1.81664732
O -3.48007278 1.30403687 0.47338927
Ti -2.14241711 -1.33106468 -5.03239397
O 2.42127697 2.49567342 -2.81350204
O 1.75716360 -2.10434566 -3.99516148
O 3.00297938 -1.62208093 -1.37400071
O 2.20500361 -0.52009046 3.66158149
O -0.17575450 0.50699496 4.95267115
Ti -3.90547844 0.43640932 2.00971419
O -2.52757151 0.38281168 -4.70453686
O 0.01964628 -2.47385791 -1.60784496
Ti 1.17632378 1.46887635 -3.61995688
Ti -2.29358366 1.26501995 -0.87511663
O -0.43597603 -1.34389321 -5.66776658
Ti 0.72818757 1.84427821 0.75768961

O -2.73099978 1.04471498 3.26628872
O -1.67575424 -3.37803942 2.18496116
Ti 2.29642451 -0.99334049 1.91185724
O -0.70571880 -0.66294541 2.43317568
O -2.71424020 -3.09894581 -0.51356787
O -3.71025075 -1.32557142 1.69096984
H -4.70710211 -5.00721512 1.16714594
H -6.38543458 0.28163878 2.49853227
O 0.18966674 -2.34182049 4.49476745
O 5.91728394 -1.22991010 -0.99402487
H 5.39852958 4.01293991 -1.16786240
H 6.31736386 -2.09958888 -1.03543130
H -3.36850175 4.14535588 -4.90930418
H -3.88385468 -1.59743023 -6.84508249
O 0.02749979 2.09794955 2.41828391
O 2.01587977 2.91152245 0.09020521
Ti -3.17237998 -3.00238710 1.22338695

63
(TiO2)16(H2O)5 Energy = -448799.271203031
H -1.00373557 5.52318213 -6.27870219
O -4.71800979 0.60957760 -0.11594319
H -2.90775775 -4.14130911 -4.09234772
O 2.17297551 3.31988986 -0.86817029
O 2.03116160 -2.72279962 2.42610134
O -2.60934033 4.06912851 -3.75056539
Ti -1.24114560 0.78968825 -3.42055815
O -6.16616295 2.97372138 0.99576872
O 0.19178776 4.17163865 -2.99118941
O -0.26081553 -1.51657326 0.32058987
Ti 2.75868422 -3.32966170 0.90427989
O 1.34535380 -2.07124499 5.25011376
O -1.85055854 0.65781674 -0.16392072
Ti -0.22331852 -4.33571411 -0.66261924
O -4.52147950 3.21317687 -1.49960975
Ti 3.61185951 -0.48831433 -0.77474431
O 1.25940280 0.04956391 3.16794106
O -1.81752061 -0.80490100 -4.41092776
Ti -3.28189282 -0.48246568 -0.25632348
Ti 3.29009426 2.75206027 0.45723329
O -1.24342176 -4.02692678 0.81515638
Ti -0.93625893 3.82160885 -4.37284965
O 4.67683048 3.87423518 0.61265950
O -2.82474667 1.34988041 -2.84550741
Ti 0.99860012 -1.71088591 3.52673929
O 0.53901939 1.22368934 0.51017423
O -0.99462871 -3.46918405 -2.06587810
Ti -1.45917860 2.26149295 0.80382335
O 3.86221023 1.08114028 0.11288311
O -5.08891268 2.57704631 -4.32492967
Ti 0.18067491 -0.13868338 -0.84730573
O 2.36403662 2.66837973 2.02568771

O -0.27382738 -6.08912134 -1.03705203
O -0.69552252 -2.12291049 3.11662222
O -2.99886506 -1.56393027 1.16087552
O -0.57647420 4.78911150 -5.83653926
Ti -4.69364926 2.40909880 0.14431682
O 3.76187678 -1.96477242 0.22829250
O -3.20521232 2.74101411 1.07004102
Ti 0.95515848 1.56008621 2.22839256
Ti -3.81515946 2.87052645 -3.09716536
O 0.02196855 1.51753428 -2.09743223
Ti 0.49618761 3.19118701 -1.51330677
O 3.82452693 -4.72844531 1.27349474
O -0.68433885 2.31061103 2.45041267
Ti -1.37849746 -2.34616547 1.43926598
O 1.48599325 -3.90044253 -0.25391306
O -3.22257426 -1.56303721 -1.70678467
O -0.77886464 2.02313692 -4.66358799
H 5.00727298 -1.30204691 -2.72465784
H -6.01452014 2.35227645 -4.21615507
H 0.80188779 -2.45095338 5.94160819
H 0.31582634 -6.77758238 -0.72409454
O 1.87385092 -0.50629521 -1.25709250
O -0.79332495 3.52841187 -0.28425699
O 4.68863024 -0.55997239 -2.20930883
H -2.42846215 -0.86098596 -5.15104209
H 5.61648628 3.71744165 0.71321605
H 4.39842786 -4.86071570 2.02991129
H -6.29406145 3.39580157 1.84637180
Ti -1.99207872 -2.20312828 -2.87008139
O -0.68577736 -0.77466330 -2.37554226
O -2.87788917 -3.18239363 -4.12519385

66
(TiO2)16(H2O)6 Energy = -450880.708071367
H -6.67519934 0.89993136 -0.82970907
O -0.14176501 0.13687949 -4.97119617
H -5.52999900 -2.90553749 -4.08171397
O -0.73417250 -2.87472281 1.85180834
O -3.97094802 4.72855216 -4.58916905
O 3.53046920 -0.14997237 -0.94655859
Ti 1.27858227 2.86563389 -0.57117662
O -1.16862765 -1.19215353 -0.39502760
O 0.75866705 4.53469561 -1.09385319
O -4.28500238 -0.18859202 -1.65084577
Ti 3.32330981 0.90391810 -2.42661842
O -1.50408185 0.80628844 4.56683764
O -5.36069192 -2.04672673 -3.69257181
Ti 2.42648541 2.01317457 2.42971970
O -2.71531150 1.35220158 -0.06335313
Ti -0.99511925 0.68409181 -0.51808132
O 2.26548251 3.00430412 0.90104265
O 0.95168019 0.67445228 -0.34405235

Ti 1.05958048 -1.02815224 -4.31745798
Ti -0.85914674 5.31029774 -1.20762105
O 1.72444612 -2.13838764 0.43706715
Ti -2.97769588 3.62843504 -3.57936972
O -6.07454032 1.59547221 -0.54966388
O -4.01426078 2.52280837 -2.57517487
Ti -1.56918228 0.79990276 -4.07847441
O -2.02064550 2.46247234 -4.58339947
O 2.34615603 2.34366868 -1.94528932
Ti -2.23517929 3.18095339 0.70124872
O -2.96447999 -0.32079200 -4.22414461
O -2.57646719 -1.41049768 3.46289983
Ti -0.91503898 1.49444631 3.04825611
O -1.99619330 2.84632472 2.42595323
O -1.80556362 4.88330253 0.28724180
O -4.09937507 3.27214283 0.15676794
O -0.31555067 -3.80826993 -0.84844181
O -3.45255729 -1.87418233 0.91150943
Ti -1.91069365 -1.50110107 1.74593384
O -0.72653261 7.08669952 -1.40490930
O 2.45053787 -0.10917615 -3.63264157
Ti 2.26231749 -0.41312540 0.28820908
Ti 0.53909769 -3.47587494 0.73866781
O 2.77465779 0.34138091 1.85812157
Ti -1.01599129 -2.42689056 -1.74222463
O 4.91695766 1.42222205 -3.06259119
O 3.69568632 2.64850712 3.52139026
Ti -3.87373362 -1.30940608 -3.00266546
O -1.05399208 0.19104509 1.76253909
O 1.61919893 -2.16114675 -5.58996597
O -2.69301230 -2.55517971 -2.43112904
H -1.99149166 -0.03941694 4.47946020
H -4.59591968 4.56248992 -5.29594515
H 1.22403219 -2.44591171 -6.41481456
H 0.03344427 7.67007550 -1.38473173
O 1.32595395 -4.94562378 1.39250909
O -1.84878656 4.56062919 -2.54337493
O -0.57604294 2.53016940 -0.02210557
H -3.79806530 -1.44147676 0.12042949
H 4.62419661 2.44619324 3.64117329
H -3.47855502 -1.70747086 3.61036624
H 2.17502775 -5.36314389 1.24466171
Ti -4.34345582 1.57734867 -1.07675878
O 0.15531613 -1.89321767 -2.99574700
O -1.12767526 0.83496130 -2.30876774
H -4.63158664 4.06869221 0.10211549
H 5.49918475 1.01884486 -3.70784379
O 0.80490733 2.01977772 3.20986995

69
(TiO2)16(H2O)7 Energy = -452962.039211837
H -6.39177730 1.34496014 2.42901876

O -0.88774013 -1.21388836 -0.14908516
H -0.84557636 -6.38979408 -1.83390411
O -0.61669080 2.91378410 -3.03868501
O -5.49694553 1.11758384 2.69271392
O 1.86886613 -1.07847067 4.28479680
Ti 3.00796332 2.32147130 1.51587140
O 1.18201653 -1.02893980 1.48865197
O -0.84778130 1.48327984 -0.57627783
O 4.02786362 2.08586730 -0.25193205
Ti -1.87069768 1.63037453 4.22669033
O 0.17531815 -2.81173812 -2.55354850
O 1.65515264 -0.97425563 -4.31641034
Ti -4.22043894 0.70640608 1.48624001
O 0.83259086 -3.58621232 3.05506363
Ti 2.82298110 1.05426615 -1.45033636
O 4.62947263 2.59492210 2.28983571
O -0.27785945 1.02186375 1.80645851
Ti -1.37579000 2.45690710 1.28344380
Ti 0.92344601 4.77590909 0.38374769
O -3.08419263 2.04833382 0.99665279
Ti -1.47150340 1.49739356 -2.29437739
O 1.37611528 -0.29355883 -1.49079780
O -5.13631282 0.64952968 -0.05612228
Ti -2.47196571 -2.01745569 -0.04477939
O -0.89509933 -0.01375338 -3.12319242
O -0.67581072 4.01367544 0.68925233
Ti -2.41199767 -1.48319796 2.97930752
O -1.84720527 -2.84475326 1.69176618
O -0.63591577 -1.30057824 3.19821152
Ti 0.04124883 -2.60650942 1.73848931
O 0.89938393 6.52221288 0.79252310
O -3.25736444 1.49566273 -2.27646519
O 1.87426034 1.34441725 0.20069874
O -2.59792496 2.15221580 5.78002882
O -0.21032311 -5.67517920 -1.77728257
Ti 0.52357921 -1.10126268 -2.91674836
O 2.14975086 3.91028792 1.37652888
O -2.12469723 -3.60361786 -0.89529739
Ti 1.05633254 3.58719836 -2.88354568
Ti 1.01746659 0.00670710 3.14462261
O -1.63604365 2.92754724 3.09904903
Ti -0.40935161 -3.96750340 -1.25204124
O 0.45703839 -3.65716400 0.31428285
O -3.19274037 -2.42557360 4.28674922
Ti 0.37947280 0.18790480 0.21284789
O 2.20575081 2.15478675 -2.69668468
O 2.26662224 1.27906927 2.81470038
O -2.84380778 0.37290491 3.35895183
H 0.18231669 0.73335256 5.48959774
H 4.98600589 2.13299304 -0.29470836
H 1.66969898 -0.26687239 -4.96558988
H -6.10335506 -0.84725930 -3.32168865

O 4.13826266 -0.02676716 -2.04006821
O 1.48062697 4.53718180 -4.34512825
O -3.49158685 -1.05188925 1.37882041
H 1.87439727 5.40714484 -4.42648370
H -2.91410134 3.00514084 6.08199322
H 4.87804477 2.18833166 3.12279373
H 1.19761203 6.99087469 1.57307615
Ti -4.47293103 0.23891763 -1.69945279
O -5.77535311 -0.04995614 -2.90515381
O 1.24517649 4.55723769 -1.40357210
H 1.61720510 -2.01296856 4.32535001
H 4.12746540 -0.51715808 -2.86681442
O -0.08634994 0.98036597 4.59992872
H -2.83689628 -3.16976454 4.77581907
H 1.33134691 -4.36297746 2.78465450
O -3.52764843 -1.21536411 -1.34016318

72
(TiO2)16(H2O)8 Energy = -455043.707090292
H 1.11730585 5.46791497 -1.50655618
O -0.79071882 -3.65132244 -1.53125862
H 6.29067871 2.43237762 0.45272882
O -4.11031255 3.59949682 -4.02754611
O 3.14203367 -1.33876663 -0.84372373
O -1.53696994 1.76950944 -0.79734813
Ti 3.54366547 -0.41163745 3.47983649
O 2.11767258 0.28729572 4.37771177
O 0.54084123 2.78295784 0.50297295
O 0.48043016 2.45959377 -2.13921407
Ti -3.12403023 2.61489191 0.45435858
O 5.36887742 2.69229453 0.43522490
O 0.73675579 0.39122436 -0.66683728
Ti -0.53204548 0.95777586 0.75473827
O -3.45933358 1.74183532 4.28047410
Ti 2.01113751 -0.83625048 0.53025139
O -1.79109111 4.00792431 0.47216734
O -3.21737148 -0.93040643 2.93067287
Ti -3.32741497 -1.05730256 1.19055182
Ti -0.61858204 3.68213193 -0.95399376
O -1.54009078 -0.58147298 0.59118520
Ti -3.04852127 2.97046710 -2.72930642
O -4.74307426 4.40051042 4.43771469
O 2.89745519 1.01447187 0.39632223
Ti -0.78843522 0.85599120 -2.32411330
O -3.88931630 0.68703322 0.52606350
O 0.31974166 2.59400040 3.46488366
Ti -3.60642618 3.37909808 3.49854205
O 2.83693712 6.05572489 0.75909607
O -1.10850492 -0.91837079 -2.06648009
Ti 0.54856328 0.85233779 3.69721990
O -2.52895659 -2.67557377 0.29935139
O 4.58153963 -1.43274951 4.53484800

O 0.51874821 4.95531022 1.99750765
O -2.01814527 4.19606534 3.33617198
O 2.84449511 3.53126324 -0.72387034
Ti 1.90210238 1.86843018 -1.08154696
O 2.98131580 3.47516377 1.96937447
O -3.94884039 2.88107111 -1.15862957
Ti -0.66521416 3.61967193 2.27221516
Ti -2.72906819 0.10759063 4.39870093
O 2.92137741 -1.30790858 2.06366670
Ti 1.90185213 4.52891428 0.92210988
O 0.67143409 0.32477791 -3.77258847
O 0.72284463 -2.08500984 0.21232936
Ti -0.87548264 -2.06024967 -0.66055914
O 2.84027902 1.01851342 -2.41338187
O 0.65146971 5.07822099 -0.76169535
O -4.96420287 -1.79076359 0.82595852
H 3.79473303 3.64043041 -0.86260195
H -4.75835553 5.35341941 4.54108686
H -4.83192479 4.22948470 -4.00116143
H -3.08112500 -3.39564610 -0.01425697
O -0.94683590 0.15809537 4.49088170
O -2.12461283 1.46719674 -3.31904054
O -1.71353728 1.87834359 1.80397993
O -4.17764894 3.20764430 1.76506401
O 4.44408707 1.02537514 2.79883190
O -3.35387730 -0.69229784 5.87714349
H -2.85860092 -1.17927146 6.53819744
H 4.88771977 -2.33552975 4.44363225
H -5.62615732 -1.92413219 1.50877527
H 3.27545238 0.21438407 -2.06960968
H -0.49547741 -4.49798185 -1.19253539
H 0.66618150 -0.62120992 -3.95037465
H 1.58114697 0.56565215 -3.44846572
H 2.98688363 -2.21083581 -1.21666462
H 2.49327166 6.92959350 0.95757167
H -4.80698053 0.68146649 0.23519759
O -1.72309465 4.12232881 -2.32331532
O 0.68130069 0.23549954 1.97490870
Ti 3.97486212 2.09270502 1.44219126