Stability of Mixed-oxide Titanosilicates: Dependency on Size and Composition from Nanocluster to Bulk

Andi Cuko[1,2], Monica Calatayud[2,3,*], Stefan T. Bromley[1,4,*]

[1] *Departament de Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, E-08028 Barcelona, Spain*

[2] *Sorbonne Universités, UPMC Univ Paris 06, CNRS, Laboratoire de Chimie Théorique CC 137 - 4, place Jussieu F. 75252 PARIS CEDEX 05 - France*

[3] *Institut Universitaire de France, France*

[4] *Institució Catalana de Recerca i Estudis Avançats (ICREA), E-08010 Barcelona, Spain*

* Corresponding authors: s.bromley@ub.edu, calatayu@lct.jussieu.fr

Supplementary information

1. Normalization of mixing energies

In table S1 and S2 we report mixing and total energies of global optimized clusters and crystalline bulk systems respectively as plotted in Fig. 4 of this work.

Table S1. Total energies and mixing energies of global optimized silica, titania and titanosilicate clusters. Systems are ordered by size (smallest to biggest) and for a specific size are ordered by composition (x TiO_2 from 0 to 1).

System	x TiO_2	Total energies (eV)	ΔE_{mix}/unit (eV)
(SiO2)2	0.000	-23998.628948781	0.0000
Ti1Si1O4	0.500	-39395.821093405	-0.0167
(TiO2)2	1.000	-54792.946306103	0.0000
(SiO2)3	0.000	-36000.645793516	0.0000
Ti1Si2O6	0.330	-51397.838677881	-0.0145
Ti2Si1O6	0.667	-66794.761616984	0.0609
(TiO2)3	1.000	-82192.093849742	0.0000
(SiO2)4	0.000	-48002.639028013	0.0000
Ti1Si3O8	0.250	-63399.803085355	0.0144
Ti2Si2O8	0.500	-78797.770370337	-0.1719
Ti3Si1O8	0.750	-94194.492950979	-0.0471
(TiO2)4	1.000	-109591.52638539	0.0000
(SiO2)5	0.000	-60004.627962668	0.0000
Ti1Si4O10	0.200	-75401.541009197	0.0564
Ti2Si3O10	0.400	-90799.333800403	-0.0631
Ti3Si2O10	0.600	-106196.86047662	-0.1294
Ti4Si1O10	0.800	-121593.78698265	-0.0757
(TiO2)5	1.000	-136990.60356196	0.0000
(SiO2)6	0.000	-72006.617106618	0.0000
Ti1Si5O12	0.167	-87403.888230548	0.0159
Ti2Si4O12	0.333	-102802.40371295	-0.1754

Ti3Si3O12	0.500	-118199.99675263	-0.2131
Ti4Si2O12	0.667	-133597.15947250	-0.1791
Ti5Si1O12	0.833	-148994.02466230	-0.0955
(TiO2)6	1.000	-164390.81850687	0.0000
(SiO2)7	0.000	-84008.482129892	0.0000
Ti1Si6O14	0.143	-99406.641652290	-0.1088
Ti2Si5O14	0.286	-114805.17581770	-0.2713
Ti3Si4O14	0.429	-130202.68151404	-0.2867
Ti4Si3O14	0.571	-145599.55783254	-0.2123
Ti5Si2O14	0.714	-160996.59754615	-0.1612
Ti6Si1O14	0.857	-176393.13931644	-0.0390
(TiO2)7	1.000	-191790.26328829	0.0000
(SiO2)8	0.000	-96011.405525393	0.0000
Ti1Si7O16	0.125	-111409.27556127	-0.0706
Ti2Si6O16	0.250	-126807.32170324	-0.1632
Ti3Si5O16	0.375	-142204.94048643	-0.2024
Ti4Si4O16	0.500	-157602.22671239	-0.2000
Ti5Si3O16	0.625	-172999.20477183	-0.1591
Ti6Si2O16	0.750	-188396.15253490	-0.1144
Ti7Si1O16	0.875	-203792.98287985	-0.0550
(TiO2)8	1.000	-219189.84754442	0.0000
(SiO2)9	0.000	-108013.52540721	0.0000
Ti1Si8O18	0.111	-123411.42645541	-0.0706
Ti2Si7O18	0.222	-138809.70683876	-0.1834
Ti3Si6O18	0.333	-154207.48989963	-0.2410
Ti4Si5O18	0.444	-169605.36116046	-0.3083
Ti5Si4O18	0.556	-185002.34976334	-0.2776
Ti6Si3O18	0.667	-200399.24311390	-0.2363
Ti7Si2O18	0.778	-215795.91258780	-0.1701
Ti8Si1O18	0.889	-231192.52948979	-0.0980
(TiO2)9	1.000	-246589.33391945	0.0000
(SiO2)10	0.000	-120016.05808241	0.0000
Ti1Si9O20	0.100	-135414.67096072	-0.1306
Ti2Si8O20	0.200	-150812.91539109	-0.2243
Ti3Si7O20	0.300	-166210.96628318	-0.2987
Ti4Si6O20	0.400	-181608.04766648	-0.2762
Ti5Si5O20	0.500	-197005.03857150	-0.2446
Ti6Si4O20	0.600	-212402.00237762	-0.2103
Ti7Si3O20	0.700	-227798.74224502	-0.1536
Ti8Si2O20	0.800	-243195.58402226	-0.1071
Ti9Si1O20	0.900	-258592.23642913	-0.0416
(TiO2)10	1.000	-273989.44301377	0.0000
(SiO2)12	0.000	-144022.25380481	0.0000
Ti3Si9O24	0.250	-190216.38898834	-0.2120
Ti5Si7O24	0.417	-221010.91476169	-0.2229
Ti6Si6O24	0.500	-236407.83444198	-0.1998
Ti9Si3O24	0.750	-282598.13722054	-0.1385
(TiO2)12	1.000	-328788.61783104	0.0000
(SiO2)14	0.000	-168029.35750224	0.0000
Ti4Si10O28	0.286	-229619.94416664	-0.1705
Ti5Si9O28	0.357	-245017.07648010	-0.1764
Ti7Si7O28	0.500	-275810.82349600	-0.1512
Ti10Si4O28	0.714	-322001.22704360	-0.0980
(TiO2)14	1.000	-383588.05321771	0.0000
(SiO2)16	0.000	-192035.44996292	0.0000
Ti4Si12O32	0.250	-253625.63452931	-0.1386
Ti6Si10O32	0.375	-284419.92512328	-0.1578

Ti8Si8O32	0.500	-315213.54039826	-0.1348
Ti12Si4O32	0.750	-376800.54162855	-0.0745
(TiO2)16	1.000	-438387.21836150	0.0000
(SiO2)24	0.000	-288060.06629464	0.0000
Ti12Si12O48	0.500	-472823.84752340	-0.0363
(TiO2)24	1.000	-657585.88426394	0.0000

Table S2. Total energies and mixing energies of SiO_2 (quartz), TiO_2 (rutile) and a selection of titanosilicate bulk systems.

System	x TiO_2	Total energies (eV)	ΔEmix/unit (eV)	n of units/cell
(SiO2)quartz	0.000	-36010.12399679	0.0000	3
Sodalite-like	0.083	-159436.37868418	0.0742	12
quartz-like 1_2	0.333	-51406.65217968	0.0817	3
Ti-Si_wired	0.333	-102813.42794212	0.0611	6
quartz-like 3_3	0.500	-118209.76116476	0.1344	6
quartz-like 2_1	0.667	-66803.17680510	0.1646	3
(TiO2)rutile	1.000	-54800.29585748	0.0000	2

In table S3, we report ΔE_{mix}/unit for a range of $(Ti_{0.5}Si_{0.5}O_2)_n$ systems according to two definitions of normalisation unit: (i) MO_2 (M= Si, Ti) used in this study and (ii) $TiSiO_4$ unit typically employed for reporting experimental mixing enthalpies of bulk systems.

Table S3. Calculated mixing energies per unit for a set of titanosilicates (clusters and bulk) with 50% molar fraction composition of titania using two different definition of unit. [a)] the bulk system is referred to titanosilicate having quartz-like structure shown in Fig. 1a) while all the other systems are referred to clusters at different size shown in Fig 3.

System	ΔE_{mix}/unit [MO_2 (M=Ti, Si)] (eV)	ΔE_{mix}/unit [$TiSiO_4$] (eV)
$(Ti_{0.5}Si_{0.5}O_2)_2$	-0.0167	-0.0335
$(Ti_{0.5}Si_{0.5}O_2)_4$	-0.1719	-0.3439
$(Ti_{0.5}Si_{0.5}O_2)_6$	-0.2131	-0.4263
$(Ti_{0.5}Si_{0.5}O_2)_8$	-0.2000	-0.4001
$(Ti_{0.5}Si_{0.5}O_2)_{10}$	-0.2446	-0.4892
$(Ti_{0.5}Si_{0.5}O_2)_{12}$	-0.1998	-0.3998
$(Ti_{0.5}Si_{0.5}O_2)_{14}$	-0.1512	-0.3026
$(Ti_{0.5}Si_{0.5}O_2)_{16}$	-0.1348	-0.2697
$(Ti_{0.5}Si_{0.5}O_2)_{24}$	-0.0363	-0.0727
$(Ti_{0.5}Si_{0.5}O_2)^a{}_{bulk}$	0.1344	0.2689

2. Performance of the employed interatomic potentials (IP1 and IP2)

In Fig S1 we compare how well IP1 and IP2 perform with respect to yielding low energy $(Ti_xSi_{1-x}O_2)_n$ nanocluster isomers (where relative energies are refined using DFT-based calculations) with respect to x for three intermediate cluster sizes, n. Focussing on the global minima candidates (i.e. data point at zero relative energy) we clearly see that the performance of IP1 is distinct to IP2. In all cases for $x \leq 0.25$ IP2 tends to give the lower energy candidates than IP1 (we note that in some cases IP1 can also provide good candidates for x = 0.1). Conversely, in all cases for $x \geq 0.45$ IP1 tends to provide lower energy isomers than IP2 (although again IP2 is sometimes able to reproduce the global minima predicted by IP1). For the intermediate composition region of $0.25 > x > 0.45$ both IPs are able to provide low energy isomers, where

the performance in this region depends more sensitively on the size n and the structures of the low energy isomers for this size. These IP performance tendencies were found to hold over the full range of nanocluster sizes and compositions studied.

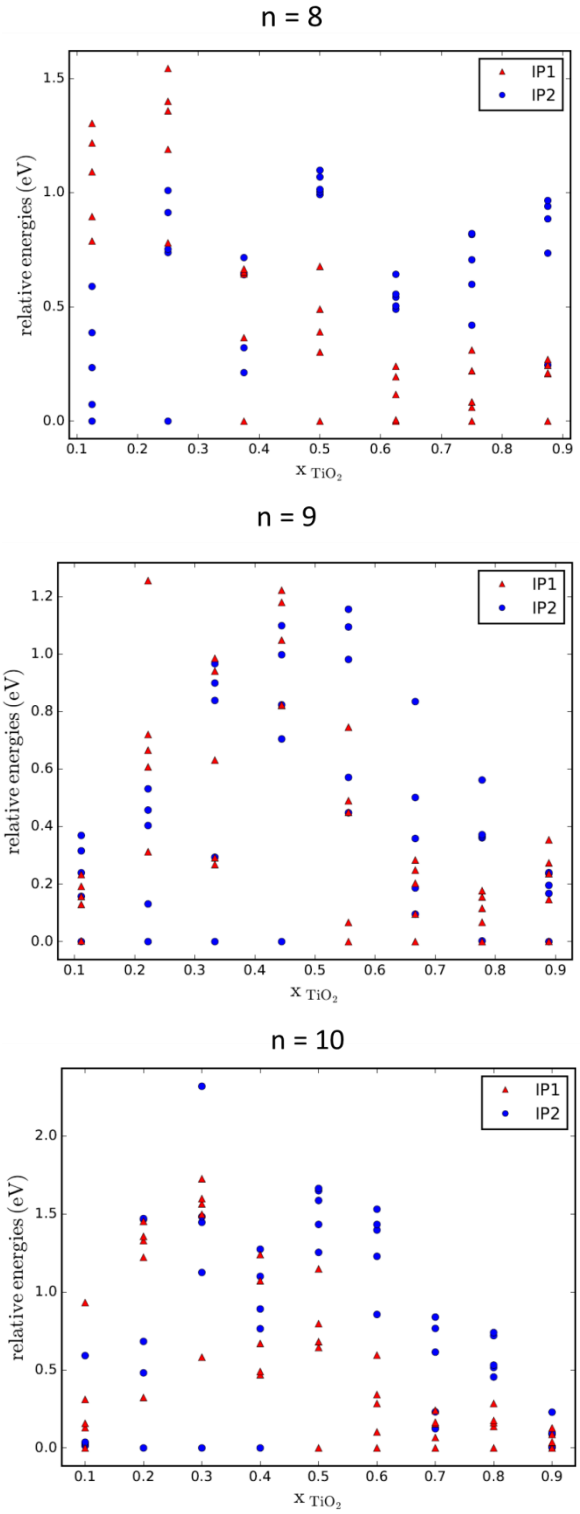


Figure S1. DFT-optimised energies of low energy $(Ti_xSi_{1-x}O_2)_n$ titanosilicate nanocluster isomers coming from IP-based MCBH global optimisations using IP1 (red filled triangles) and IP2 (blue filled circles) for n = 8 (upper), n = 9 (middle) and n = 10 (lower).

3. Relative energies of few energetically low lying isomers with respect to the corresponding global minimum for a set of $(Ti_{0.5}Si_{0.5}O_2)_n$ clusters

In Fig S2 we report the energy separations between our titanosilicate global minima nanoclusters and the respective first few energetically low lying isomers. In Fig S2 we also include the probability of the isomers to be thermally accessible considering different temperatures (298, 500, 700, 900K) according to calculated Boltzmann factors as shown in eq S1. The large separation between the global minimum and the second most stable isomer for systems with n ≤ 10 allow us to neglect the configurational entropy in the calculation of the mixing free energies. However, for systems with n > 10 neglecting the contribution of low ling isomers in configurational entropy may introduce some errors in estimating mixing free energies.

$$N_i/N_0 = e^{\frac{E_i - E_0}{RT}} \qquad \text{eqn. S1}$$

N_i/N_0 is the Boltzmann factor and represents the probability of the configurational isomer N_i being thermally accessible at temperature T and having energy difference $E_i - E_0$ with respect to the global minimum.

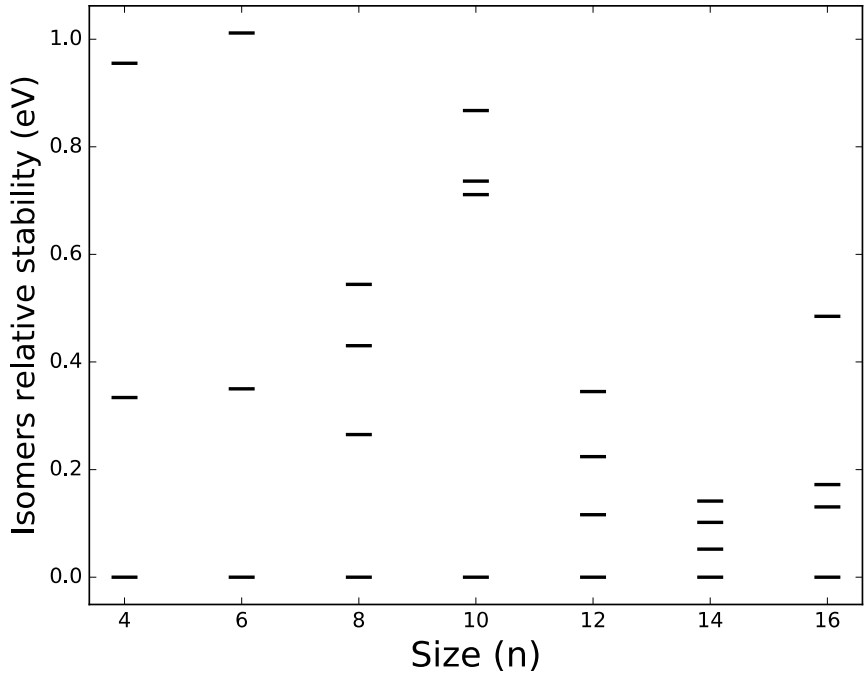
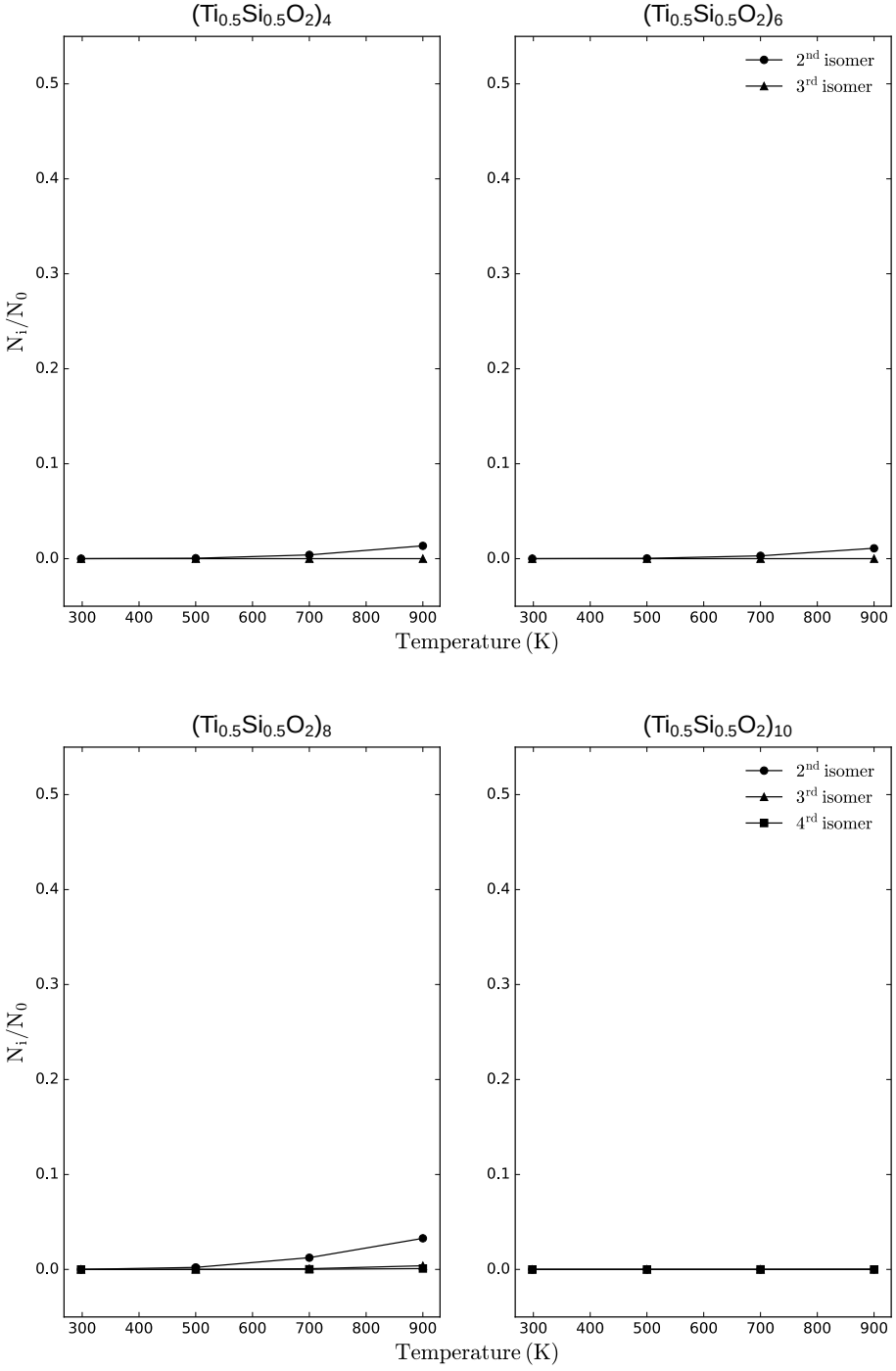


Figure S2. Energy separations between our titanosilicate global minima nanoclusters and the respective first few energetically low lying isomers.


(Ti0.5Si0.5O2)4
(Ti0.5Si0.5O2)6
(Ti0.5Si0.5O2)8
(Ti0.5Si0.5O2)10
2nd isomer
3rd isomer
4rd isomer
Ni/N0
Temperature (K)
0.0
0.1
0.2
0.3
0.4
0.5
300
400
500
600
700
800
900

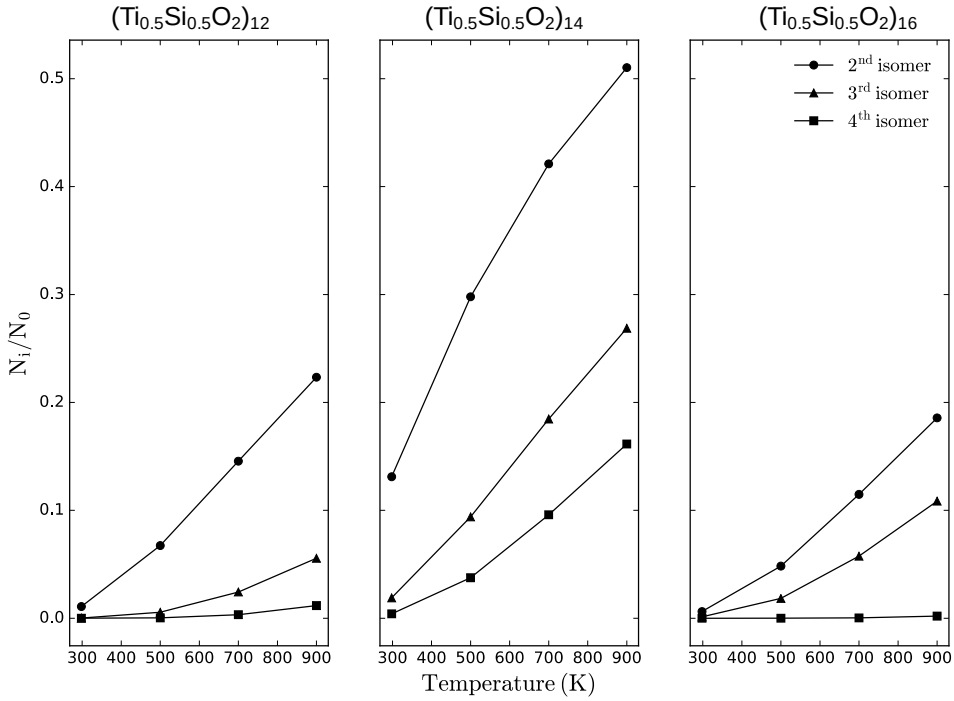
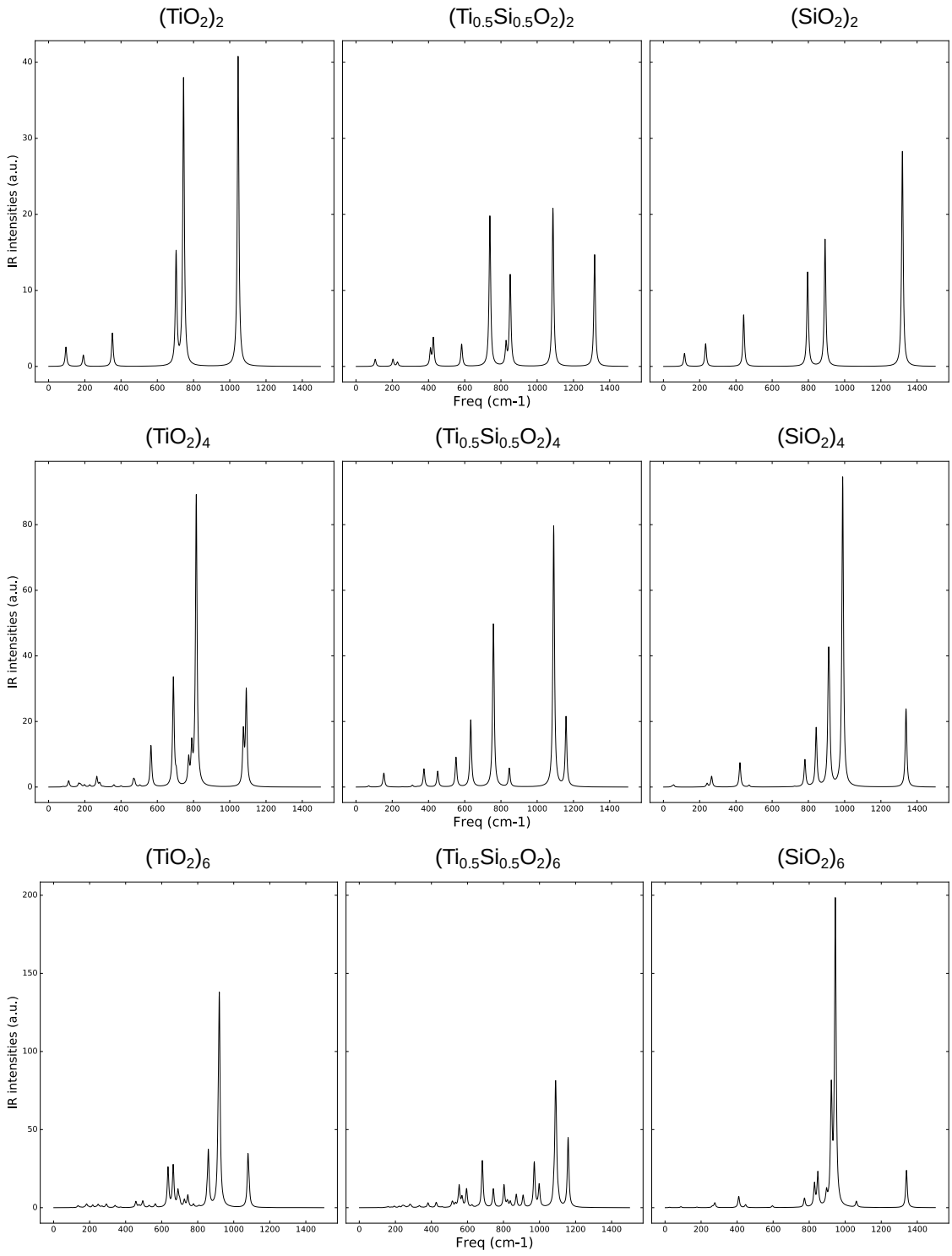
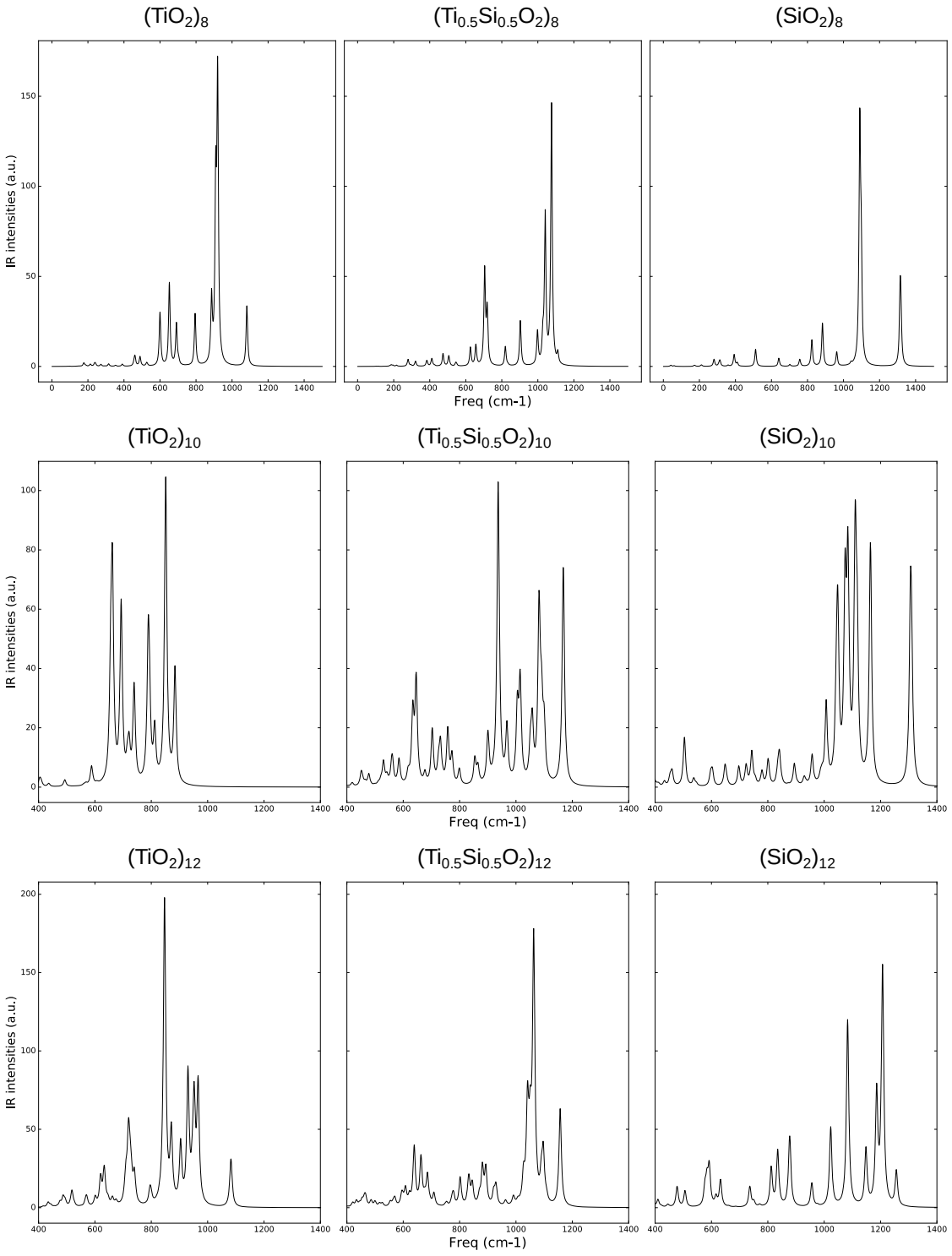


Figure S3. Boltzmann factors at different temperatures for the $(Ti_{0.5}Si_{0.5}O_2)_n$ set of clusters with relative energies shown in Fig S2. Energetically low lying isomers are represented with filled circles, triangles and squares for the 2nd, 3rd and 4th energetically most stable isomers respectively. Notice that for $(Ti_{0.5}Si_{0.5}O_2)_{10}$ Boltzmann factors are zero for all first energetically low lying clusters at all temperatures considered.

4. Calculated Infrared (IR) spectra

In Fig S4 we report calculated IR spectra for each $(Ti_{0.5}Si_{0.5}O_2)_n$ nanocluster and the corresponding pure counterparts.


$(TiO_2)_2$
$(Ti_{0.5}Si_{0.5}O_2)_2$
$(SiO_2)_2$
$(TiO_2)_4$
$(Ti_{0.5}Si_{0.5}O_2)_4$
$(SiO_2)_4$
$(TiO_2)_6$
$(Ti_{0.5}Si_{0.5}O_2)_6$
$(SiO_2)_6$
IR intensities (a.u.)
Freq (cm-1)


$(TiO_2)_8$
$(Ti_{0.5}Si_{0.5}O_2)_8$
$(SiO_2)_8$
$(TiO_2)_{10}$
$(Ti_{0.5}Si_{0.5}O_2)_{10}$
$(SiO_2)_{10}$
$(TiO_2)_{12}$
$(Ti_{0.5}Si_{0.5}O_2)_{12}$
IR intensities (a.u.)
Freq (cm-1)

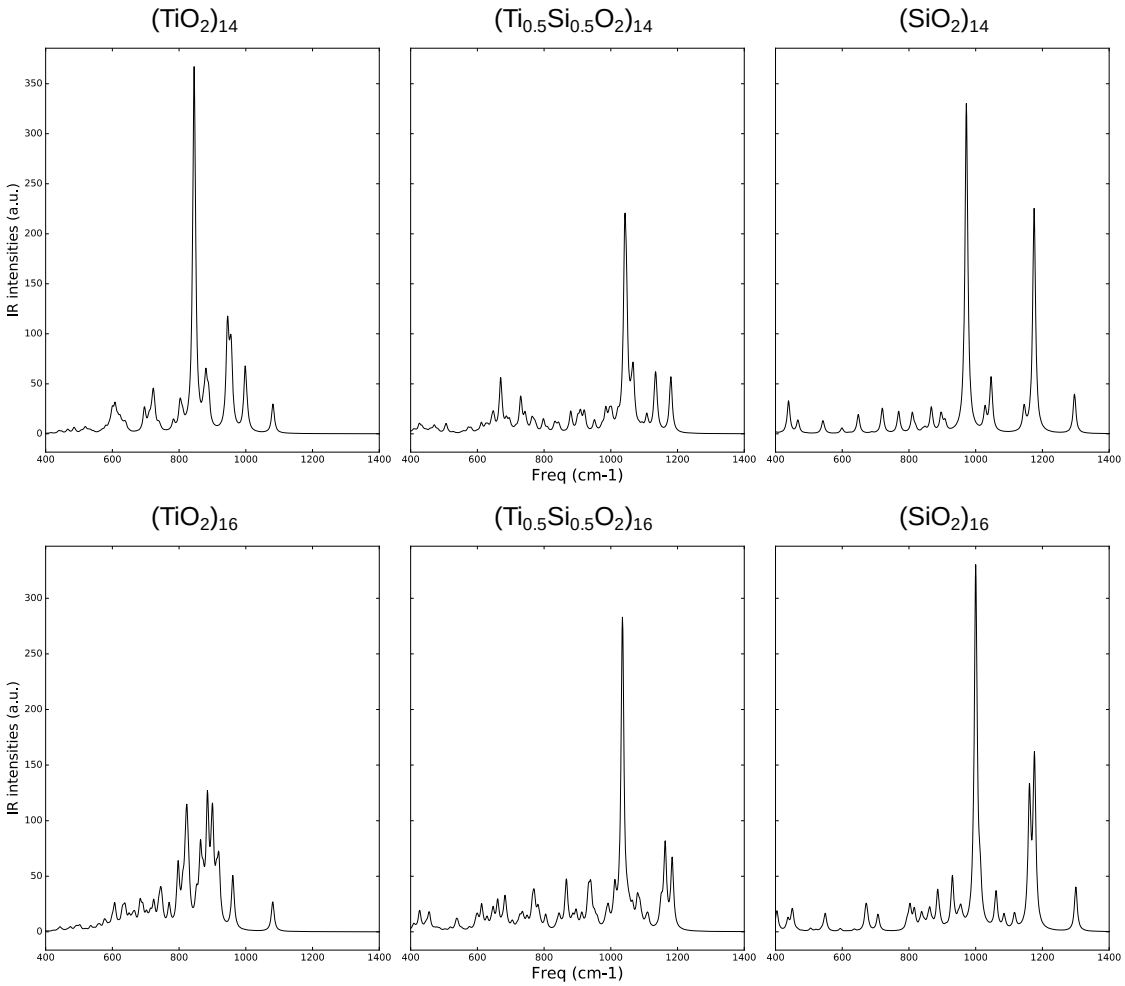


Figure S4. Calculated IR spectra for $(TiO_2)_n$ left, $(Ti_{0.5}Si_{0.5}O_2)_n$ centre and $(SiO_2)_n$ right with n=2, 4, 6, 8, 10, 12, 14 and 16.

5. Structures and energies of global minima clusters

Here, we report the xyz coordinates for all the global optimized titanosilicate, titania and silica clusters investigated in this work in the xyz file format. In the title for each case we indicate the chemical composition, the corresponding short two number notation as presented in Fig 2 and Fig 3 of the main text (i.e. indicating size (n) and number of incorporated Ti atoms), total DFT energies from an optimisation calculation using the PBE0 functional and a tight/tier-1 numerical basis set, and any relevant references to previous reports of the structure. Notice that structures without reference are new to this study.

6
Si2O4 (2-0) Energy= -23998.628948781 ref[49]
Si -0.7764 -0.8925 -0.0000
O -0.8856 0.7705 0.0000
Si 0.7767 0.8925 -0.0000
O 0.8859 -0.7705 0.0000
O -1.7649 -2.0302 -0.0000

O 1.7653 2.0302 -0.0000

6
Ti1Si1O4 (2-1) Energy= -39395.821093405 ref[29]
Ti -0.8730 -1.0178 -0.5359
O -0.8807 0.8299 -0.2339
Si 0.7378 0.8503 0.0394
O 0.9507 -0.7596 -0.1989
O -1.6378 -1.8745 0.5698
O 1.7041 1.9717 0.3594

6
Ti2O4 (2-2) Energy= -54792.946306103 ref[32]
Ti -1.3494 -0.0025 0.0084
Ti 1.3491 -0.0015 -0.0076
O -0.0006 1.2431 -0.0015
O 0.0003 -1.2471 0.0022
O 2.2292 -0.0032 -1.3581
O -2.2295 -0.0007 1.3589

9
Si3O6 (3-0) Energy= -36000.645793516 ref[49]
Si -2.3510 -0.0002 0.0000
O -1.1715 -0.3084 -1.1346
Si 0.0000 -0.0001 0.0000
O 1.1716 -1.1347 0.3082
Si 2.3510 -0.0001 -0.0000
O 1.1715 1.1345 -0.3082
O -3.8582 -0.0002 0.0000
O 3.8582 -0.0000 -0.0000
O -1.1716 0.3081 1.1346

9
Ti1Si2O6 (3-1) Energy= -51397.838677881 ref[29]
Ti -2.5343 0.4197 -0.1142
O -1.1222 -0.0685 -1.2452
Si -0.0412 0.1288 -0.0356
O 1.0269 -1.1156 0.3034
Si 2.3051 -0.1016 0.0277
O 1.2677 1.1436 -0.3119
O -3.5883 -0.7342 0.2005
O 3.8081 -0.2454 0.0679
O -1.1218 0.5721 1.1074

9
Ti2Si1O6 (3-2) Energy= -66794.761616984 ref[29]
Ti -2.4838 0.4437 0.0089

O -1.2156 -0.0718 -1.2509
Si 0.0001 0.0816 -0.1401
O 0.9868 -1.2198 0.0811
Ti 2.4841 -0.2226 -0.3843
O 1.2149 1.1279 -0.5458
O -3.6105 -0.6335 0.3847
O 3.6099 -0.0266 0.7405
O -0.9858 0.5200 1.1058

9
Ti3O6 (3-3) Energy= -82192.093849742 ref[32]
Ti -0.3936 0.2102 -1.8243
Ti -1.2848 -0.1087 0.8030
Ti 1.4987 0.0998 0.2266
O -2.3702 -0.9665 1.6241
O 2.9308 -0.5689 0.5265
O 0.2968 0.4304 1.5891
O -1.6888 0.8636 -0.9001
O 1.0536 1.0690 -1.4681
O -0.0424 -1.0289 -0.5768

12
Si4O8 (4-0) Energy= -48002.639028013 ref[49]
Si -1.1682 0.0000 0.0000
Si -3.5200 -0.0000 -0.0000
O -2.3420 1.1753 -0.0002
O -2.3419 -1.1753 0.0002
O 0.0000 -0.0002 -1.1774
O -0.0000 0.0003 1.1775
Si 1.1682 0.0000 0.0000
O 2.3420 1.1753 -0.0002
O 2.3419 -1.1753 0.0002
Si 3.5200 -0.0000 -0.0000
O -5.0276 -0.0001 -0.0000
O 5.0276 -0.0001 -0.0000

12
Ti1Si3O8 (4-1) Energy= -63399.803085355 ref[29]
O -2.3106 1.1761 0.0793
Ti -3.6269 -0.1506 -0.0365
O -5.1324 0.3650 0.0724
Si -1.7619 0.5576 1.4897
Si 0.0041 1.1928 2.8928
Si 1.7812 1.8297 4.3024
O 2.9235 2.2341 5.2023
O -2.8358 -0.6720 1.5784
O -0.1286 0.1810 1.5984

O -1.5949 1.5782 2.8068
O 1.1526 2.4049 2.8797
O 0.6448 0.6221 4.3253

12
Ti2Si2O8 (4-2) Energy= -78797.770370337 ref[29]
O -1.7506 0.7327 -1.3031
Si -0.7673 -0.4466 -0.8626
O -0.8620 -0.1321 0.8352
Ti -1.4306 1.8161 0.3324
O -2.6622 2.4760 1.0864
O 0.3928 1.9801 1.1064
Si 0.7673 0.4466 0.8627
O 0.8620 0.1321 -0.8352
Ti 1.4306 -1.8161 -0.3324
O -0.3928 -1.9801 -1.1064
O 1.7506 -0.7327 1.3031
O 2.6622 -2.4759 -1.0864

12
Ti3Si1O8 (4-3) Energy= -94194.492950979 ref[29]
O 1.5100 -1.6808 -0.4531
Ti 2.0544 -0.0130 0.4766
O 1.6835 1.6886 -0.3519
Ti 0.0083 1.4430 -0.9346
O 0.0254 -0.0385 -1.9715
Si 0.0197 -1.1903 -0.7627
O -1.4713 -1.6955 -0.4811
Ti -2.0495 -0.0332 0.4380
O -2.9490 -0.0963 1.7523
O 0.0015 0.0471 0.5186
O -1.6798 1.6721 -0.3835
O 2.9296 -0.0673 1.8076

12
Ti4O8 (4-4) Energy= -109591.526385395 ref[32]
Ti -1.6231 0.6666 0.9230
Ti 2.2871 -0.2592 0.6006
O 0.3200 0.1903 0.6546
O -2.1537 1.0062 2.3920
O 3.1339 -0.2457 1.9563
O 1.4813 -1.9117 -0.0214
Ti 0.4709 1.3732 -0.9137
O 0.0389 -0.1235 -1.8555
Ti -0.1366 -1.3339 -0.5071
O -1.7453 -1.1476 0.2446
O -1.0174 2.0956 -0.2424

O 2.2091 1.3316 -0.5084

15
Si5O10 (5-0) Energy= -60004.627962668 ref[49]
Si 4.6897 -0.0001 -0.0000
Si -2.3374 0.0001 -0.0000
Si -4.6897 -0.0001 0.0000
O -3.5124 -0.8227 0.8394
O -3.5125 0.8227 -0.8393
O -1.1706 0.8407 0.8239
O -1.1706 -0.8405 -0.8240
Si -0.0000 0.0001 0.0000
O 1.1706 -0.8238 0.8407
O 1.1706 0.8241 -0.8406
Si 2.3374 0.0001 0.0000
O 3.5125 0.8393 0.8227
O 3.5124 -0.8394 -0.8227
O 6.1974 -0.0003 -0.0000
O -6.1974 -0.0003 0.0000

15
Ti1Si4O10 (5-1) Energy= -75401.541009197 ref[29]
Si 2.2391 -2.3713 2.0500
Ti -1.8195 0.4400 0.9986
Si 1.1143 -0.6633 0.0789
O -1.2554 1.0940 -0.6940
O 3.1280 -3.4720 2.5727
O -0.3354 -1.0223 0.8809
O -3.2900 -0.1469 1.0639
O -0.8440 0.6191 2.7327
O 1.4764 0.5017 1.2033
Si 0.4072 -0.2169 2.2638
Si -0.2580 0.8920 -1.9250
O 0.9122 -0.1983 -1.4359
O 1.2633 -1.4109 2.9806
O -0.2296 1.4921 -3.3119
O 2.0680 -1.9371 0.4671

15
Ti2Si3O10 (5-2) Energy= -90799.333800403 ref[29]
Si 1.7261 -0.0867 -0.7441
Ti 1.4256 0.9706 1.7078
Ti 0.3288 -0.7658 -2.9208
O 1.8480 2.4145 2.2177
O 0.2681 -1.8097 -4.1189
O -0.0285 0.1408 2.5860
O 0.5340 -1.3269 -0.8141

O -1.7206 -0.5019   0.6957
O   1.9894   0.0443 -2.3132
Si -1.4705 -0.4951   2.3361
Si -0.7382 -0.2125 -0.5349
O   2.6712   0.0319   0.5186
O -2.5084 -1.0346   3.2941
O   0.4312   0.9555 -0.1437
O -1.2598 -0.0866 -2.0396

15
Ti3Si2O10 (5-3) Energy= -106196.860476626 ref[29]
Si -0.3050   1.2813 -0.4243
Si -0.1249 -0.9370   0.7431
Ti   2.8080 -1.6570   0.3481
O -4.0719 -0.1886   0.0552
O   0.9657 -2.0799   0.8158
O   0.6690   0.5938   0.8310
O -1.4976 -0.9487   1.5826
O   3.9441 -2.7735   0.2039
O -1.7220   1.8704   0.0206
Ti -2.5607   0.1614   0.4318
Ti   2.3535   0.8747 -0.4063
O   3.2894   0.1615   0.8884
O   2.3164 -0.5925 -1.2514
O   0.9045   1.9754 -1.1899
O -0.8226 -0.3400 -0.7388

15
Ti4Si1O10 (5-4) Energy= -121593.786982650 ref[29]
Ti -0.9979 -0.4644   0.5976
Si   1.5033 -0.3641   1.7497
Ti -0.0954   1.5070   2.5324
O -1.5054 -3.2367 -2.6714
O   0.6681   0.7597   0.8168
O -2.1059 -1.6447 -0.1196
O -0.1216   3.0951   2.7158
O -1.6489   0.5396   1.8686
O   2.6377 -1.2096   0.9796
Ti   1.3365 -2.2736 -0.0030
Ti -1.0644 -2.8462 -1.1843
O   1.3906   0.3648   3.1629
O   0.2890 -1.5922   1.5257
O   0.4621 -3.7477 -0.2992
O   0.2865 -1.3524 -1.0673

15
Ti5O10 (5-5) Energy= -136990.603561966 ref[32]

Ti -0.2614 0.9035 -0.7682
Ti -1.3679 -1.3444 0.7874
Ti 1.2504 -1.5172 -0.0255
O -3.0721 -1.1816 0.3676
O 0.1305 -2.3751 1.1913
O 1.5238 0.2253 0.2616
O -1.2207 0.4064 1.1134
O 3.9610 1.1573 -1.3620
O -1.8740 1.5125 -1.1093
Ti -3.0187 0.7719 0.2538
Ti 2.5522 0.4046 -1.4749
O 2.4257 -1.5442 -1.3388
O 0.9369 1.3271 -1.9817
O -4.0163 1.6832 1.1131
O -0.4200 -1.0159 -0.8709

18
Si6O12 (6-0) Energy= -72006.617106618 ref[35]
O 7.8100 9.5789 7.2917
O 7.8053 7.2282 7.2919
O 10.1470 8.3990 8.4730
O 10.1511 8.3988 6.1187
O 12.4922 9.5710 7.2998
O 12.4875 7.2174 7.3000
O 14.8286 8.3898 8.4812
O 14.8328 8.3896 6.1269
O 17.1742 9.5608 7.3081
O 17.1701 7.2102 7.3083
O 5.1231 8.4090 7.2873
O 19.8567 8.3808 7.3129
Si 6.6309 8.4059 7.2899
Si 8.9833 8.4012 7.2938
Si 11.3209 8.3966 7.2979
Si 13.6589 8.3919 7.3020
Si 15.9964 8.3876 7.3062
Si 18.3489 8.3835 7.3102

18
Ti1Si5O12 (6-1) Energy= -87403.888230548
Si -0.3873 1.7911 1.6428
O -0.6533 0.1825 -2.3285
O -3.7291 -0.8842 1.9814
O -1.2079 0.7720 2.5042
O -1.1541 3.1019 1.0123
O 1.1728 2.0264 -1.5639
Si 1.1610 1.1641 -0.2453
O -1.5690 -1.3263 -0.0798

O -3.1018 1.4312 0.1881
Si -1.8747 2.3131 -0.2892
O -0.6260 1.0443 0.0116
O 1.1225 -0.4631 -0.4480
Ti -2.5430 -0.1526 1.2368
O -1.4376 2.6835 -1.7667
O 1.2466 1.7525 1.2993
Si -0.2177 1.8360 -2.6703
O 0.0194 2.2470 -4.1085
Si -0.4997 -0.5213 -0.9041

18
Ti2Si4O12 (6-2) Energy= -102802.403712957
O -0.2979 -1.0592 1.1123
Si -0.7451 -0.2701 -0.1892
O 0.9827 -3.5529 -0.3450
Si 0.6790 -1.1356 -3.1516
O 1.9753 -2.6015 2.3319
Ti -2.1632 -1.4900 -2.5430
O 0.2644 -1.2651 -1.3688
Si 0.2447 -3.0866 -1.6565
O 1.8201 -0.0156 -2.7173
Ti 1.3644 -2.1064 0.9556
O -2.1284 -0.3222 -0.9415
O 2.4791 -0.7270 -0.0221
Si 1.5726 -0.0109 -1.0790
O -1.2997 -3.1788 -2.0071
O 0.3590 0.9528 -0.5456
O -0.7155 -0.8115 -3.7858
O 1.1397 -2.7040 -3.0327
O -3.5916 -1.6518 -3.2108

18
Ti3Si3O12 (6-3) Energy= -118199.996752633
O 1.8409 3.2509 -0.0324
Ti 1.7050 -0.6426 -1.8707
O 2.8468 0.8586 -1.2045
Si 0.5099 -0.0231 0.8300
O 2.4696 -1.7749 -2.6846
Ti 0.0203 3.3879 -0.5132
O -0.4960 2.8210 -2.1475
Si -0.6721 1.1776 -1.9284
O -1.2362 3.1318 0.5872
Ti -2.1460 1.3032 0.6707
O 0.1824 0.1802 -2.8034
O 1.8372 0.8448 1.3433
Si 2.1035 1.6539 -0.0679

O -2.0587 0.8567 -1.2105
O -3.6112 1.3044 1.2865
O -0.8745 0.1281 1.5733
O 0.3524 1.3292 -0.4556
O 0.9281 -1.1934 -0.1523

18
Ti4Si2O12 (6-4) Energy= -133597.159472500
O 0.0166 0.8082 0.3193
Ti 0.9081 -0.9651 -0.2544
Si -1.6008 1.4213 0.8992
O 0.0535 -1.7644 0.9835
Ti 0.3412 3.5919 0.1586
O 0.4962 5.1753 0.0777
Si 1.5149 1.1209 1.3120
O -2.2107 1.1410 -0.6125
Ti -0.6862 1.1139 -1.5994
O 0.1825 -0.4818 -1.8713
O -1.9477 0.4177 2.0711
O 1.7937 2.6533 1.0380
O 1.0266 0.5149 2.7013
Ti -0.4708 -0.7095 2.6301
O 2.3075 -0.0185 0.4124
O -1.2322 2.9586 1.0913
O -0.7199 -1.5616 3.9528
O 0.0752 2.6375 -1.6072

18
Ti5Si1O12 (6-5) Energy= -148994.024662301
O 0.2233 0.7153 0.4487
Ti 1.1858 2.5171 0.7838
O -0.2842 0.4038 -2.2515
Si -1.2801 1.5408 1.0524
O -1.2198 3.1475 -3.0104
Ti 0.1103 -0.7399 -0.9927
O -1.9962 -2.4445 2.6854
Ti 1.7611 -0.2934 1.2661
O -1.8962 2.0600 -0.3209
Ti -0.6836 2.2413 -1.8113
O 2.4797 1.4036 1.4298
O 0.7051 -1.0864 2.3691
Ti -1.2110 -1.3152 1.8783
O -0.3381 2.7089 1.7492
O 0.9481 2.9354 -0.8588
O -1.0976 -1.5644 -0.0603
O 1.8120 -1.1003 -0.3291
O -1.9611 0.4575 1.9837

18
Ti6O12 (6-6) Energy= -164390.818506874 ref[32]
O -1.7827 -2.7812 0.4670
O -1.2613 2.1392 1.0643
O 2.0854 -0.2503 1.4911
Ti 1.1682 -0.3983 -0.1170
Ti -2.2432 -1.0932 0.5227
Ti -1.1899 1.6083 -0.8463
O -0.1497 0.4234 3.5415
Ti 0.0534 -3.2852 0.7229
O 0.9362 -2.0680 -0.5265
O -2.7992 -0.1522 2.0242
O 0.5864 0.9240 -1.1057
Ti -1.3984 0.9299 2.2907
Ti 0.8498 -0.8342 2.6473
O 0.3918 -4.8342 0.5323
O 0.5517 -2.5287 2.4882
O -1.6700 2.7296 -1.8770
O -2.2201 -0.0530 -0.8654
O -0.4274 -0.4139 1.1504

21
Si7O14 (7-0) Energy= -84008.482129892 ref[35]
O 5.0234 -1.3214 1.2273
Si 3.6854 -0.9809 0.6189
O -4.6005 -1.3215 1.2274
Si -3.2626 -0.9810 0.6190
O 0.2113 4.9247 -1.1605
Si 0.2113 3.4686 -0.7642
O 0.2114 -2.1792 -1.9815
O -1.1371 2.5599 -0.5286
Si -1.1749 1.0085 -0.0168
O 2.8153 -2.0157 -0.3368
O 2.8856 0.4398 0.8230
O 0.2114 -1.6757 0.2998
O 1.5598 2.5600 -0.5286
O -1.1595 0.0061 -1.3094
O 0.2114 0.8860 0.8475
Si 1.3542 -1.5725 -0.9037
Si -0.9313 -1.5726 -0.9037
Si 1.5977 1.0086 -0.0168
O 1.5823 0.0061 -1.3094
O -2.3924 -2.0158 -0.3368
O -2.4628 0.4396 0.8230

21

Ti1Si6O14 (7-1) Energy= -99406.641652290
Si 0.4449 -0.0985 -3.5960
Si 0.0611 -0.2318 -1.1874
Si -0.7890 2.3680 -3.7255
Si -2.5094 0.0054 -2.9029
O -0.7667 -0.8120 0.0228
O -0.9309 -0.5571 -2.6034
O -0.0790 -0.4595 -5.0518
O -1.3310 2.0425 -5.1832
Si -1.2272 2.3426 -1.3225
Si -1.5283 0.3502 -5.6741
Ti -2.5445 0.1469 0.1368
O -3.4338 -0.2324 1.3891
O 0.0836 1.4010 -1.0263
O -0.7402 3.4814 -2.4697
O 1.3109 -0.6178 -2.2546
O 0.6046 1.5279 -3.5737
O -2.6694 -0.1574 -4.4718
O -2.0233 1.6261 -2.7181
O -3.3346 -0.3397 -1.6073
O -2.2383 2.1285 -0.1315
O -1.8469 0.1140 -7.1360

21
Ti2Si5O14 (7-2) Energy= -114805.175817704
Si -0.7099 -0.6906 -2.1963
Si 1.9894 -0.3767 -0.7198
Si -0.1318 0.6369 1.2900
Si -0.1991 1.8040 -0.8559
O 0.5979 -1.2723 -1.1627
O 0.1085 -2.8023 0.9650
O -1.5792 -1.9102 -1.4407
O 0.5509 2.5307 -2.0375
Si -0.6421 -1.8577 -0.0504
Ti 1.4794 -1.7245 1.9827
Ti 1.3120 1.1435 -3.2916
O 2.6203 -1.1596 0.4969
O 2.2365 -2.5008 3.1392
O -1.2230 0.7125 -1.5232
O -1.1504 -0.5437 0.7864
O 1.0341 0.8593 -0.0172
O -0.0355 -0.3328 -3.5761
O 0.6943 0.0611 2.5036
O -0.7637 2.0746 0.7004
O 2.5386 0.2350 -2.0673
O 1.9905 1.7111 -4.6072

21
Ti3Si4O14 (7-3) Energy= -130202.681514043
Si -1.3746 -2.1713 0.3439
Si -0.7263 0.6758 1.3859
Si -1.2529 0.0884 -1.2527
Si 1.5687 0.4916 -0.1237
O 2.2479 -0.8083 0.5990
O 0.6166 -2.2373 2.8662
O -1.1626 0.9355 -2.6025
O -1.9320 -1.9237 4.5494
Ti 0.8090 1.1739 -2.6659
Ti -1.3189 -1.5360 3.1371
Ti 1.1331 -2.1721 1.2476
O 0.7399 1.3183 1.0588
O -0.0552 -3.1415 0.1960
O 1.4426 0.6027 -4.0048
O -1.9112 -1.4176 -1.0164
O -0.3636 -0.9447 0.9972
O 2.1645 1.4502 -1.2629
O -2.2751 -2.4198 1.6314
O -1.6727 0.9811 0.0798
O -1.3108 0.4403 2.8379
O 0.4213 -0.1992 -1.1893

21
Ti4Si3O14 (7-4) Energy= -145599.557832541
Ti 2.1569 -1.6158 -0.5474
Ti 2.3123 1.1202 1.1396
Ti -1.6047 0.3184 2.3374
Ti -2.5368 2.1565 -0.1339
O 0.6659 -0.8129 -1.4653
O 1.5732 -0.0441 2.2467
O 0.6859 1.3916 0.0322
O 3.0103 -2.6642 -1.3905
Si 0.1214 2.6023 1.1536
Si -0.2829 0.1937 -0.6959
Si 0.4741 -1.2562 1.8944
O -1.0847 3.3523 0.4482
O -0.5547 1.7391 2.4183
O -3.7871 2.8773 -0.8087
O -1.5782 0.9143 -1.2513
O -0.6586 -1.2306 3.0528
O -2.9140 0.8973 1.3888
O -0.6699 -0.5240 0.8005
O 3.0745 0.0896 -0.0033
O 1.2770 -2.3389 1.0591
O 1.6611 2.9126 1.5516

21
Ti5Si2O14 (7-5) Energy= -160996.597546154
Ti 0.2321 0.6208 -1.5166
Ti 1.1731 -2.5259 2.1929
Ti -2.2063 0.5426 -3.0365
Ti -2.2519 -1.5624 -1.0917
O 0.6962 1.4526 0.0718
O -0.2346 -1.0708 0.5042
O 1.1410 -0.9702 -1.6310
O -2.7593 -1.6838 0.7303
Si 0.5374 -2.1134 -0.6337
Si -1.4858 -1.4163 1.6942
Ti 0.3756 0.4935 1.6013
O -1.5711 0.1771 -1.2013
O -0.8253 -2.6785 -1.3494
O -3.2544 1.7383 -3.0698
O 2.0135 -3.4170 3.2087
O -0.7572 -2.5603 2.5298
O 1.4426 -3.0091 0.3048
O -3.0453 -1.2035 -2.6035
O 1.5494 -0.5359 2.2947
O -1.2885 0.0986 2.3043
O -0.3363 1.1683 -3.0823

21
Ti6Si1O14 (7-6) Energy= -176393.139316446
Ti 0.5005 4.1223 -1.0589
Ti 2.8374 2.2042 -2.1237
Ti -2.8591 0.1360 -1.4238
Ti -1.0067 0.7717 1.1138
O 0.5737 0.8704 2.0967
O -1.2285 4.8069 -0.9368
O -4.0087 -0.8200 -1.9819
O -0.5297 2.6167 -1.7230
Ti -2.1070 3.1754 -0.7384
Si 0.0165 1.0264 -1.9758
Ti 1.6009 1.7186 0.7934
O -2.1401 -0.3145 0.3691
O 0.3055 0.7919 -0.3168
O 4.1781 2.1520 -2.9878
O -1.2142 0.1281 -2.4109
O -3.2372 2.0823 -1.4776
O -1.7081 2.4170 0.8531
O 2.9720 1.5416 -0.2589
O 1.4076 1.0799 -2.7329
O 1.0250 3.4095 0.5171

O 1.8748 3.9384 -2.1059

21
Ti7O14 (7-7) Energy= -191790.263288290 ref[32]
Ti -0.3603 -3.7893 -0.6633
Ti 0.0695 -1.7639 1.3242
Ti -0.1107 3.2346 0.3723
Ti 1.7772 0.7785 0.8687
O -1.3776 -0.7202 1.7023
O 1.2869 2.3325 1.4503
O -0.1988 4.8012 0.6487
O 1.5748 -0.8004 1.7830
Ti -1.7152 0.5571 0.4566
Ti -0.9467 -1.2557 -1.8774
Ti 0.9400 1.1972 -1.7696
O -2.2545 -0.2814 -1.0610
O -1.7712 2.2718 0.7465
O -1.3710 -2.9438 -2.1204
O 0.8070 -4.7414 -1.1850
O 0.3485 2.8017 -1.5069
O 2.4693 0.9074 -0.8157
O 0.1135 0.6010 -0.1168
O 0.1171 -0.0714 -2.8105
O 0.2217 -1.8945 -0.5472
O -0.2929 -3.4830 1.2761

24
Si8O16 (8-0) Energy= -96011.405525393 ref[35]
Si 9.3972 9.3972 4.0000
Si 6.6028 9.3972 4.0000
Si 9.3972 6.6028 4.0000
Si 6.6028 6.6028 4.0000
Si 11.4348 8.0000 2.4090
Si 4.5652 8.0000 2.4090
Si 8.0000 11.4348 5.5910
Si 8.0000 4.5652 5.5910
O 9.4496 8.0000 4.8513
O 6.5504 8.0000 4.8513
O 8.0000 9.4496 3.1487
O 8.0000 6.5504 3.1487
O 10.6690 9.3280 2.9846
O 10.6690 6.6720 2.9846
O 12.6327 8.0000 1.4928
O 5.3310 9.3280 2.9846
O 5.3310 6.6720 2.9846
O 3.3673 8.0000 1.4928
O 9.3280 10.6690 5.0154

O 6.6720 10.6690 5.0154
O 8.0000 12.6327 6.5072
O 9.3280 5.3310 5.0154
O 6.6720 5.3310 5.0154
O 8.0000 3.3673 6.5072

24
Ti1Si7O16 (8-1) Energy= -111409.275561272
O 0.3344 1.4509 -1.5125
Si -0.2526 0.4670 -0.4259
O 1.9618 4.0025 -1.4350
Si 0.8273 -2.2850 3.6433
O -0.1512 1.3726 3.0943
Si 1.1724 -4.2324 2.3883
O -0.1537 -3.5164 3.3783
Si 0.9293 0.1461 3.2325
O 1.4347 -5.7223 2.3213
Si 2.5329 0.5348 1.0618
O 0.8644 -0.8725 4.5247
O 2.4278 0.5594 2.7211
O 0.8622 0.8403 0.8632
Si -0.3061 1.9296 1.5442
O 0.4607 -1.1909 2.2513
Si 1.0035 -1.7918 0.7066
O 0.9716 -3.3584 0.8978
Ti 1.5217 2.7731 -0.5446
O -1.4083 1.1332 0.5861
O 2.1812 -3.0255 3.1957
O -0.0633 -1.1508 -0.3928
O 3.0948 1.7398 0.2192
O 2.4587 -1.0186 0.5420
O 0.2773 3.2847 0.9947

24
Ti2Si6O16 (8-2) Energy= -126807.321703247
O 0.4989 1.6021 -0.2032
Si 1.7874 0.3562 -0.4200
O 0.4440 -0.5367 -4.4701
Ti -2.5527 2.6806 1.3771
O 2.3204 -0.2906 2.8729
Si 0.4092 -0.0409 -3.0472
O -2.5762 0.9126 2.3330
Si -1.1418 1.0761 -0.7431
O -3.7361 3.7075 1.6488
O 3.1654 0.8928 0.1130
Si 0.9697 -0.5976 2.1263
O -0.8648 0.5954 -2.2629

Ti 3.3070 1.2408 2.0232
O -1.4131 -0.2066 0.2337
Si -1.3954 -0.0164 1.8654
O   4.7451 1.6238 2.5836
O   0.0702 0.9164 2.1559
Si 0.5137 2.3946 1.4289
O -0.5076 -1.2821 2.4956
O -2.1970 2.2108 -0.4785
O   1.9871 2.6686 1.8942
O   1.6409 -0.0204 -1.9865
O   1.2332 -0.8570 0.5256
O -0.7305 3.3363 1.5947

24
Ti3Si5O16 (8-3) Energy= -142204.940486433
O -0.0540 -1.3307 -0.3394
Ti -3.9260 -0.5936 -0.2301
O   1.2599 -0.3791 1.8497
O -2.0122 0.0189 0.6351
Si 0.8966 -1.7811 1.1263
O   1.7632 -0.7427 -2.0446
O -0.9142 0.5399 -1.8279
Ti 3.1560 -1.4011 -0.7608
O   1.0618 1.0981 -0.3186
O   1.0607 4.1842 -0.3990
Si -1.9132 1.2036 -0.6503
O   2.1231 -2.5480 0.5117
O -3.4430 1.0165 -1.1111
Si 0.5183 -0.0609 -1.3624
O -1.2967 2.5284 -0.0347
O -0.5803 -2.2751 1.7106
Si -1.5041 -1.5613 0.5464
O   3.4095 0.1262 0.3949
O   1.8726 2.2466 1.6509
Si 2.1093 0.7944 1.0297
O -2.8164 -2.2135 -0.0507
O   4.4759 -2.0371 -1.3815
Ti 0.5187 2.9552 0.4455
O -5.1876 -0.5004 0.7294

24
Ti4Si4O16 (8-4) Energy= -157602.226712390
O -0.4111 -1.0571 0.1163
Ti 0.6510 -2.6679 0.1539
O   2.1629 -1.8870 0.1318
Ti 3.0845 -0.0912 0.0856
O   2.4322 0.8282 -1.5085

Si 0.8740 1.1251 -1.5662
O 0.1637 2.6038 -1.6725
Ti -0.6509 2.6738 0.0245
O 0.1700 2.6872 1.7197
Si 0.8801 1.2050 1.6837
O 2.4380 0.9056 1.6348
Si -0.8799 -1.1991 -1.5053
O -0.1699 -2.6813 -1.5413
Si -0.8739 -1.1191 1.7446
O -2.4320 -0.8223 1.6869
Ti -3.0843 0.0971 0.0928
O -2.1627 1.8929 0.0466
O 4.6671 -0.2433 0.0863
O 0.4112 1.0630 0.0621
O -2.4379 -0.8997 -1.4564
O -4.6670 0.2493 0.0921
O -0.0045 -0.0556 -2.2864
O 0.0046 0.0615 2.4648
O -0.1636 -2.5978 1.8509

24
Ti5Si3O16 (8-5) Energy= -172999.204771836
O 0.3859 1.0830 -0.0165
Ti -3.0983 0.1328 0.1299
O 0.0477 0.0934 2.3857
O 0.1646 2.7196 1.6525
Ti 0.7597 -2.6364 0.1628
O -0.3739 -1.0911 0.0361
O -2.3771 -0.8107 1.6577
Ti 3.1333 0.0037 0.0080
O 2.4585 0.9608 -1.5542
O 4.7211 -0.1127 0.0104
Ti -0.8891 -1.3202 -1.7387
O 0.0536 0.0849 -2.4362
O -4.6774 0.3000 0.2270
Si 0.8961 1.2288 -1.6328
O 0.1674 2.7074 -1.6918
O -0.0085 -2.9412 -1.4708
Si 0.8942 1.2459 1.5956
O 2.2497 -1.7904 0.0770
O 2.4577 0.9961 1.5453
Si -0.8164 -1.1111 1.6875
O -0.1005 -2.5702 1.8540
O -2.5458 -0.9328 -1.4252
Ti -0.6741 2.7042 -0.0198
O -2.1903 1.9146 -0.0009

24
Ti6Si2O16 (8-6) Energy= -188396.152534902
O -0.3812 -1.0990 0.0562
Ti 3.1450 -0.1395 0.1424
O 0.0042 0.0606 2.4073
O -0.1863 -2.5989 1.8807
Ti -0.6903 2.6977 0.0806
O 0.3811 1.1018 0.0003
O 2.4324 0.9015 1.6092
Ti -3.1446 0.1482 0.1462
O -2.5919 -0.9481 -1.3916
O -4.7244 0.3269 0.2431
Ti 0.9426 1.2985 -1.7746
O -0.0046 -0.0621 -2.5250
O 4.7251 -0.3132 0.2423
Ti -0.9491 -1.3837 -1.7048
O -0.0974 -3.0200 -1.3986
O 0.0920 2.9481 -1.5473
Si -0.8697 -1.1241 1.6969
O -2.2176 1.8997 0.0403
O -2.4267 -0.8184 1.6604
Si 0.8756 1.2087 1.6360
O 0.1926 2.6908 1.7485
O 2.5866 0.8789 -1.4461
Ti 0.6906 -2.6889 0.2121
O 2.2177 -1.8939 0.1269

24
Ti7Si1O16 (8-7) Energy= -203792.982879852
O -0.2527 -1.7701 4.8331
Ti 1.0387 2.7118 -0.9579
O 1.4742 -4.0121 5.9312
O -0.0997 1.5019 -1.9940
Ti 0.8869 -2.2034 -0.2063
O 2.2713 1.2142 -1.2854
O 1.1765 -1.7785 -1.8775
Ti -0.7455 -3.5737 1.9940
O 0.6531 2.3508 0.9250
O 0.2986 -1.9208 2.2345
Ti 1.0414 -3.2569 4.5971
O 2.4820 -2.4189 3.6319
O -2.0707 -2.5273 2.6786
Ti -1.0807 -1.1934 3.4408
O 2.0320 -0.0138 2.3010
O 2.3890 -2.2353 0.8483
Si 2.0290 -1.6408 2.3263
O 1.3923 4.1590 -1.5474

O 0.3437 -0.3754 0.0225
Ti 0.9965 0.1634 -1.7609
O -0.2706 -3.5578 0.2278
O 0.1294 -4.3807 3.2377
Ti 0.5217 0.7544 1.5721
O -0.8460 0.4781 2.7507

24
Ti8O16 (8-8) Energy= -219189.847544426 ref[32]
O 0.4191 1.1514 0.1443
Ti -3.1923 0.2489 0.0091
O -0.0181 -0.1853 2.6228
O 0.1511 2.8389 1.9037
Ti 0.7009 -2.6741 -0.1656
O -0.3676 -1.0974 -0.0538
O -2.6280 -0.9620 1.4324
Ti 3.2438 -0.1949 0.0814
O 2.6795 1.0161 -1.3419
O 4.8178 -0.4513 0.0871
Ti -0.9175 -1.1273 -1.8621
O 0.0696 0.2393 -2.5322
O -4.7664 0.5053 0.0035
Ti 1.0296 1.4755 -1.6151
O 0.2056 3.1048 -1.3233
O -0.0996 -2.7848 -1.8132
Ti 0.9689 1.1814 1.9526
O 2.2472 -1.8789 -0.0742
O 2.6283 0.7681 1.6640
Ti -0.9781 -1.4214 1.7056
O -0.1542 -3.0507 1.4138
O -2.5769 -0.7141 -1.5734
Ti -0.6494 2.7282 0.2561
O -2.1958 1.9330 0.1648

27
Si9O18 (9-0) Energy= -108013.525407219 ref[35]
O 4.1908 -0.0001 3.8083
Si -0.6509 1.4016 -0.5717
O -2.1884 1.3406 -0.0459
O -0.2412 -2.6713 -1.5070
Si 1.2017 3.4393 -1.5996
O 1.5057 4.6443 -2.4541
O 2.8431 1.3280 1.7435
Si 1.9841 -1.3974 0.3613
O 1.5055 -4.6443 -2.4541
O -0.4179 0.0000 -1.3853
Si -0.6509 -1.4016 -0.5717

O -0.2411 2.6713 -1.5070
O 2.2621 2.6690 -0.6183
Si 3.3695 -0.0000 2.5435
O -3.8800 0.0001 1.6722
O 2.8431 -1.3280 1.7435
Si -3.0853 0.0001 0.2115
O 0.3834 -1.4536 0.6964
O 2.3174 -0.0000 -0.4236
Si 1.2016 -3.4393 -1.5996
O -2.1884 -1.3405 -0.0459
O 0.3835 1.4536 0.6964
Si 1.9842 1.3973 0.3613
O 2.2620 -2.6691 -0.6183
Si -5.3395 0.0001 0.8767
O -6.7854 0.0001 1.3049
O -4.5462 0.0001 -0.5840

27
Ti1Si8O18 (9-1) Energy= -123411.426455410
Si 0.9792 1.9752 -2.1684
Si -0.7033 2.1721 -4.6164
Si -0.2311 -1.6968 -1.3067
O 0.6279 0.7985 0.5972
Si -2.0929 0.9640 -0.5300
Si -1.2588 2.9675 -1.9285
Si 1.7770 0.0853 -0.3705
O 0.2838 3.3432 -1.5393
O 0.7931 1.9129 -3.7431
O 0.2360 -2.9297 -0.4375
O -1.5256 0.6860 -4.2897
O -1.5836 3.1526 -3.4587
O 2.5408 -0.9926 0.5107
O -2.3116 2.6362 -0.7576
O 1.9266 -3.5559 2.0241
Si -0.6057 -0.1155 1.1738
Si -1.6839 0.0133 -2.8754
Ti 1.2849 -2.3815 1.1697
O -0.0972 -1.2780 2.1031
O -1.9294 0.9112 1.1151
O -1.2277 -0.7660 -0.2780
O 1.0459 -0.7305 -1.6083
O 2.2169 1.4119 -1.3056
O -2.9255 0.3226 -1.8201
O -0.6103 2.6563 -6.0473
O -1.1360 -1.5056 -2.6782
O -0.6995 1.1700 -1.8388

27
Ti2Si7O18 (9-2) Energy= -138809.706838764
Si 0.7819 0.6178 -1.1343
Si -1.0442 1.3887 2.6944
Si -0.9207 -1.6316 2.1088
O -2.5340 -1.2064 1.9441
Si -0.4240 -1.9002 -0.5895
Si 1.1305 1.1173 1.5662
Si -2.0532 0.4908 -1.4523
O -2.0262 0.0545 -2.9589
O -0.3895 0.0239 1.6886
O -2.4920 1.3700 1.9604
O 0.1038 2.3386 2.0211
O -3.3010 0.8332 -0.3899
O 1.4420 -0.5395 5.6132
O -1.8065 -0.8746 -0.4135
O -0.2358 -1.8758 3.5002
Si -2.5931 0.0816 0.9171
Ti 0.7500 -0.3188 4.2019
Ti -0.3353 -0.9053 -3.4078
O -0.7569 0.9648 4.1812
O -0.5379 -2.6363 0.8710
O 0.8145 -0.8728 -0.4199
O -0.7279 1.3302 -0.9777
O 1.9138 0.4590 2.7695
O -0.4942 -2.3965 -2.0868
O -0.1593 -1.3220 -4.9313
O 1.6597 1.3831 0.0544
O 1.0027 0.3557 -2.6898

27
Ti3Si6O18 (9-3) Energy= -154207.489899632
Si -3.4365 1.3741 0.9080
Si -2.3244 -0.5626 2.6550
Si 0.6312 0.9593 -0.8509
O -3.1538 0.3052 -0.3422
Si -3.3144 -1.3108 -0.0416
Si 0.3763 -0.4122 2.0438
Si -0.9659 2.4160 0.4130
O -0.7707 -0.6584 3.1812
O 0.1214 3.0245 1.3751
O -4.7388 -1.7028 0.5017
O -4.9337 1.1885 1.4017
O -2.5566 2.7034 0.4220
O -2.1519 -1.4322 1.2047
O -0.3525 0.5327 0.6457
O -3.7059 -1.0192 3.2757

Ti -0.7070 -1.3582 -0.2888
Ti -5.2558 -0.6354 2.0916
Ti 1.8975 2.1363 1.5069
O -2.4390 0.9914 2.1695
O -0.4276 2.1778 -1.1282
O -6.7019 -0.9240 2.6900
O -2.2364 -2.0248 -1.0715
O 3.1145 3.0276 2.0058
O 0.4700 -1.7357 1.0632
O 2.0396 1.4123 -0.3252
O 1.6125 0.4624 2.4633
O 0.2707 -0.4500 -1.5589

27
Ti4Si5O18 (9-4) Energy= -169605.361160460
Si -1.3082 0.5911 0.4273
Si 1.1565 -3.3660 -0.6499
Si 0.0689 -1.8281 1.3975
O 1.4685 -1.0086 0.9454
Ti -0.4492 -3.7614 -3.1529
Si 1.1052 -1.2984 -3.0882
Si 1.5281 0.7022 0.9589
O 2.8576 0.6079 -0.0126
O -1.0614 -1.1313 0.3798
O -1.6673 1.0323 1.9018
O -0.0871 -0.2079 -3.0424
O 0.8629 -2.5703 -3.9873
O 0.2310 1.0930 0.0196
O 2.5729 -0.7651 -2.6031
O 0.6245 -4.4444 -1.6640
Ti 2.5862 -1.0522 -0.7975
Ti -0.3536 0.5161 3.2602
Ti -1.1867 -0.9065 -1.7245
O -1.0622 -4.8663 -4.1154
O 2.7197 -2.8707 -0.4860
O -1.7186 -2.4037 -2.3784
O 0.7386 -1.8183 -1.4078
O 0.3750 -3.3108 0.7916
O -0.6571 0.9531 4.7617
O -2.1483 0.5274 -0.9605
O 1.3237 1.1787 2.4515
O -0.2477 -1.4211 2.8858

27
Ti5Si4O18 (9-5) Energy= -185002.349763347
Si -3.0076 2.9271 1.8696
Si -2.8242 1.7204 -0.8019

Si -0.3138 2.6637 -1.5378
O 3.0658 0.0233 -2.4235
Si -2.7039 0.0697 1.6351
Ti 1.6308 2.2623 1.2339
Ti -0.2157 0.0907 0.8170
O -0.4690 4.2049 -1.0137
O -2.3265 1.5103 2.3841
O -4.3860 1.5163 -0.8768
O -1.4218 -0.9003 1.8714
O -4.5880 2.8321 1.8971
O 0.7410 -0.4655 -0.4987
O -2.5267 2.9980 0.2363
O -0.0483 2.0911 0.1356
Ti 1.9842 0.7290 -1.4954
Ti -5.3041 1.3155 0.8622
Ti -0.7214 3.9534 0.8156
O -1.9524 4.1384 2.2116
O -2.1456 0.4394 0.0341
O -4.2655 -0.1704 1.6104
O -6.8890 1.1454 0.8341
O 0.8666 3.9423 1.5920
O 2.7012 1.8437 -0.0359
O 0.9015 2.0803 -2.3581
O 1.0084 0.8101 2.0178
O -1.7615 2.0403 -1.9960

27
Ti6Si3O18 (9-6) Energy= -200399.243113905
Si 0.5736 -0.1252 1.4324
Si -1.8680 0.9301 0.1858
Si -0.7733 -1.5858 -0.7089
O 3.8492 2.0908 -0.1716
Ti 3.0065 3.6118 -1.0688
Ti -0.0226 2.4162 -0.9066
Ti 1.5773 -0.9291 -1.9026
O 0.6662 -1.1162 0.0817
O 1.5211 1.0015 -1.2532
O -1.6627 -2.4143 0.3064
O -2.7898 0.2466 1.2706
O -0.3090 -0.8473 2.5245
O 0.0455 2.3753 -2.7592
O 2.8779 2.8304 -2.8540
O 3.1763 -0.9009 -1.0310
Ti -2.0919 -1.4518 1.9649
Ti 1.6248 1.6803 -3.1386
Ti 3.0129 0.6011 0.0104
O 1.7916 -0.1392 -3.4868

O -1.8543 2.4052 -0.4990
O 3.7776 5.0007 -0.9853
O -1.4855 -0.1270 -1.0437
O -2.9776 -2.2206 3.0473
O 0.0759 -2.0291 -2.0370
O -0.2700 1.1846 0.8114
O 2.1072 0.3993 1.5825
O 1.1242 3.6288 -0.4696

27
Ti7Si2O18 (9-7) Energy= -215795.912587809
Si -0.6698 -2.4406 2.2127
Si -2.6324 -0.4321 3.1489
Ti -1.8283 -2.6590 5.0025
O -1.3080 0.4295 3.6865
Ti -2.0577 0.3871 0.7126
Ti -0.8650 -0.0260 -2.2977
Ti 0.2157 -0.3167 4.3103
O -3.3848 0.5014 2.0535
O -0.2871 -1.5006 5.4651
O 0.0299 -0.0118 0.5798
O 1.7516 1.7789 1.0416
O -0.1128 -2.9085 0.7606
O 1.7603 0.5267 3.6291
O 0.4107 -1.4183 -1.8097
O 2.3493 -1.0800 0.7033
Ti 0.8508 -1.6596 -0.1599
Ti 0.2737 1.8586 -0.0555
Ti 1.6729 0.1770 1.8607
O -1.3524 2.0884 0.6283
O -2.3459 -3.6837 6.1115
O -2.2963 -0.0787 -0.9298
O 0.1909 1.5182 -1.7476
O -3.1463 -1.3975 4.2946
O -1.3522 -0.0149 -3.8136
O 0.5013 -1.3955 2.7881
O -1.1374 -3.4270 3.3577
O -1.9091 -1.3598 1.8850

27
Ti8Si1O18 (9-8) Energy= -231192.529489798
Si -0.6428 0.4514 -1.9398
Ti 1.1719 -2.0375 -1.2877
Ti -0.4962 0.0780 2.9089
O 1.0810 -2.3137 -3.0054
Ti -0.5726 -1.8314 -3.9511
Ti -1.3529 2.2577 0.2619

Ti -2.0406 -2.2437 -1.1244
O -2.9923 1.5173 0.6274
O -0.6612 0.0370 -3.4676
O 2.3793 -1.5111 -0.0108
O -2.0465 -2.5324 -2.8358
O 0.8716 -0.9044 2.3466
O -2.2312 -0.5009 2.6388
O -3.2225 -1.8216 0.2652
O -0.4438 3.3772 1.2052
Ti 1.0532 2.7372 2.2889
Ti 1.4158 -0.1298 0.7547
Ti -2.5702 -0.2412 0.8910
O 0.7038 -0.1762 -1.1751
O -0.7864 1.9945 -1.4554
O -0.3722 -2.6498 -0.5349
O -0.6431 0.5997 1.0147
O 0.0414 1.6071 3.5150
O -0.6324 -2.1611 -5.5127
O -1.8373 -0.3718 -1.1074
O 2.0301 1.4343 1.1790
O 1.9495 3.8592 2.9801

27
Ti9O18 (9-9) Energy= -246589.333919454 ref[32]
Ti 1.9572 -2.0305 -0.9979
Ti -1.6088 -1.3444 1.2468
Ti -0.4367 0.7673 2.7448
O 2.4412 -0.9903 -2.4970
Ti 1.5623 0.5534 -2.6268
Ti -0.8285 3.3216 0.5399
Ti 2.2014 2.5033 -0.6617
O 1.3652 0.4753 2.8782
O 2.5627 -1.2922 0.6101
O 2.4582 2.1437 -2.4527
O -1.7598 -0.4867 2.8778
O -0.8067 2.3832 2.2458
O -1.3787 1.9300 -0.6545
O -1.7391 4.6336 0.5254
O 1.6393 -3.7377 -0.8538
Ti 1.9017 0.2539 1.1415
Ti -0.2777 -3.5816 -0.5354
Ti -0.8411 0.3258 -0.9799
O -1.2233 -4.3099 -1.6000
O -0.1561 -0.0489 1.0189
O 0.1920 -1.7118 -0.9794
O -2.2418 -0.6936 -0.2924
O 1.2177 0.8345 -0.7379

O 0.9821 3.6005 -0.1409
O -1.1198 -3.0138 1.1198
O -0.2005 0.4187 -2.7618
O 2.9913 1.6747 0.7509

30
Si10O20 (10-0) Energy= -120016.058082410 ref[35]
O -1.3833 2.4708 2.4563
O 1.3833 -2.4708 2.4563
Si -1.4423 4.0020 1.8495
Si 1.4423 -4.0020 1.8495
O 0.0000 0.0000 2.5846
O -0.3437 -1.8322 0.6780
O 0.3437 1.8322 0.6780
Si -0.7451 1.1687 1.7099
Si 0.7451 -1.1687 1.7099
O 3.3788 2.9401 -2.9274
O -3.3788 -2.9401 -2.9274
Si 2.3389 2.2578 -2.0722
Si -2.3389 -2.2578 -2.0722
O 2.4490 0.6986 -1.5965
O -2.4490 -0.6986 -1.5965
O 0.9914 3.0048 -1.5295
O -0.9914 -3.0048 -1.5295
Si 1.5106 -0.4050 -0.8658
Si -1.5106 0.4050 -0.8658
O 1.5078 -1.9993 -1.2800
O -1.5078 1.9993 -1.2800
O -1.8411 0.4361 0.7399
O 1.8411 -0.4361 0.7399
O 0.8769 -4.0389 0.3091
O -0.8769 4.0389 0.3091
Si 0.2619 -2.7723 -0.5268
Si -0.2619 2.7723 -0.5268
O 1.9585 -5.1968 2.6129
O -1.9585 5.1968 2.6129
O -0.0000 -0.0000 -1.2959

30
Ti1Si9O20 (10-1) Energy= -135414.670960728
O 3.1369 -1.5368 -1.2442
Si 1.5883 -1.5941 -0.9908
O 0.3700 -1.2553 -1.9889
Si -0.6412 -0.0186 -1.3940
O -0.9014 -1.1573 0.0939
Si -2.2981 -1.3426 1.0660
O -1.4312 -2.5769 1.8151

Si 0.0141 -2.1069 1.1497
O 0.9388 -1.2693 2.1964
Si 1.7977 0.0239 1.6613
O 1.4170 0.0016 -0.0432
Si 1.5838 1.5730 -1.0313
O 1.0727 2.7478 0.0292
Si 0.0080 2.1357 1.0954
O -0.9048 1.1571 0.0641
Si -2.3020 1.3632 1.0312
O -1.4387 2.6187 1.7484
Ti 4.0182 0.0013 -0.3557
O 5.5967 0.0017 -0.4941
O 3.3690 0.0248 1.5501
O 3.1325 1.5136 -1.2833
O 1.0805 -2.7429 0.0994
O 0.9350 1.3279 2.1632
Si -3.7018 -0.0192 -1.0847
O -3.5171 1.3362 0.0222
O -2.1682 -0.0267 -1.8496
O -3.5131 -1.3451 0.0567
O -4.9511 -0.0321 -1.9429
O -2.3173 0.0224 1.9889
O 0.3665 1.2053 -2.0204

30
Ti2Si8O20 (10-2) Energy= -150812.915391096
O 3.2764 -1.7746 -0.6839
Si 1.7271 -1.6543 -0.4504
O 0.5560 -1.3478 -1.5093
Si -0.3591 0.0402 -1.1355
O -0.7684 -0.8730 0.5217
Si -2.1541 -0.8172 1.5535
O -1.3488 -1.9908 2.4564
Si 0.0959 -1.7319 1.7030
O 1.1070 -0.8685 2.6464
Si 2.0811 0.2591 1.9679
O 1.6925 0.0538 0.2776
Si 2.0118 1.4589 -0.8942
O 1.5957 2.7981 -0.0068
Si 0.4750 2.4187 1.1111
O -0.5577 1.4340 0.1922
Si -1.9047 1.9131 1.1638
O -0.8813 3.1285 1.7260
Ti 4.2955 -0.2230 0.0056
O 5.8689 -0.3837 -0.1123
O 3.6470 0.1034 1.8781
O 3.5514 1.2324 -1.1125

O 1.1023 -2.5991 0.7624
O 1.3396 1.6846 2.2822
Ti -3.5157 0.3755 -0.8005
O -3.1754 2.0268 0.2450
O -1.8337 0.0924 -1.7114
O -4.8245 0.3653 -1.7079
O -2.0254 0.6745 2.2477
O -3.4475 -0.9540 0.6704
O 0.7785 1.0844 -1.8560

30
Ti3Si7O20 (10-3) Energy= -166210.966283184
Ti 4.0913 0.0024 -0.2810
Ti -3.8964 -0.0183 -1.0092
Si 1.6812 -1.6462 -1.0064
Si 0.0011 -2.1249 1.1091
Si 1.7564 0.0231 1.6024
Si -2.3059 -1.3866 1.1095
Si -2.3101 1.4084 1.0737
O 3.2456 -1.5590 -1.1371
O -2.2309 -0.0298 -2.0898
O -3.6174 -1.5101 0.2406
O 0.9109 1.3227 2.1135
O -2.2822 0.0221 1.9701
O 3.3298 0.0248 1.5508
O 0.5664 1.3520 -2.1670
O -5.2772 -0.0306 -1.7977
O -3.6220 1.5058 0.2021
O 1.0961 -2.7590 0.0853
O 0.9150 -1.2657 2.1467
O -1.4003 -2.5986 1.8553
O 3.2412 1.5389 -1.1768
Si -0.0052 2.1525 1.0543
Ti -0.5979 -0.0209 -1.5763
O 5.6787 0.0040 -0.3351
O 1.3795 0.0005 -0.1226
O -1.4079 2.6414 1.7882
O -0.9696 1.2297 0.0196
O 1.0882 2.7634 0.0147
Si 1.6766 1.6247 -1.0481
O 0.5702 -1.4054 -2.1318
O -0.9657 -1.2312 0.0513

30
Ti4Si6O20 (10-4) Energy= -181608.047666486
O 3.1771 -1.6354 -1.0432
Si 1.6460 -1.6315 -0.6867

O 0.3883 -1.4071 -1.6503
Ti -0.6168 0.0651 -1.0159
O -0.8108 -1.0267 0.7195
Si -2.0265 -1.1752 1.9131
O -1.0355 -2.3695 2.5830
Si 0.2651 -1.9210 1.6659
O 1.3206 -1.0187 2.5130
Si 2.1193 0.1989 1.7643
O 1.5188 0.0680 0.1074
Si 1.7605 1.6144 -0.9663
O 1.3878 2.8487 0.0643
Si 0.4081 2.4225 1.2994
O -0.7444 1.4399 0.5467
Ti -2.0555 1.8290 1.8690
O -0.7162 3.2059 2.1509
Ti 4.1889 -0.0700 -0.4063
O 5.7556 -0.1476 -0.6623
O 3.6707 0.1086 1.4982
O 3.2826 1.4243 -1.3129
O 1.1869 -2.6519 0.5444
O 1.4124 1.5688 2.2773
Ti -3.8185 0.0386 -0.1493
O -3.4482 1.6936 0.8851
O -2.2953 0.0356 -1.3754
O -5.2651 -0.0703 -0.8019
O -1.9555 0.2336 2.7532
O -3.4184 -1.3403 1.1790
O 0.4805 1.3276 -1.8862

30
Ti5Si5O20 (10-5) Energy= -197005.038571508
Ti 4.2115 -0.0602 0.2958
Si 1.8446 1.6729 0.9081
Ti -2.4200 -1.6502 -1.0112
Si 1.7809 -1.5612 1.2012
Si 0.0892 -2.3007 -0.8471
Si 1.8395 -0.1827 -1.5681
Si 0.1759 2.0970 -1.2462
O -2.4841 -0.1377 -2.0162
O 5.8012 -0.0887 0.3277
O -3.5582 1.6109 -0.0714
O 0.7037 1.5397 2.0261
O 0.9849 -1.5110 -1.9688
O 1.3072 2.7190 -0.2494
O 3.4169 -0.2084 -1.5123
O -2.0453 0.2347 2.1905
O -1.1848 -3.0627 -1.4810

O -5.0488 0.2948 2.1941
O -3.6190 -1.4646 0.2073
O   1.1987 -2.7769 0.2494
O   3.4047 1.5592 1.0699
Ti -2.3574 1.5272 -1.2994
Ti -0.4591 0.1437 1.5299
O   3.3449 -1.4815 1.3451
O   1.0359 1.0841 -2.2045
O -0.8419 1.2420 -0.1995
O   0.6504 -1.1844 2.2732
O   1.4911 -0.0192 0.1579
Ti -3.7511 0.1861 1.2789
O -1.0693 2.7823 -2.0113
O -0.8905 -1.2318 0.0251

30
Ti6Si4O20 (10-6) Energy= -212402.002377629
O -2.2983 2.7955 0.6285
Ti 2.2662 0.3983 2.4519
O -3.5969 0.1731 0.8237
Ti -3.3885 -1.4158 -0.4475
O   2.7680 -1.2376 2.0512
Ti 2.1321 2.0069 0.1937
Ti 2.2843 -0.1922 -2.3622
O -4.7866 -2.0125 -0.9331
Ti -2.8885 1.4015 1.7318
O -2.2607 -0.8352 -1.8602
Si -0.8195 -2.2116 0.9056
O -0.8332 -1.4071 2.3600
Si -0.7844 -0.2653 -1.6236
O -0.9172 1.3429 -1.2348
Si -0.7687 0.1471 2.7806
O   1.4423 0.3713 0.7919
O   0.5957 -3.0231 0.9223
Ti 1.7278 -1.6026 0.4824
O   2.5864 -1.5764 -0.9881
Si -0.8713 2.1612 0.1394
O   0.5249 2.9557 0.2811
O -0.2361 -1.1117 -0.2456
O   0.6649 0.5358 3.4194
O -0.9770 0.9776 1.3352
O   3.0914 1.8747 1.7816
O   3.1598 -0.3616 -3.6838
O -2.2767 -2.6790 0.5024
O -2.1839 0.7401 3.3449
O   2.6823 1.4739 -1.3386
O   0.4203 -0.3682 -2.6690

30
Ti7Si3O20 (10-7) Energy= -227798.742245023
O -3.1281 -2.3372 1.8409
Si -1.6577 -1.8049 2.0738
O 0.6466 0.6433 1.2861
Si -1.6867 -0.5555 -0.8565
O -1.1104 -0.9971 0.6820
Ti -4.2623 -1.3213 0.6520
O -0.2564 -2.6273 2.2146
O -1.5886 -0.6884 3.2984
Ti 0.8757 -1.3653 1.4374
O -0.0333 3.1432 0.1582
Ti -1.6998 2.4487 0.2370
O -4.4036 0.4955 1.5405
Ti 1.5216 1.0064 2.8818
O -5.6829 -1.9941 0.3762
Ti 1.3847 -0.7023 -1.6682
O -1.7853 1.4354 1.7876
Ti -3.6733 1.8872 2.1726
O -0.4993 -0.9005 -1.8667
Si -1.5087 0.9219 3.3757
O 2.4175 2.2262 1.8820
Ti 1.4384 2.0397 0.3061
O 1.9640 -0.6939 2.8563
O -3.1726 -1.1394 -0.9045
O 1.6951 -1.7220 -0.0128
O -3.2995 3.1150 0.8565
O -1.8232 1.1162 -0.8857
O 1.8874 1.1286 -1.0815
O -0.0408 1.4209 3.8373
O -2.8904 1.6239 3.8786
O 2.2080 -1.2169 -2.9329

30
Ti8Si2O20 (10-8) Energy= -243195.584022268
O 0.6493 1.2004 2.7752
Ti -2.5404 0.6388 -1.4315
O 0.4383 1.7095 0.1464
Ti 1.5032 -0.9335 -2.7214
O 2.9348 -0.1350 -2.0598
Ti 0.8488 3.8918 -2.4967
O -1.2848 3.1022 1.5350
Si -0.7837 2.8913 0.0343
O -1.7052 2.1803 4.2960
Ti 2.1824 1.3146 -1.0894
O -2.2584 0.1513 2.1212

Ti -2.6232 -0.9490 0.8778
O 2.7002 1.1119 0.6952
Ti -0.1032 -1.7259 -0.0576
O 0.5774 0.5413 -2.0559
O 0.7046 -2.1907 -1.6264
Ti -0.3190 0.9387 -3.6675
O 2.3686 2.8314 -1.8399
O -1.3173 -0.3781 -0.4517
O -2.0369 0.4859 -3.1617
O 0.7574 -0.4343 -4.3030
Ti -1.2156 1.7214 2.8476
O -2.0484 2.2007 -0.8202
O 0.0517 2.6136 -3.7836
O -1.5026 -2.4476 0.8365
Si 1.2382 0.8293 1.3563
O 0.9537 -0.7766 0.9974
O -3.7634 -0.2527 -0.4030
O -0.1982 4.0332 -0.9148
O 1.2340 5.3025 -3.1348

30
Ti9Si1O20 (10-9) Energy= -258592.236429135
O 2.9916 0.2621 -1.1440
Ti -0.1387 -0.9573 3.9616
O 0.3495 0.1868 -3.0567
Ti 0.6377 -2.5002 -0.2814
O -1.8932 1.1209 0.4264
Ti -0.6762 -1.1559 -2.3649
O -1.3925 -2.2888 3.5281
Ti 1.2956 0.7498 -1.5828
O 4.1093 -0.5233 1.8948
Ti 0.5604 2.1699 4.1259
O -0.1202 2.3047 2.3475
O 0.6505 1.9274 -0.5250
Ti 2.7010 0.0173 3.0368
O -4.6189 0.2268 -0.3198
Ti -0.2641 1.1816 1.0332
Ti 3.0963 -0.6827 0.4278
O -0.5008 -2.8931 1.0351
O -0.5595 -0.5005 2.1457
O -0.3595 0.5511 4.7629
O 0.0118 -2.8281 -1.9335
Si -1.4851 -1.9115 1.9413
O 1.8032 0.1711 1.3883
O -2.8344 -1.6005 1.1727
O 1.6527 -1.2420 3.8202
Ti -3.0979 -0.2376 -0.1605

O -2.2737 -0.8404 -1.8717
O 0.4433 3.4674 5.0518
O 2.3928 -2.3457 0.1009
O 0.2627 -0.6860 -0.6950
O 2.3926 1.5293 3.8086

30
Ti10O20 (10-10) Energy= -273989.443013773 ref[48]
Ti 1.8304 0.9803 -2.6540
Ti -2.8203 -1.4820 -1.1873
Ti -0.0712 -0.1287 2.4951
Ti -1.0282 2.5685 2.0103
Ti 0.5280 2.3033 -0.4242
Ti -0.2487 -1.0010 -2.2335
Ti -2.2238 1.1455 -0.1073
O -0.5140 1.1309 0.9647
O -3.6432 0.0699 -0.7204
O -1.9830 -1.4976 -2.7654
O -1.3117 -0.6111 -0.5629
O 0.8202 -0.2193 -3.5727
O 1.3817 2.6488 -2.0241
O -0.5718 1.4591 3.3758
O -2.6467 2.3274 1.2932
O -1.2969 2.0958 -1.2177
O 0.0511 3.5283 0.8719
O 2.1376 1.6128 0.5430
O 1.3084 -1.1108 3.3132
O 0.8291 0.3869 -1.2153
Ti 1.9309 -2.0225 1.9085
Ti 2.4565 0.0288 -0.0769
O 3.3076 -1.2653 0.9947
O 3.2340 0.3254 -1.7635
O 0.3326 -2.3515 -1.3205
O -1.2605 -1.3128 2.0725
O -2.2250 -2.8576 -0.1218
Ti -0.5716 -2.2811 0.4629
O 0.7052 -3.2752 1.3514
O 0.9094 -0.8624 0.8911

36
Si12O24 (12-0) Energy= -144022.253804812 ref[35]
O 1.5710 0.1870 2.7384
Si 0.0467 0.0411 2.1343
Si 2.6615 0.0859 1.5171
O 0.2067 -1.3677 1.3673
Si -2.5925 -0.0252 1.6342
O 3.3994 -1.2812 1.2762

O 1.8363 0.3405 -0.0467
O 3.3026 1.6198 1.2890
Si 2.4821 1.9691 -0.0922
O -1.4496 -0.0801 2.8098
O -0.1479 1.4194 1.3214
Si -0.2756 2.2887 -0.0380
O 1.2547 3.0206 -0.0856
Si 2.5925 0.0252 -1.6341
Si 0.2757 -2.2887 0.0381
O -1.8362 -0.3405 0.0468
Si 3.3285 -2.4449 -0.0256
O 3.2416 1.5662 -1.4935
O -3.3413 1.3323 1.3733
Si -2.4821 -1.9691 0.0923
O -3.2416 -1.5662 1.4936
Si -0.0467 -0.0411 -2.1342
Si -2.6614 -0.0859 -1.5170
O 4.4152 -3.5022 -0.0290
O 3.3414 -1.3323 -1.3732
Si -3.3285 2.4449 0.0257
O -1.7015 2.9944 -0.0205
O -0.2067 1.3677 -1.3672
O 1.7015 -2.9944 0.0206
O 0.1480 -1.4195 -1.3213
O 1.4496 0.0801 -2.8097
O -1.2547 -3.0206 0.0857
O -3.3025 -1.6198 -1.2889
O -3.3994 1.2812 -1.2761
O -4.4152 3.5022 0.0290
O -1.5710 -0.1870 -2.7384

36
Ti3Si9O24 (12-3) Energy= -190216.388988345
Si 0.4572 -0.4101 -2.8379
Ti 1.5792 -3.1111 -3.9466
Si -1.0431 -1.6785 -0.3771
Si 3.3235 -2.5617 -1.4204
Si 2.7070 0.0001 -0.6732
Si 1.2288 -1.3181 1.7843
Si 0.3549 -3.8903 -1.1863
Ti 0.1369 1.3275 2.9527
Si 2.1579 -3.6202 0.4980
Si -1.6356 0.8806 0.4004
Si 1.2996 2.1942 0.1682
Ti -0.6360 2.2327 -1.6979
O -1.0781 -3.3075 -0.6453
O 1.0834 -4.7719 0.0446

O 1.7696 -3.7879 -5.3732
O -2.1545 1.9628 -0.7481
O 0.6873 3.2345 -0.9730
O 3.9039 -1.0775 -1.0386
O 0.5189 -4.2270 -2.7066
O -0.1480 -1.5656 0.9606
O 3.2666 -2.9974 -2.9233
O 0.9402 -0.4459 3.0714
O 2.2099 -0.5102 0.7744
O -0.2355 1.1044 -3.0242
O 1.9225 -2.8494 1.8890
O -0.0533 2.0049 4.3808
O 3.6596 -3.6188 -0.1585
O 0.7796 -1.3486 -4.0769
O 1.1725 2.4451 1.7122
O -0.5543 -1.1771 -1.8288
O 2.7334 1.6195 -0.3997
O 1.6121 -2.6379 -0.8461
O 0.0053 1.0567 -0.2447
O -1.5359 1.2328 1.9266
O -2.2261 -0.6004 -0.0078
O 1.8234 -0.1129 -2.0164

36
Ti5Si7O24 (12-5) Energy= -221010.914761693
Si -1.0111 -1.0338 -1.1728
Ti -2.4824 -1.8515 3.1449
Ti 1.4588 -1.0714 -2.0207
Ti -1.1409 1.0994 2.8968
Si 3.4708 0.3146 0.4383
Ti -2.5555 2.2524 0.6866
Si 1.3406 1.0924 2.0608
Ti 2.9415 1.8001 -2.2309
Si 0.1577 1.9485 -0.7326
Si -3.1348 -0.2968 0.4935
Si 0.2346 -1.9016 1.6021
Si 2.6729 -1.9664 0.1887
O 2.3249 0.0449 -2.9576
O -1.7585 0.5476 1.0860
O -0.4147 -1.8390 0.1068
O 2.0315 -0.4015 -0.1891
O -1.3137 2.6746 -0.5691
O -3.2660 -2.7664 4.1856
O 1.2552 2.5493 -1.7111
O -0.7791 -2.5770 2.6133
O 0.7530 1.9104 0.7886
O -3.9465 1.1146 0.2656

O 4.0095 1.3181 -0.6447
O 2.4717 -2.5244 -1.3035
O 4.0722 -1.2320 0.6654
O 2.9468 0.9121 1.8809
O 0.5813 1.7310 3.3397
O -1.9456 -0.0606 3.8373
O 1.7406 -2.5635 1.3739
O 0.4986 -0.3451 2.1379
O 3.7321 2.7086 -3.2703
O -2.1715 2.6024 2.3669
O -3.5382 -1.3723 1.5718
O -2.6069 -0.8540 -0.9703
O -0.2647 -1.6905 -2.4544
O -0.1637 0.3978 -1.2731

36
Ti6Si6O24 (12-6) Energy= -236407.834441988
Ti -1.2517 -1.9757 2.0766
Ti -2.0279 0.9153 -2.9775
Si -2.7230 0.4062 -0.1285
Si -0.8436 -2.2078 -0.5157
Ti -3.4695 0.2225 2.9493
Ti 1.4864 0.4177 -2.3909
Si -0.5658 1.3215 2.9107
Ti 0.1883 3.4165 -2.6042
Si 1.6737 -0.3875 0.1420
Si -0.1781 2.2357 0.2469
Ti -0.4774 -1.3450 -3.4169
Si 0.9181 -0.6005 2.8021
O -1.9310 -1.0683 0.0089
O 1.5597 2.0264 -2.9445
O -2.6751 -1.6164 2.9194
O 2.1357 -0.5078 1.7119
O -2.0033 1.3819 3.5464
O -0.9208 -2.5709 -2.0889
O 0.3436 -2.0555 3.1488
O 0.9323 1.0564 -0.1754
O -3.2413 0.5034 -1.6792
O 0.7475 0.7121 3.7724
O -0.4929 -0.1123 1.9349
O -1.4402 2.5107 -3.2348
O -0.4623 0.1019 -2.2266
O 0.1092 3.4784 -0.6997
O -1.6496 1.6281 -0.0478
O 0.6477 -1.6194 -0.1595
O 0.4757 4.8305 -3.2814
O -4.7963 0.3661 3.8181

O 2.6753 -0.3195 -1.1241
O -0.0777 2.4750 1.8734
O -3.7520 0.4771 1.0796
O 1.2214 -0.8987 -3.7006
O -1.1463 -3.2438 0.7032
O -1.7943 -0.4455 -4.2303

36
Ti9Si3O24 (12-9) Energy= -282598.137220546
Si 0.8387 1.9893 1.4212
Ti -2.2526 -0.4719 -1.3562
Ti -3.1188 2.9222 1.0308
Ti -1.9325 -0.0689 2.5853
Ti -1.0797 2.8786 3.7324
Ti -0.9528 2.8278 -1.2360
Ti 2.8344 1.2608 -0.7658
Ti 0.1095 -0.2731 -2.7262
Ti 1.4367 2.6170 -3.4828
Si 1.9264 -1.1444 -0.9492
Ti -4.2179 0.3552 0.9433
Si -0.0216 -1.1123 1.0410
O 1.9436 3.4217 -4.7608
O 1.2890 -1.7144 -2.3109
O -2.4101 3.5572 2.4673
O -1.2690 1.0403 -1.7333
O 1.1697 0.3869 -1.1002
O 0.6996 0.8281 -3.8906
O -3.7121 -0.5683 2.3928
O -3.9805 -0.3830 -0.6977
O -2.4712 1.0954 1.0412
O 0.5823 2.6999 2.8205
O 0.0662 2.7882 0.2230
O 1.3675 -1.7576 0.4722
O -2.5359 3.4975 -0.5815
O -1.6691 1.0041 3.8794
O 2.3846 1.8271 0.9051
O -1.1136 -1.2123 -0.1789
O -4.7660 2.0638 1.0626
O 2.8254 2.3131 -2.1291
O -0.8367 -1.5868 2.3546
O -0.0361 3.4607 -2.5740
O 0.1321 0.4702 1.5068
O 3.4226 -0.5306 -0.8524
O -1.5785 -1.1299 -2.8546
O -0.9808 3.6786 5.1106

36

Ti12O24 (12-12) Energy= -328788.617831048 ref[33]
Ti -0.6484 0.4372 3.1666
Ti 2.5148 -1.6152 -1.8548
Ti 2.3796 0.6892 2.4504
Ti -1.3129 1.2899 -0.2137
Ti -3.5792 -2.9481 2.2406
Ti -3.7080 -2.1277 -0.4071
Ti -0.4580 -2.8912 2.2597
Ti 1.9945 -1.9451 1.3748
Ti -4.5718 1.1514 -0.2236
Ti 1.8366 1.2755 -0.2069
Ti -0.6542 -1.9422 -1.1542
Ti -3.2934 -0.1059 2.5322
O -2.2372 0.6082 3.9312
O 2.9513 1.8176 1.1625
O 1.2516 -3.3151 2.4489
O -4.4334 0.8687 1.7141
O -4.0830 -1.6150 3.3110
O -2.2999 -2.7351 -1.3641
O 2.8498 -2.3236 -0.0550
O 0.9965 1.2044 3.5127
O 0.7093 -2.2183 -2.1910
O 3.0356 -0.9628 2.5825
O -2.0210 -3.8297 2.5601
O -5.8364 2.0031 -0.6964
O 1.2959 -0.0452 1.0830
O 2.4244 0.2920 -1.5080
O -4.5039 -3.3371 0.7399
O 3.5793 -2.0480 -2.9630
O 0.2843 2.1842 -0.3869
O -4.5211 -0.6727 -0.8840
O -2.8608 1.9524 -0.6327
O -1.0467 -0.1948 -1.1796
O -2.8008 -1.5744 1.1965
O -0.0026 -2.2808 0.5796
O -1.5199 0.6980 1.5618
O -0.4919 -1.3553 3.1971

42
Si14O28 (14-0) Energy= -168029.357502248 ref[36]
Si 3.5358 1.5342 -0.2401
O 0.8868 1.3272 -0.2079
Si 1.3445 1.1946 -1.7594
O 1.5883 0.3515 2.2433
Si -1.3445 -1.3094 1.6758
O -2.8332 -1.0126 2.3600
Si 1.3440 -1.6760 -1.3096

O 2.8326 -2.3605 -1.0129
O 2.8331 2.3598 1.0133
O 0.0001 2.5061 1.8269
Si -1.3441 1.7597 1.1946
O 0.0005 1.8270 -2.5060
Si 3.5354 -1.5350 0.2406
O 2.8326 -1.9373 1.6865
O -0.0003 -1.8268 2.5061
O -0.0003 -2.5060 -1.8269
O 1.5885 -0.3518 -2.2431
O 2.8333 1.9367 -1.6861
Si 1.3443 1.6758 1.3098
O -1.5882 2.2435 -0.3517
Si 1.3439 -1.1948 1.7596
O 0.8864 -1.3273 0.2080
O 3.0996 -0.0003 0.0002
O 5.1668 1.3733 -0.2148
Si 6.0537 -0.0008 0.0001
O 5.1664 -1.3746 0.2154
O 7.5645 -0.0011 -0.0003
O -0.8867 0.2082 1.3272
Si -1.3439 1.3099 -1.6759
Si -1.3444 -1.7592 -1.1948
O -1.5888 -2.2429 0.3516
O -0.8866 -0.2078 -1.3273
O -2.8331 -1.6859 -1.9371
O -2.8326 1.0135 -2.3603
O -2.8329 1.6867 1.9368
Si -3.5357 0.2409 1.5344
Si -3.5356 -0.2398 -1.5348
O -3.0997 0.0005 -0.0002
O -5.1668 0.2157 1.3737
O -5.1666 -0.2145 -1.3743
Si -6.0538 -0.0002 -0.0002
O -7.5646 -0.0016 -0.0000

42
Ti4Si10O28 (14-4) Energy= -229619.944166649
O 3.2346 -2.2135 0.7021
O -3.4435 2.0480 0.7674
O 5.2185 -0.3624 0.8656
Si 3.2786 1.8081 -1.2600
O -0.4893 -0.5026 2.4641
O -1.6449 0.4299 4.5997
O 0.7651 -2.7519 2.1176
Ti 3.2941 -0.7236 -3.0547
O -1.3601 1.9865 2.4370

O 3.4867 1.2030 -2.6917
Si 1.8703 1.0075 2.4197
O -1.0902 -1.3759 -1.5686
Si 4.0947 -1.0960 -0.1191
O -3.7757 -0.3468 2.4522
O 3.2160 0.4419 -0.1548
Ti 4.5313 1.3018 1.0436
Si -1.9898 -1.2771 -0.2310
O -3.6170 -1.1512 -0.3341
Si 1.7731 -1.7553 1.3068
O -3.8205 -1.4345 5.2939
O 3.7735 -1.1524 -4.5138
Ti -3.8840 0.2307 0.8744
O 1.0694 1.5061 1.1065
O 4.5232 2.4416 -0.3566
Si -0.6756 0.8310 3.4018
O 4.4156 -1.4366 -1.6181
O -1.5541 -2.3362 0.8972
Si 0.4773 -0.8359 -1.4931
O 0.9532 -1.2683 0.0038
O -1.7028 -2.5183 3.5466
O 0.8879 1.3231 3.6787
O -1.8752 0.2836 0.4339
O 1.9519 2.7328 -0.9857
Si -1.8249 1.9113 0.8982
O -0.8138 2.7140 -0.1057
O 0.3430 0.7922 -1.4305
Si -0.7577 -2.1183 2.3259
Si 0.6344 1.9695 -0.3758
O 2.2249 -0.5658 2.3269
Ti -2.8032 -1.0411 4.1306
O 3.3722 1.7145 2.3563
O 1.4886 -1.2568 -2.6372

42
Ti5Si9O28 (14-5) Energy= -245017.076480109
O 1.4346 2.1032 -0.1997
O 1.6788 -2.6932 1.0320
O -0.7142 1.8089 1.1936
Si 0.3044 -0.5307 -2.4645
O -3.0337 -1.9920 -1.1346
O -0.3342 -2.4914 2.8247
O -0.8618 2.9114 -2.0811
Ti -0.1141 -3.5517 4.5708
O 0.8759 -0.2873 0.7469
O -1.8512 -3.8965 4.0066
Ti -2.1601 1.6514 -1.5269

O 1.6005 1.4331 2.5287
Ti -0.1694 -0.2724 6.1892
O 1.1914 0.7421 -3.0274
O -2.9969 0.6950 -2.6477
Si 0.8224 1.2922 1.1015
Si 1.1590 0.2777 3.6329
O 1.2767 0.5334 5.2013
Si -2.0200 -2.6780 2.9302
O -2.7096 1.1714 2.8603
O -2.6302 -1.3620 3.6220
Si -2.1880 1.1037 1.3163
O 1.5208 -3.7212 3.6779
O -0.6513 -2.3553 -0.0968
Ti -2.7084 -1.2658 -2.8782
O -1.8260 0.3939 5.4577
O -0.0463 -0.0706 7.7667
Si -1.9542 0.1182 3.8926
O -2.6417 -2.9435 1.4631
O -3.6105 -1.9258 -4.0135
O 1.2830 -1.4687 -1.5361
O -0.8047 -1.2622 -3.3109
O -0.0896 -2.2587 5.6484
Si 0.8210 -1.7192 0.0129
O 1.9376 -1.1197 3.2097
O -2.9952 1.8328 0.0926
Ti 0.6416 2.0150 -1.8279
Si 1.3475 -2.4943 2.6184
O -0.5551 0.5494 -1.3860
Si -2.1987 -1.9422 0.2164
O -2.1498 -0.4587 0.8831
O -0.4283 0.0392 3.2962

42
Ti7Si7O28 (14-7) Energy= -275810.823496006
O -1.7125 -0.9229 -1.5979
O 1.6809 1.7053 2.7828
O -3.1281 -3.2521 3.0271
Ti -1.8635 -3.5648 1.9154
O -1.9753 3.5501 -0.5238
O 2.6545 -1.2378 -0.3812
O -2.5357 1.7689 1.5801
Ti 0.0888 -2.0893 4.5583
O 3.1293 1.6775 -1.8480
O -3.0155 -0.1678 3.4724
Si -0.9328 0.5136 -1.8490
O -0.5622 0.3812 2.5675
Ti 0.7932 -4.0230 2.6517

O -0.4088 -2.5549 2.7400
O 0.8829 3.5276 -1.7714
Si 1.3348 2.5286 1.4224
Ti 2.3000 3.0768 -0.9755
O -1.4517 -2.1083 5.2868
Si -2.1586 0.3063 2.2128
O -1.9391 -3.1444 0.1295
O 0.9659 -0.4737 4.4669
Si -1.4871 2.4444 0.5182
O 1.8089 -3.3111 1.3041
O 1.6023 1.5005 0.0850
Ti -1.1168 3.4213 -2.2311
O -0.6560 -4.9581 2.1891
O -1.5667 4.5566 -3.2587
Ti -3.1927 -1.8186 4.3821
O -2.2888 -0.8646 1.0679
O 0.6545 0.1302 -2.1939
O 1.1118 -3.6334 4.3753
O 2.3458 3.6513 0.8181
O -0.1967 3.0054 1.3883
Si -1.4716 -1.5995 -0.1318
O -1.4441 1.6232 -2.8689
O 1.8052 -0.7906 2.0416
Si 1.6160 -1.7765 0.7656
Si 0.9758 0.2296 2.9997
O -0.9123 1.1707 -0.3508
Ti 2.1228 0.2944 -1.2365
O 0.1467 -1.5707 0.1146
O -4.4521 -1.8781 5.3586

42
Ti10Si4O28 (14-10) Energy= -322001.227043601
O -0.9890 1.3657 -0.0740
O -0.2708 2.6049 -5.4279
O 0.2854 -1.7473 0.8235
Si 1.4673 -0.8642 1.5098
O -1.2583 -3.2984 -0.4998
O -1.2321 1.7710 -2.7488
O 1.2202 2.8316 -0.1350
Si -1.5930 0.8822 -1.4894
O -0.7747 -2.0324 4.9000
O 1.5041 -1.1689 3.1069
Si 0.2544 1.9286 0.8120
O 2.7768 -1.1602 0.5763
Si -1.1493 -2.4786 0.9166
O 2.3400 -1.7013 -2.4725
O -3.1056 1.2843 3.1812

Ti -3.2622 -0.4074 2.4152
Ti -3.7775 -0.8069 -0.3968
O -0.4992 -2.6108 -3.2409
Ti 0.1404 1.8596 -4.0757
O -2.3705 -1.3035 0.7663
O -2.7010 -4.3367 4.7075
Ti -1.3360 1.5505 3.3635
O 0.5709 -0.0432 -4.2365
O -0.3176 0.9907 4.7513
Ti 0.6249 -1.1257 -2.9202
O -1.1683 -0.2066 2.7738
O 1.6614 2.6013 -3.1197
Ti -2.1626 -3.0255 3.9700
O 3.6407 1.0304 -1.3917
O -1.0680 -0.7079 -1.7906
O 1.2857 0.3161 -1.4925
O -1.4268 -3.3172 2.2305
O -3.5035 -1.6657 3.5405
Ti 0.0390 -0.7193 4.1442
O -3.1915 0.6839 -1.1803
O -4.6355 -0.4116 1.1167
Ti -1.7613 -2.4569 -1.9892
Ti 2.0942 2.0310 -1.5560
O 1.1919 0.7298 1.3759
Ti 2.8750 -0.5934 -1.1603
O -3.5445 -2.0941 -1.6956
O -0.4608 2.5800 2.1304

42
Ti14O28 (14-14) Energy= -383588.053217711 ref[33]
O 0.5979 -1.4465 -2.0118
O -2.3509 0.9766 1.7333
O -0.4969 1.6390 -0.3361
Ti -1.0814 0.6543 2.9980
O -2.8940 0.3829 -4.2482
O 2.9088 0.8441 3.1282
O -1.0493 -0.9865 3.6686
Ti -2.0000 0.7052 -0.0376
O -1.7170 3.1967 -3.6185
O 1.7515 -1.8038 3.7620
Ti -2.0861 -1.3328 -4.7205
O -0.3974 1.1272 -3.1177
Ti 0.5778 -3.8381 0.7503
O -2.9944 1.3165 -1.4393
O 2.1579 0.8157 -1.1166
Ti 0.3721 -1.8014 2.7557
Ti 2.2215 -0.7401 -2.0332

O 1.7117 2.6642 1.0274
Ti 1.1607 2.2199 -0.6304
O 0.9034 2.1791 -4.9627
O 0.9873 3.3669 -2.0837
Ti 0.0627 2.9367 -3.5660
O -1.8801 -2.2639 -3.0494
O 3.3368 -1.8765 -1.1717
Ti 1.4800 1.5899 2.4976
O 2.2693 -0.2691 -3.7990
O -1.7212 -1.0262 -0.3609
Ti -2.3139 1.5196 -3.1014
O 2.3329 -4.2776 0.5311
O -0.1328 -3.5486 2.3611
O 4.5374 -1.1585 4.6116
O 0.0429 1.9646 3.5826
O -2.8910 -2.1569 -5.8262
Ti 3.4793 -0.9869 3.4271
O 0.3877 0.1280 1.9609
O -0.5400 -3.7558 -0.6604
Ti -0.9829 -2.2073 -1.5541
Ti 3.0265 -2.5763 0.4866
O -0.3269 -0.7169 -5.2972
Ti 0.7444 0.3837 -4.5129
O 1.2373 -2.0820 0.8715
O 3.9522 -1.9130 1.7984

48
Si16O32 (16-0) Energy= -192035.449962924 ref[36]
Si -3.9520 -0.6667 -1.5474
O -1.3153 0.1297 -1.5168
Si -2.2833 1.4328 -1.4749
O -1.3740 -2.1074 0.0001
Si 1.3935 -1.4918 1.5071
O 2.8915 -1.7728 2.1702
Si -2.2832 1.4329 1.4749
O -3.6646 0.8308 2.1841
O -2.8931 -1.7706 -2.1700
O -0.0009 -2.0071 -2.2217
Si 1.3934 -1.4919 -1.5070
Si -3.9520 -0.6665 1.5476
O -2.8931 -1.7705 2.1702
O -0.0009 -2.0069 2.2219
Si 0.0011 2.9165 1.1996
O -3.6647 0.8306 -2.1841
Si -1.3948 -1.4908 -1.5070
O 1.3152 0.1287 -1.5168
Si -1.3948 -1.4907 1.5071

O -1.3153 0.1298 1.5169
O -3.5014 -0.5345 0.0001
O -5.5129 -1.1297 -1.3803
Si -6.3735 -1.3829 0.0001
O -5.5128 -1.1296 1.3805
O -7.8222 -1.8103 0.0002
O 1.3721 -2.1085 0.0001
Si 2.2842 1.4310 -1.4749
Si 2.2842 1.4311 1.4748
O 1.3152 0.1288 1.5168
O 2.7244 1.9633 -0.0001
O 3.6651 0.8278 2.1840
O 3.6651 0.8277 -2.1842
O 2.8915 -1.7729 -2.1701
Si 0.0010 2.9164 -1.1997
O -1.3668 2.6723 -2.0834
O 1.3687 2.6714 2.0832
O 1.3686 2.6712 -2.0834
O -1.3667 2.6725 2.0833
O -2.7231 1.9654 -0.0000
O 0.0015 4.1038 -0.0001
O 0.0006 1.7805 -0.0001
Si 3.9512 -0.6698 -1.5475
Si 3.9513 -0.6697 1.5475
O 3.5008 -0.5373 -0.0000
O 5.5118 -1.1339 1.3804
Si 6.3723 -1.3879 -0.0000
O 5.5117 -1.1340 -1.3804
O 7.8207 -1.8162 -0.0000

48
Ti4Si12O32 (16-4) Energy= -253625.634529310
O 1.3132 2.3298 -0.1053
O -0.0383 0.5380 5.9766
O 1.5090 -1.4763 1.9275
O -2.2087 0.8318 1.9315
O -0.8582 -1.1756 -1.6460
O 1.3980 -0.3429 -0.6281
O 2.9130 0.6863 1.1786
O -0.3495 -0.0176 -4.7825
O -0.0667 -3.4095 2.4335
O 0.4974 0.9726 2.0805
O 2.2554 0.0916 3.8530
O -1.0620 1.9121 3.9433
O -0.3990 -0.7396 3.9736
O -3.0051 -0.4240 -0.2748
O -0.8259 3.0418 1.3313

O -2.1735 0.6638 -2.7987
O 0.6740 -2.7815 -0.2373
O 0.4937 1.3134 -2.6283
O 1.7894 3.2081 -3.2014
O -2.0375 -2.8702 4.5777
O -1.0739 -1.3960 1.1767
O -3.5114 -1.3893 2.3017
O 2.5447 0.6438 -4.2136
O 3.0820 1.3540 -1.6388
O -4.9015 -1.9528 4.8213
O 1.8414 -1.8291 -5.7239
O -0.3908 3.6564 -1.4554
O -2.6901 0.0084 5.0922
O 1.3690 -1.8870 -2.8179
O 0.9773 -2.3274 5.2893
O -0.8875 2.6841 -3.9909
O -1.1078 1.2928 -0.5300
Ti -0.4334 -2.6871 4.0710
Si 2.2258 1.5896 -3.0078
Si 0.2062 3.0293 -2.8257
Si -2.5224 -0.6473 1.2988
Si -1.2325 0.5432 4.8333
Si 2.2234 0.9894 -0.2811
Si -0.2771 2.6161 -0.1521
Ti -3.4885 -1.5441 4.2099
Si 0.6969 -1.6074 -1.4042
Si -0.9234 1.7181 2.3234
Si -1.8354 0.0560 -1.2992
Si -0.8930 1.0177 -3.7421
Si 1.8315 0.0738 2.2650
Si 0.2593 -2.3098 1.2662
Ti 1.1433 -0.5768 5.1353
Ti 1.3860 -0.9311 -4.4910

48
Ti6Si10O32 (16-6) Energy= -284419.925123286
O 3.2022 0.8498 -2.9803
O 1.8604 0.3283 3.8352
O -0.7349 1.2446 5.1571
O 3.0062 -0.3033 -0.7081
O -2.5214 0.2793 2.7548
O 0.6722 3.2365 0.1974
O -1.6722 3.7019 1.0955
O -3.7630 1.1933 5.2548
O 1.8535 1.1526 1.3792
O 1.3311 -3.6969 -3.2706
O 3.6321 -1.8019 -3.5952

O 0.6518 -1.3535 -0.3129
O 1.0086 1.2698 -1.6467
O -0.2358 5.0066 2.9959
O -1.0520 1.2091 0.7152
O 2.0778 -0.0559 -5.2136
O -0.4621 1.2211 -3.8481
O 1.1506 -0.9486 -3.1841
O 2.8125 -2.9000 -0.6798
O -1.2452 -0.1209 -1.7722
O 3.0700 2.3554 -0.5631
O -0.0391 -0.4977 2.3811
O 4.1556 -4.5752 -2.6748
O 2.5281 3.6647 1.9018
O -1.2389 2.5458 -1.4874
O -0.5397 -1.7082 -4.8312
O -1.0158 -2.6581 -1.7866
O 1.6625 3.2898 4.7534
O 0.1152 2.6356 2.9254
O 2.3725 -1.3853 1.6275
O -2.3667 3.2706 3.6726
O -1.8198 -1.2640 0.5583
Ti 0.0698 -2.5680 -3.2536
Si 2.6066 1.0597 -1.4667
Ti 0.7658 1.6443 4.4696
Ti 3.1470 -3.3525 -2.5074
Ti -2.5228 1.4280 4.2800
Si -0.5086 1.2559 -2.2036
Si -0.8955 -1.3758 -0.7763
Si -0.8556 2.6840 0.1063
Si -1.2404 3.7355 2.6747
Si 2.0742 2.6093 0.7226
Ti 0.3132 -0.1633 -4.7438
Si -1.4369 -0.0794 1.6466
Si 2.2418 -1.5710 -0.0112
Si 1.5434 -0.1553 2.3008
Ti 1.3462 4.1032 3.2227
Si 2.7465 -0.5118 -3.7713

48
Ti8Si8O32 (16-8) Energy= -315213.540398264
O 0.8306 -1.9921 -1.7841
O 2.2971 2.7763 -1.7134
O 0.6976 0.3449 2.1699
O 0.6084 0.6091 -3.0495
O 2.3304 1.6188 -4.5291
O -0.1892 3.2619 -3.3140
O -1.0912 0.0312 4.0162

O 3.0252 -3.2971 2.2159
O 0.1663 2.0837 -0.1133
O -0.8572 -0.2749 -0.6117
O -1.5009 -1.5665 -2.7904
O 2.6886 1.8242 1.4490
O 3.0199 -0.7738 1.7901
O -1.9222 1.0279 -4.1629
O -1.7183 1.0789 1.4352
O -1.2211 -2.8481 -0.3141
O 3.3274 -2.3343 4.7870
O 1.6601 -4.5245 4.1560
O -2.2173 1.9525 -1.1885
O 2.1479 0.1224 -0.7734
O 0.9248 -2.2899 3.6491
O -1.2928 -1.4752 1.9802
O 0.9779 -0.8172 5.9872
O -0.9657 -3.0438 5.0725
O 2.8961 -1.0600 -3.0102
O 0.5045 -0.7723 -5.1108
O -0.6970 -3.9996 2.1694
O 0.9769 -2.3385 0.9407
O 3.8412 -0.0181 6.5841
O 2.6894 0.6558 3.9686
O -3.1538 3.6405 -3.3882
O 3.1338 -2.2521 -0.4376
Si -0.5785 -2.6893 1.1827
Ti -0.2142 -1.3170 4.8961
Si 2.2903 -1.3240 -1.5116
Si -0.8794 0.0583 2.3926
Ti 2.8782 -0.5471 5.4273
Si 2.3056 0.5591 2.4244
Ti 1.9141 1.7940 -0.2026
Si 2.4603 -3.1366 3.7450
Si 2.5795 -2.1656 1.1097
Si -0.7193 -1.6945 -1.3698
Si -1.2441 1.2442 -0.1424
Ti -0.0516 -3.9553 3.8633
Ti 1.3132 2.4349 -3.1720
Ti -0.8638 -0.2915 -3.9364
Ti -2.0125 2.6067 -2.9756
Ti 1.9176 -0.0897 -4.2412

48
Ti12Si4O32 (16-12) Energy= -376800.541628553
O 0.9696 0.5523 -0.9698
O -0.0403 -3.4688 4.4940
O 0.7571 -3.4131 2.1120

O 2.4510 -1.9628 0.5957
O -1.8567 -2.5327 2.1060
O 0.3704 3.1755 -4.1724
O 1.4514 3.1861 -1.3348
O -0.6020 0.6758 1.9380
O -1.5072 -0.7212 4.2626
O -0.1813 -2.2538 0.0723
O -2.5081 1.9614 2.8611
O -3.5392 2.9226 -2.6777
O -2.7352 -2.5305 -0.4527
O -1.9856 1.3496 -4.9038
O 0.7833 -1.0885 2.9067
O 1.5790 1.9810 1.1206
O -1.1952 -4.6111 0.6396
O -2.6846 0.2993 0.1107
O 0.5231 1.5693 3.9536
O -1.1522 4.6000 -1.9023
O 1.5067 -4.2141 -0.3617
O -3.0437 3.0829 0.1637
O -1.0080 -0.9053 -2.0598
O 0.7572 0.2161 -3.6131
O -1.3989 1.7330 -2.5260
O 1.4814 5.6770 -2.9178
O -0.7329 2.4207 -0.1029
O 2.9457 -0.1102 2.6495
O 2.7928 -3.2125 3.5939
O 1.1599 -5.7564 2.5322
O -3.6119 -0.1234 -2.5889
O 1.4581 -1.8459 -1.8975
Ti -2.5921 -0.8499 -1.2540
Ti -1.2040 0.9853 3.5951
Ti -0.7146 -2.0939 3.4331
Ti -2.1598 1.7938 1.0213
Ti 1.3040 0.8539 2.5016
Ti 1.3416 -4.2648 3.6311
Ti -3.0389 1.4021 -3.4156
Si 1.3460 -2.5664 -0.4408
Si -1.5648 -2.9923 0.5630
Ti 2.4291 -1.7826 2.4030
Ti 0.6541 4.3400 -2.6206
Si 0.5692 -0.4798 -2.1588
Ti -0.3470 1.6167 -4.1034
Si 0.8756 2.0676 -0.3580
Ti -2.1213 3.2567 -1.4468
Ti 0.5477 -4.8849 1.0341

Ti16O32 (16-16) Energy= -438387.218361503
Ti 3.2609 -1.5876 1.4430
Ti 2.3268 0.3569 -2.6655
Ti -0.3488 1.5297 -2.3970
Ti 1.6922 0.4567 3.3621
Ti 1.8881 2.5408 1.5704
Ti 1.5303 -5.2341 -2.1922
Ti 0.4143 -0.4292 -0.0743
Ti -1.3494 -1.2284 -2.7005
Ti -1.1672 -2.9566 1.7662
Ti 1.3471 -2.6108 -3.2150
Ti 1.7837 -3.8343 0.3125
Ti -2.9579 -1.7368 -0.4397
Ti -3.5259 1.1985 1.4933
Ti 3.8394 1.0120 -0.4082
Ti -1.2869 -0.6687 3.3250
Ti -0.9754 2.9728 -0.0168
O -2.6372 -3.1060 0.7608
O 4.3662 -0.4583 0.5227
O 0.1804 0.0186 4.2003
O -3.5958 -0.2832 0.2516
O -2.5745 0.4325 3.0039
O 0.4997 3.5177 0.9810
O -3.0128 -1.8575 -2.2517
O 0.1545 -6.0282 -2.3549
O 1.2046 -3.3651 -1.4920
O -2.4742 2.6816 0.7983
O -4.9913 1.6692 1.9155
O 2.2111 2.2064 3.3298
O 0.2878 -3.9522 1.3681
O 1.9179 -4.1601 -3.7629
O -1.6177 -2.4705 3.4456
O 2.2067 -5.3731 -0.3977
O 3.3620 -3.3369 1.2453
O 2.5414 -1.2281 -3.4890
O 3.4129 2.4913 0.6099
O 2.8668 -0.8875 3.0939
O 4.0230 1.0127 -2.1843
O -0.3872 -2.3077 -3.7494
O -0.9577 3.1693 -1.8269
O 2.1413 0.5172 -0.7394
O -1.1363 -1.4114 -0.7498
O -0.4320 1.2420 -0.4209
O 1.6986 -1.6747 0.4771
O 0.4970 -0.4420 -2.0555
O -0.6281 -1.1307 1.6283
O 1.2435 1.6776 -3.2763

O -1.5935 0.5288 -3.1935
O 1.2078 0.7888 1.6040
Si24O48 (24-0) Energy= -288060.066294640 ref[37]
Si 2.5075 3.0255 -1.5209
Si 2.5076 3.0254 1.5208
Si 1.2047 4.8968 0.0000
Si 1.2052 -4.8967 -0.0001
Si 2.5079 -3.0252 1.5207
Si 4.5249 -1.1654 1.4571
Si 4.5248 1.1658 1.4571
Si 2.5078 -3.0252 -1.5209
O 3.9340 2.5243 -2.1796
O 3.9341 2.5243 2.1794
O 2.1535 4.6382 1.3255
O 3.9344 -2.5239 2.1794
O 3.3492 0.0002 -1.3098
O 1.2840 -2.2766 2.2356
O 2.5973 -2.4690 -0.0001
O 5.1547 -1.5858 -0.0002
O 2.5971 2.4692 -0.0000
O 0.0002 -3.7626 -0.0000
O 1.2836 2.2767 -2.2357
O 3.3492 0.0002 1.3097
O 2.1534 4.6382 -1.3255
O 5.5258 0.0003 -2.1490
O 5.1545 1.5864 -0.0001
O 5.5259 0.0003 2.1487
O -0.0002 3.7626 0.0000
O 2.1539 -4.6380 1.3254
O 1.2838 -2.2765 -2.2357
O 0.0003 -6.0791 -0.0001
Si 4.5247 1.1658 -1.4573
Si 4.5249 -1.1654 -1.4573
O 1.2837 2.2766 2.2356
O 3.9343 -2.5239 -2.1796
O -0.0003 6.0791 0.0001
O 2.1539 -4.6380 -1.3256
Si -2.5078 3.0252 1.5209
Si 0.0000 -1.4753 -1.6164
Si 0.0001 -1.4753 1.6163
Si -2.5079 3.0252 -1.5207
Si -1.2052 4.8967 0.0001
Si -1.2047 -4.8968 -0.0000
Si -0.0000 1.4753 1.6164
Si -2.5076 -3.0254 -1.5208
Si -4.5248 -1.1658 -1.4571
Si -4.5249 1.1654 -1.4571

Si -2.5075 -3.0255 1.5209
Si -0.0001 1.4753 -1.6163
O 0.0001 -0.0000 2.2683
O -3.9343 2.5239 2.1796
O -3.9344 2.5239 -2.1794
O -2.1539 4.6380 -1.3254
O -3.9341 -2.5243 -2.1794
O -3.3492 -0.0002 1.3098
O -1.2837 -2.2766 -2.2356
O -2.5971 -2.4692 0.0001
O -5.1545 -1.5864 0.0001
O -2.5973 2.4690 0.0001
O -0.0001 0.0000 -2.2683
O -1.2838 2.2765 2.2357
O -3.3492 -0.0002 -1.3096
O -0.0001 1.3052 0.0000
O -2.1538 4.6380 1.3256
O -5.5258 -0.0003 2.1490
O -5.1547 1.5858 0.0002
O -5.5259 -0.0003 -2.1487
O -2.1535 -4.6382 -1.3255
O -1.2836 -2.2767 2.2357
Si -4.5249 1.1654 1.4573
Si -4.5247 -1.1658 1.4573
O -1.2840 2.2766 -2.2356
O -3.9340 -2.5243 2.1796
O 0.0001 -1.3052 -0.0000
O -2.1534 -4.6382 1.3255

72
Ti12Si12O48 (24-12) Energy= -472823.847523400
Ti 1.5271 -4.3940 3.2978
O -0.6879 3.2144 2.1433
O 3.5770 -0.6080 3.8210
O -1.3628 -2.0311 2.8448
O -2.2975 0.1672 -2.1849
Ti 3.4351 -2.0675 -0.2870
Ti 0.0500 0.9012 5.4754
O 1.0795 -4.0076 1.5886
O -0.3554 3.9022 -0.4271
O 1.9382 1.1975 5.0575
O 3.8739 2.0094 0.2225
O 0.8782 0.1070 -4.4084
O -0.5530 0.6026 2.2931
O -0.1599 -0.9506 4.9984
O 2.0707 0.9047 2.4036
O -0.0959 -3.8846 -1.0332

O -1.2530 1.9166 4.4286
O 3.6539 -3.7863 -0.9978
O 0.2614 -3.5192 4.2117
O -1.0267 -5.7369 0.5554
O 1.7955 3.9517 1.4761
O 1.7973 -5.7857 -0.4397
Ti 0.7774 0.1613 1.2513
Ti 2.8911 2.4713 1.6488
Si 2.9488 -1.8581 2.9697
Si 0.3670 3.3558 0.9219
Ti -3.6893 1.2049 -2.1016
Ti -1.1464 2.5806 -1.4624
Ti 3.4102 0.6708 -0.9526
Ti -2.9212 -1.0944 -3.4476
Si 0.9861 0.8634 -2.9260
O 2.3233 -0.3348 0.0391
O 0.4791 -2.6559 -5.4340
Si -2.9148 0.8755 0.7133
Si 0.4191 -3.6041 -4.0369
O -0.3462 -1.3450 0.5026
O 1.7489 -2.4455 -1.0628
O -1.0801 -4.2139 -3.8193
O -0.2119 1.1193 7.0339
O 0.3438 -0.1421 -1.7962
O 2.5323 1.1154 -2.5017
O -2.1216 -3.2962 0.6306
O 2.9922 -3.3342 3.6542
O 3.6544 -2.0428 1.5181
O 4.4390 -0.8060 -1.1429
O -4.1643 1.0977 -0.3153
O 1.0192 1.8640 0.4779
O -1.5541 -0.9549 -4.7009
Ti 1.9905 -4.3004 -1.4811
Si -2.2549 -3.6445 -2.8058
Si -0.0386 -1.9532 3.7976
Si 2.9154 0.9103 3.8584
Si 0.0267 -1.2643 -4.6051
O -1.5885 1.4537 -0.0977
O -2.8886 1.6753 2.1453
Ti 0.7603 -5.6954 1.0381
O 1.3179 -6.1368 2.7249
O 0.0586 2.1787 -2.7994
O -4.3201 0.0651 -3.4467
Ti -0.0273 -1.8246 -1.3286
O 3.7914 2.1811 3.2539
O -1.7701 -2.2254 -2.0568
Si -1.4788 -4.4571 -0.3303

O -2.7591 2.8068 -2.2215
O 1.2873 -1.5042 2.7702
O -3.4646 -2.9087 -3.5908
O -2.5086 -4.7136 -1.5939
O -2.8433 -0.7407 0.9967
Si -1.4159 1.9260 2.8588
O 1.5993 -4.4522 -3.3520
Si -1.7282 -1.8688 1.2924
O 0.4282 -2.1420 -3.2191

72
Ti24O48 (24-24) Energy= -657585.884263940 ref[33]
Ti 0.1766 3.8291 -3.1552
O 3.8771 -0.4377 -1.4316
O 1.4510 -1.2320 4.2235
O 2.6064 -0.0054 1.5167
O 0.2744 3.3725 3.5585
Ti -2.1019 -2.4892 -2.7337
Ti -4.4629 -2.0407 1.9932
O 4.1202 -0.7387 3.2910
O 3.3458 4.5934 -1.2971
O -1.5812 -1.1265 2.9563
O 0.9266 0.0445 -0.9106
O -2.8123 -0.7607 -1.6619
O 2.2643 2.8699 -3.3008
O -1.0750 -2.3003 5.0350
O -5.1872 -0.4108 -1.3252
O -0.8325 0.7824 5.1612
O 5.2900 2.2192 -2.0279
O -2.4511 1.0352 -4.6438
O 2.0932 2.3329 -5.8321
O -3.6624 1.2412 0.3528
O -1.8041 1.4689 -1.7487
O -1.6202 4.0050 -3.2925
Ti 4.0188 0.7848 2.3379
Ti -0.3237 -0.7650 4.3617
Ti 3.9320 3.4011 -2.4806
Ti 4.5101 1.1514 -0.8056
Ti 2.0116 3.7040 -0.3472
Ti 1.6815 3.1004 2.4294
Ti 1.1798 1.1559 -4.7691
Ti -2.9053 0.3366 1.7069
Ti -3.8670 0.8513 -1.4000
O -2.3101 1.7146 2.7788
O 0.5918 4.0485 -1.3749
Ti 2.5252 3.8021 -4.8378
Ti 0.3445 -3.3323 -1.5861

O	-3.6288	-3.1497	3.1809
O	5.1097	1.1085	0.9177
O	-4.3691	-0.3325	2.5839
O	-0.8584	-2.1147	-1.0603
O	1.0557	4.7948	-4.4401
O	-0.1026	2.0849	-3.7823
O	0.7789	-4.2044	-0.0417
O	0.2572	0.7418	2.8814
O	-3.6289	-3.1217	-1.9828
O	-2.3668	-1.9574	-4.4630
O	-0.6617	-3.8430	2.5748
O	-0.8453	-3.8381	-2.8438
O	3.0263	2.1595	-0.9191
Ti	0.6857	0.3234	1.0390
Ti	2.2284	-0.6747	-2.1076
Ti	-0.8261	1.9259	3.7404
Ti	-1.4152	-0.4155	-4.7156
Ti	0.7981	-3.4300	1.5893
O	-3.1924	-1.5730	0.7778
O	1.8015	-2.4125	-2.1768
Ti	-0.9859	-0.1341	-1.3033
O	-0.6273	-0.6657	-3.1126
O	2.1321	4.4416	1.3329
O	-4.0102	2.1529	-2.6643
Ti	-1.8601	-2.8396	3.4989
O	0.8390	-1.6092	1.5169
O	2.3903	-3.3266	2.4658
Ti	-2.3153	2.3084	-3.3182
O	2.2070	0.0744	-3.7203
O	-5.4243	-2.5713	0.5503
O	1.1512	2.1988	0.9083
O	4.1534	4.1914	-4.1375
O	-1.0948	0.2333	0.5759
Ti	-4.3222	-1.9169	-0.7837
O	0.0921	0.0540	-5.6798
Ti	2.4961	-1.5362	2.8204
O	3.1806	2.2463	3.0307