Supplementary Information for:

Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters *versus* nanocrystals

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1. Interionic Potential (IP) parameters

In both IP-based global optimisation approaches local interactions are described by a Buckingham potential:

$$V_{ab}^{Buck} = A_{ab}\exp(\frac{-r}{B_{ab}}) - \frac{C_{ab}}{r^6}$$

In addition, long range electrostatic interactions between all ions are included.

1. Buckingham parameters employed for "mixed" MA-FB IP approach where *a*, *b* ϵ {Ti1, Si2, O1, O2}.

a	*b*	*A*	*B*	*C*	Reference
Ti1	Ti1	31120.2	0.154	5.25	MA-IP [41]
Ti1	O1	16957.53	0.194	12.59	MA-IP [41]
Ti1	O2	16957.53	0.194	12.59	MA-IP [41]
O1	O1	11782.76	0.234	30.22	MA-IP [41]
Ti2	Ti2	79502.113454	0.201010	446.779725	FB-IP [42]
Ti2	O2	10454.201954	0.207591	63.046504	FB-IP [42]
Ti2	O1	10454.201954	0.207591	63.046504	FB-IP [42]
O1	O2	1428.405811	0.357734	41.373873	FB-IP [42]
Ti1	Ti2	79502.113454	0.201010	446.779725	FB-IP [42]
O1	O2	2100	0.32	00.0	-

Where the ions are given the following partial charges: Q_{Ti1}=2.4e, Q_{Ti2}=2.4e, Q_{O1}=-1.2e, Q_{O2}=-1.2e

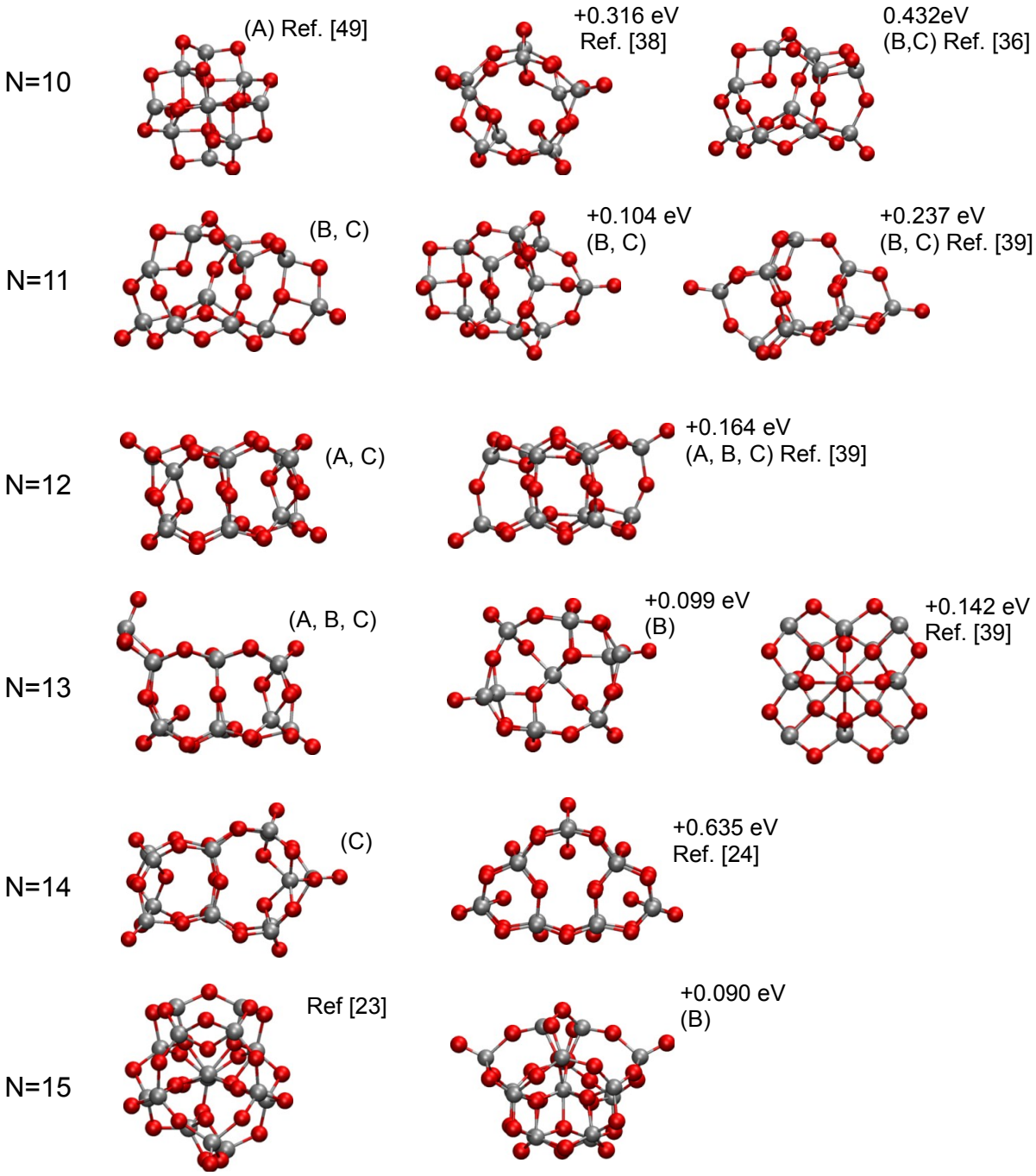
2. Buckingham parameters employed for newly parameterised IP for nano-TiO_2 where *a*, *b* ϵ {Ti, O}.

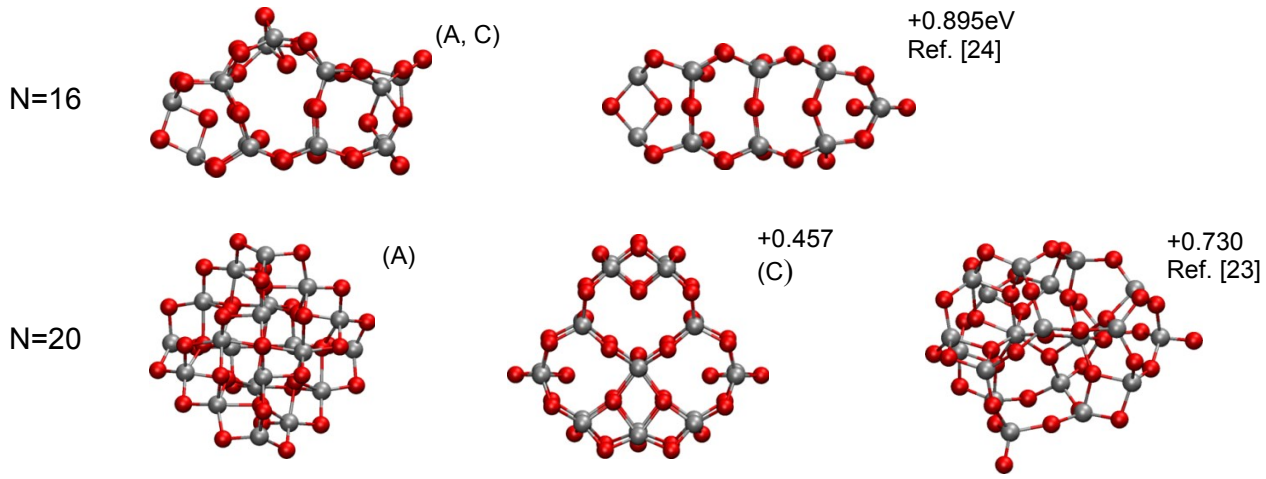
a	*b*	*A*	*B*	*C*
Ti	Ti	69000.0	0.210	500
Ti	O	22054.2	0.185	5.05
O	O	3328.5	0.297	16.48

Where the ions are given the following partial charges: Q_{Ti}=2.4e, Q_O=-1.2e

2. Comparison of nanocluster energies/structures with reported nanoclusters in the literature

For $(TiO_2)_N$ nanocluster sizes where we could find other reported candidate ground state structures we compare our results. We use A, B and C to denote how we found a nanocluster structure according to: (A) – data mining from known $(CeO_2)_N$ or $(SiO_2)_N$ structures, (B) - global optimization using the mixed IP approach (see above), (C) - global optimization using our new parametrization of the MA IP (see above). We also provide the reference to where any previously known structure was first reported and the calculated relative total energies (PBE0 Tier 1/tight level using FHI-AIMS) of clusters when found to be higher than the best candidate ground state.





3. Parameters used for fitting energy versus size data

Taking:

$a_0 = E_{bulk}$ (which for convenience we set to zero)

and

$x = N^{-1/3} a_n$

The expressions and a_n values used to fit the energy versus size data for the top-down nanocrystals and bottom-up generated nanoclusters were:

Top-down:

$E(N) = a_0 + a_1 x + a_2 x^2$

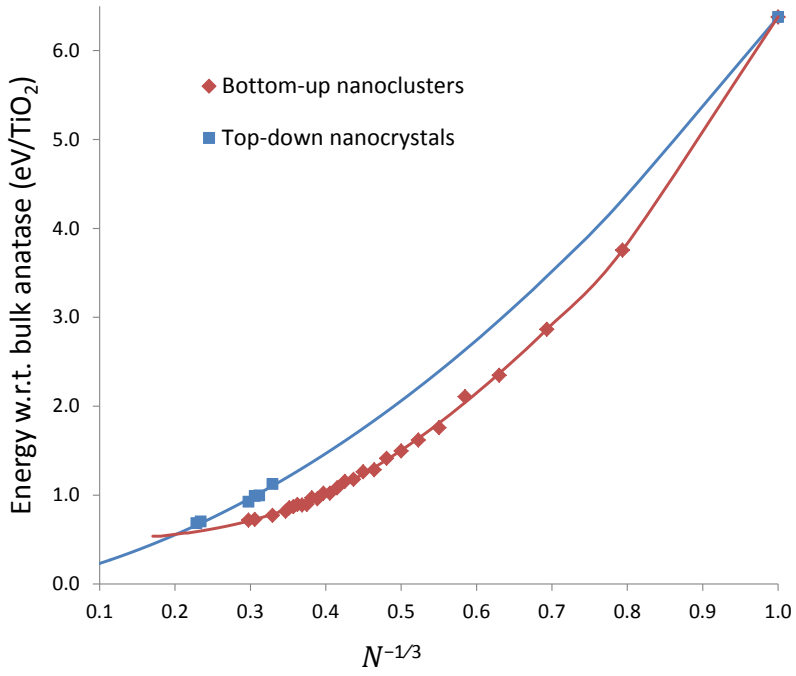
With: $a_1 = 1.86775$, $a_2 = -4.50952$

Bottom-up:

$E(N) = a_0 + a_1 x + a_2 x^2 + a_1 x^3 + a_2 x^4 + a_2 x^5$

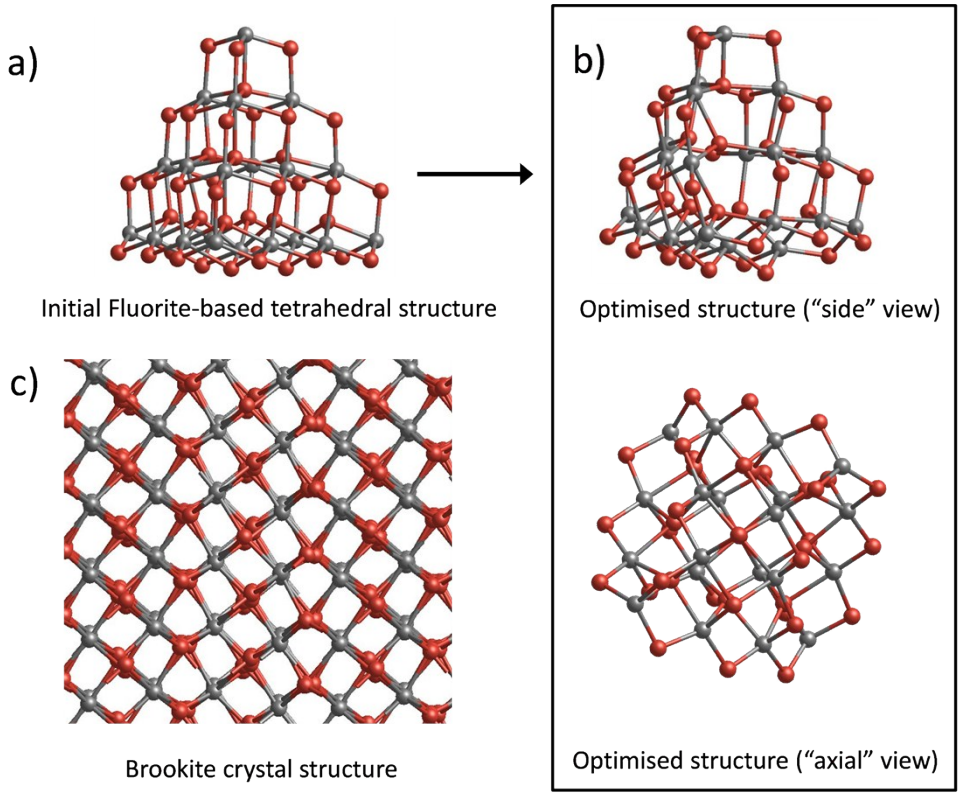
With: $a_1 = 6.68$, $a_2 = -34.60$, $a_3 = 92.36$, $a_4 = -93.32$, $a_5 = 35.26$

Below we plot the calculated energy versus size data for all considered nanoclusters and nanocrystals with respect to $N^{-1/3}$ together with their corresponding fitted curves following the above. The coefficient of determination (R^2) in each case is > 0.999.



4. Structure of fluorite-derived $Ti_{20}O_{40}$ nanocluster

Energetically stable $(TiO_2)_N$ nanoclusters for N=10, 20, 35 were found from data-mining the correspondingly sized fluorite-derived tetrahedral ceria nanoclusters in ref [16]. For the size N=20 we show below: a) the original data-mined structure, b) two views of the resulting low energy N=20 nanocluster, and c) a view through the brookite crystal structure for comparison with the lower view of the optimised nanocluster in b).



5. Coordinates of all reported structures

Here we provide the xyz coordinates of a selection of low energy nanoclusters (including the best candidate global minima we have employed and others shown in the text and SI) and of all the bulk cut nanocrystals used. The total energy (eV) at PBE0 tight/tier1 level of theory is reported on the second line of each reported structure which is in the standard xyz file format. The best global optimized clusters for N = 2 to 8 (refs 38, 39), 9 (ref 39), 10 (ref 49) and 15 (ref 23) correspond to the ones in literature where we were not able to find any lower energy cluster. Where multiple isomers are given these correspond to the structures in section 2 above. For other sizes we report clusters lower in energy with respect to those present in literature (see comparison above). For sizes where no globally optimised nanocluster is reported in literature (i.e. N = 17, 18, 19, 21, 22, 23, 24, 28, 35, 38) we report the coordinates of our best low energy candidate.

Bottom-up generated nanoclusters

Ti2O4

6
Total DFT energy = -54792.946306103
Ti -1.34940769 -0.00245198 0.00839631
Ti 1.34910745 -0.00151505 -0.00762956
O -0.00059395 1.24310043 -0.00147837
O 0.00029373 -1.24706748 0.00224443
O 2.22922453 -0.00322150 -1.35811930
O -2.22952409 -0.00074543 1.35888648

Ti7O14

21
Total DFT energy = -191790.263288290
Ti -0.36025033 -3.78933847 -0.66333567
Ti 0.06946597 -1.76387568 1.32422829
Ti -0.11073846 3.23455772 0.37226969
Ti 1.77724657 0.77854240 0.86868426
O -1.37756475 -0.72017968 1.70231514
O 1.28691860 2.33251802 1.45034340
O -0.19880500 4.80119888 0.64869816
O 1.57480857 -0.80038620 1.78300693
Ti -1.71517727 0.55714159 0.45660955
Ti -0.94670058 -1.25566387 -1.87742363
Ti 0.93998860 1.19718099 -1.76963761
O -2.25454441 -0.28144333 -1.06099692
O -1.77121540 2.27179696 0.74653812
O -1.37101936 -2.94379032 -2.12038583
O 0.80699567 -4.74137131 -1.18503822
O 0.34846790 2.80174703 -1.50686791
O 2.46928174 0.90744072 -0.81569348
O 0.11348200 0.60102661 -0.11675249
O 0.11705476 -0.07139305 -2.81054714
O 0.22174222 -1.89447761 -0.54724241
O -0.29292802 -3.48295136 1.27606281

Ti3O6

9
Total DFT energy = -82192.093849742
Ti -0.39358793 0.21015746 -1.82429400
Ti -1.28483872 -0.10867205 0.80298168
Ti 1.49865122 0.09983796 0.22655090
O -2.37018897 -0.96653790 1.62411872
O 2.93079070 -0.56887227 0.52653633
O 0.29682531 0.43039963 1.58907317
O -1.68879719 0.86362839 -0.90012181
O 1.05357335 1.06895859 -1.46808585
O -0.04242977 -1.02889879 -0.57675914

Ti6O12

18
Total DFT energy = -164390.818506874
O -1.78273559 -2.78122907 0.46698776
O -1.26130252 2.13918528 1.06427246
O 2.08541566 -0.25034378 1.49110154
Ti 1.16822590 -0.39829745 -0.11695762
Ti -2.24322888 -1.09320131 0.52272710
Ti -1.18989651 1.60832364 -0.84630245
O -0.14971164 0.42339502 3.54151891
Ti 0.05338958 -3.28516524 0.72286586
O 0.93624506 -2.06802153 -0.52648491
O -2.79924547 -0.15218840 2.02416974
O 0.58637751 0.92401050 -1.10566868
Ti -1.39839789 0.92990790 2.29067807
Ti 0.84979761 -0.83423770 2.64726432
O 0.39180717 -4.83416815 0.53231480
O 0.55173161 -2.52866388 2.48821820
O -1.67004922 2.72959995 -1.87703560
O -2.22009370 -0.05300383 -0.86541507
O -0.42744266 -0.41392796 1.15037857

Ti4O8

12
Total DFT energy = -109591.526385395
Ti -1.62308461 0.66663996 0.92298577
Ti 2.28711817 -0.25922464 0.60063929
O 0.32004283 0.19031678 0.65455442
O -2.15374782 1.00620074 2.39202936
O 3.13388196 -0.24567432 1.95628749
O 1.48127905 -1.91165490 -0.02137367
Ti 0.47089397 1.37324720 -0.91366055
O 0.03888422 -0.12349114 -1.85550985
Ti -0.13662357 -1.33390044 -0.50713147
O -1.74525078 -1.14760242 0.24459743
O -1.01743492 2.09555584 -0.24239360
O 2.20913451 1.33159431 -0.50838262

Ti5O10

15
Total DFT energy = -136990.603561966
Ti -0.26139738 0.90349800 -0.76818556
Ti -1.36789353 -1.34435379 0.78740697
Ti 1.25040991 -1.51717866 -0.02545209
O -3.07210318 -1.18158385 0.36757113
O 0.13050775 -2.37505679 1.19128418
O 1.52382143 0.22528297 0.26162557
O -1.22065045 0.40643039 1.11343220
O 3.96095490 1.15727671 -1.36204206
O -1.87404346 1.51246704 -1.10930439
Ti -3.01872665 0.77191851 0.25383253
Ti 2.55217128 0.40455566 -1.47492072
O 2.42573768 -1.54416564 -1.33884993
O 0.93688744 1.32705607 -1.98165032
O -4.01632948 1.68324285 1.11305877
O -0.41995625 -1.01591251 -0.87085727

Ti8O16

24
Total DFT energy = -219189.847544426
O 0.41906602 1.15137927 0.14430369
Ti -3.19230983 0.24892360 0.00910606
O -0.01807987 -0.18525193 2.62275729

Ti9O18

27
Total DFT energy = -246589.333919454
Ti 1.95717717 -2.03046234 -0.99787058
Ti -1.60877467 -1.34441164 1.24680270
Ti -0.43669769 0.76726480 2.74475758

O 0.15107203 2.83887011 1.90368084
Ti 0.70089882 -2.67414579 -0.16559313
O -0.36759240 -1.09735513 -0.05377397
O -2.62798112 -0.96203402 1.43244931
Ti 3.24378341 -0.19489921 0.08142324
O 2.67945458 1.01605874 -1.34191980
O 4.81782715 -0.45130352 0.08707719
Ti -0.91746460 -1.12734992 -1.86211746
O 0.06955360 0.23927614 -2.53222763
O -4.76635355 0.50532820 0.00345163
Ti 1.02956285 1.47546595 -1.61511265
O 0.20563953 3.10475892 -1.32329988
O -0.09959853 -2.78484591 -1.81315095
Ti 0.96893826 1.18137405 1.95264691
O 2.24724240 -1.87893337 -0.07422148
O 2.62834559 0.76807552 1.66397306
Ti -0.97808941 -1.42144151 1.70564231
O -0.15416601 -3.05073448 1.41382994
O -2.57687187 -0.71405150 -1.57344359
Ti -0.64942526 2.72817013 0.25612311
O -2.19576880 1.93295766 0.16475097

O 2.44118621 -0.99025801 -2.49702592
Ti 1.56231716 0.55340049 -2.62677788
Ti -0.82854646 3.32157950 0.53991677
Ti 2.20140972 2.50334904 -0.66173539
O 1.36519593 0.47530696 2.87819663
O 2.56270034 -1.29223256 0.61008809
O 2.45823311 2.14372044 -2.45269915
O -1.75976070 -0.48671675 2.87781659
O -0.80667644 2.38318547 2.24584515
O -1.37869279 1.93000528 -0.65452534
O -1.73912860 4.63361235 0.52540580
O 1.63928428 -3.73773976 -0.85378132
Ti 1.90169510 0.25393053 1.14149508
Ti -0.27769990 -3.58163455 -0.53538101
Ti -0.84113003 0.32576937 -0.97994435
O -1.22326193 -4.30985334 -1.60001365
O -0.15605228 -0.04889392 1.01889590
O 0.19203125 -1.71182172 -0.97939904
O -2.24182821 -0.69360854 -0.29237942
O 1.21766447 0.83449628 -0.73791823
O 0.98211061 3.60047023 -0.14087160
O -1.11977601 -3.01383162 1.11976214
O -0.20054825 0.41868639 -2.76178480
O 2.99126952 1.67470777 0.75087133

Ti10O20 (1)

30
Total DFT energy = -273989.443013773
Ti 1.83042590 0.98033005 -2.65397514
Ti -2.82034050 -1.48201430 -1.18729309
Ti -0.07117495 -0.12869914 2.49508612
Ti -1.02816296 2.56845139 2.01029992
Ti 0.52801804 2.30330355 -0.42418466
Ti -0.24873319 -1.00104492 -2.23347637
Ti -2.22380039 1.14545299 -0.10733390
O -0.51402328 1.13091994 0.96467169
O -3.64318862 0.06993642 -0.72038061
O -1.98298244 -1.49758130 -2.76543932
O -1.31169942 -0.61106703 -0.56294448
O 0.82022488 -0.21931297 -3.57266039
O 1.38172464 2.64881503 -2.02412897
O -0.57181557 1.45905474 3.37579200
O -2.64667103 2.32736728 1.29315014
O -1.29692082 2.09584226 -1.21768189
O 0.05105009 3.52830796 0.87188294
O 2.13761485 1.61282932 0.54299099
O 1.30841748 -1.11081030 3.31321864
O 0.82914595 0.38692357 -1.21533404
Ti 1.93087885 -2.02246392 1.90846186
Ti 2.45649003 0.02876430 -0.07689927
O 3.30758756 -1.26525235 0.99472208
O 3.23401737 0.32538165 -1.76349784
O 0.33264850 -2.35145159 -1.32047285
O -1.26045442 -1.31284004 2.07249324
O -2.22500011 -2.85757160 -0.12175823
Ti -0.57157057 -2.28113253 0.46286993
O 0.70522848 -3.27524315 1.35141190
O 0.90935463 -0.86237532 0.89110261

Ti10O20 (2)

30
Total DFT energy = -273989.126742073
Ti 0.82840329 -0.67276290 2.01996078
O -0.56708831 -3.56414533 0.03026051
O 4.42639154 -0.78812803 0.45071965
Ti 1.10892222 -3.77612793 0.94220787
Ti -1.92748570 -0.07600816 1.46927308
Ti -1.46696309 -2.12182194 -0.34470171
Ti -0.79955634 -0.14947898 -2.85640173
Ti -1.59216160 2.39749651 -0.84655122
Ti 1.95670202 0.07519249 -3.18150936
Ti 3.16623607 -1.54714571 -0.64199107
Ti 1.72270607 1.58872904 -0.82897161
Ti 3.43511538 0.51835150 1.28233988
O 1.37745593 -5.23784506 1.52963708
O -0.47633345 -0.73026358 0.44818163
O 2.37297737 0.20600211 2.67060979
O -2.28316852 1.42332712 0.66539331
O 3.10074221 2.01183528 0.37222538
O 0.73442989 0.07200323 -1.80007152
O -1.66272469 1.29162691 -2.44333311
O -2.30418449 3.81229921 -1.04317671
O 0.48689551 -0.17942801 -4.21774625
O 2.53495943 -3.07830805 -0.18961533
O -1.53151896 -1.63000956 -2.11098396
O 0.33240472 2.53546644 -0.52160156
O 2.45764715 1.67168755 -2.52812539
O 2.02463123 -0.23112343 0.23917840
O 3.07404604 -1.16434904 -2.43307322
O -2.78079796 -1.55170638 0.78801598
O 1.04175307 -2.35682725 2.25807482
O -0.68889074 -0.06390527 2.82434548

Ti10O20 (3)

30
Total DFT energy = -273989.011199808
O 0.78834347 3.35360844 -0.97168182
O -2.03043027 3.34875181 0.78597919
O -0.98458795 1.33454517 -0.17453888
O 0.74623268 2.50894652 1.84520077
O 0.84019837 -1.79183965 -1.63595123
O 3.62892354 -1.26355710 -0.52824853
O 2.79666419 -3.99570614 -1.43241508
O 1.43070222 -2.97402121 1.01940289
O -0.68598954 -1.10998760 0.53526187
O -4.79154148 -1.28364991 -2.40888611
O 0.53496202 0.87102499 -2.51615604
O -1.83126610 -0.86499900 -2.07904612
O -3.41980523 -1.87957658 0.22426361
O 3.56758809 1.03812882 1.45818466
O 3.42456928 1.56227257 -1.70545596
O 1.66686029 0.69754135 -0.11586938
O 1.20974653 -0.42806424 2.56453975
O -1.27102600 -2.37734963 2.57658832
O -2.72075487 0.39569251 1.84598110
O -3.75247229 1.01743650 -0.74981575
Ti -0.32971862 2.93131520 0.42366379
Ti 2.25089677 -2.67398279 -0.71831758
Ti -0.29217653 -0.48659457 -1.38954024
Ti -3.62637127 -0.82918222 -1.41206120
Ti 3.60785638 0.42890587 -0.28870988
Ti 1.61646098 1.90164472 -1.68509841
Ti 1.78735419 1.03425499 1.76239275
Ti 0.34235688 -1.92147594 1.86149415
Ti -2.32718208 -1.34905934 1.45668775
Ti -2.72738041 1.61060168 0.50578460

Ti11O22 (1)

33
Total DFT energy = -301388.641219750
Ti 1.07380441 1.36808246 1.69217082
O -3.29576682 -0.04381057 1.82445030
O -3.10016765 2.94628164 0.77845646
Ti 0.73772016 2.21287794 -1.62781831
O -1.33219668 -2.45824672 2.62797268
O -0.38247219 3.48784868 -0.94339946
Ti -1.34706666 2.77913403 0.43315702
O 2.89836437 -0.53361359 0.03847689
O 2.74512055 1.95109571 1.40845019
Ti 4.76375543 -1.13833798 -0.46160951
O -4.46251534 0.34690774 -0.77574867
O -0.14536845 1.00809647 -2.53491132

Ti11O22 (2)

33
Total DFT energy = -301388.536673684
Ti 0.67182897 5.01707737 -0.62979580
O -0.50817138 5.87532432 0.42629994
O -5.32324254 3.64680387 1.42523653
Ti -1.50647723 0.00348282 -0.53717434
O 2.07487151 3.59578355 3.29151626
O 2.42459254 -0.11363616 -1.15214033
Ti -1.67879437 5.07309487 1.60548438
O -3.25750281 5.81141107 1.62820114
O 2.17724956 4.59575471 0.25483176
Ti 0.05583181 0.68328550 1.77975259
O 0.81467617 5.06918579 -2.44596144
O 4.31845588 -0.88953433 1.00403227

Ti11O22 (3)

33
Total DFT energy = -301388.403994269
Ti 2.07148768 -1.00677479 1.40012106
O 3.79794975 -1.05942426 1.53519118
O 0.83323723 -1.87054242 2.47358923
Ti -0.89283763 -1.56568874 2.12616218
O 1.62258722 0.72324548 1.29614453
O -0.94441629 -1.30602605 0.29208892
Ti -2.16135309 1.38401945 1.67958157
O -3.74687406 0.96320742 1.15972038
O -1.51365418 0.03564451 2.72810775
Ti -0.64521796 3.16789730 0.07042631
O -1.23794479 3.06642421 -1.63363515
O -1.11310413 1.30392087 0.08474679

O -3.49370446 -2.40019358 0.21319217	O 3.39136164 1.93579045 1.04524555	O -1.66171084 3.16594780 1.59291082
O 4.88866665 0.80209219 -0.63156346	O 1.51275355 -0.22099467 1.77371319	O 1.11767372 3.30496155 0.18019433
Ti 0.17524313 -1.80448469 1.88465826	Ti -0.01925668 3.45086788 -2.78391914	Ti 2.32497836 1.85773151 0.06264166
O 1.35626395 -2.77848945 0.94815686	O -0.52785418 -0.76257093 -1.87424228	O 4.04257625 1.73129665 0.32714552
O -4.90804601 -2.12899774 -2.43363041	O -3.96732683 3.93620660 -1.22662480	O -5.99267954 0.03720947 -0.58610884
Ti -2.54851430 -1.66080616 1.46020552	Ti 2.40123928 3.27257389 1.51327264	Ti -2.20527086 -2.66072787 -0.03736303
O 5.56523714 -1.67574912 0.80812328	O -0.89200875 4.43012872 3.14972783	O -1.10847088 -3.06951297 -1.47845169
O 2.55483105 2.25662212 -1.66532162	O -0.35050535 3.50439476 -0.96092417	O -1.97942537 -2.97580743 1.76800747
O -2.10087527 -1.07603688 -2.04963864	O -0.21756472 1.40616859 3.49189932	O -3.66686100 -1.79499156 -0.37031702
Ti -0.69699835 -0.37093526 -1.36515418	Ti 0.90123649 0.39577601 -1.80830455	Ti -4.40911798 -0.00804150 -0.38723018
O 0.73820373 -1.50722776 -1.62373368	O -2.65410598 1.29022175 -1.05927470	Ti 0.03202588 -1.66693742 -1.60204099
O 0.85077382 -0.23196779 2.51161806	O -1.76976916 3.34732800 -2.98801124	O -0.79107926 -0.19877060 -2.27089408
Ti -3.55284967 1.14181180 0.47215626	Ti 0.31473459 3.10468011 3.32689461	O 1.63998729 -1.45805763 -0.38101258
O -1.82847963 1.11185375 -0.23985255	O 0.62902019 2.64814478 1.53886001	Ti 2.62439301 -0.71098019 -1.82962873
Ti 2.08624145 -2.08326163 -0.60149039	Ti 3.08056474 0.06040818 0.66181682	O 1.40385160 -1.71556718 -2.79678203
O 0.77758616 1.08698119 -0.12130708	O 0.02236821 1.02063047 -0.28504591	Ti 4.90556228 -0.02634939 0.29862989
O 3.66962282 -2.53049343 -1.24523786	O 0.85933277 1.86937778 -2.92066386	O 4.29906286 -0.85052884 -1.36956185
O -0.28189350 2.55330206 1.89947506	O -1.39485307 -0.33893827 1.22464298	O 6.48226761 -0.03900247 0.56322287
Ti -3.90315107 -1.40963580 -1.42043464	Ti -2.44334947 3.08812176 -1.23799254	O 2.07581296 0.98392106 -1.52440830
O -0.95456110 -1.17445650 0.55578330	O -2.38681690 3.64282932 0.69183003	Ti -1.70240210 1.26448670 -1.73094316
Ti 3.26140233 1.30584586 -0.26504938	Ti -4.21968851 4.46631494 0.60864153	O -3.38949572 0.94705333 -1.72255080

Ti12O24 (1)

36
Total DFT energy = -328788.617831048
Ti -0.64844894 0.43724261 3.16659554
Ti 2.51483988 -1.61523911 -1.85482292
Ti 2.37964846 0.68918678 2.45039603
Ti -1.31293457 1.28987082 -0.21365941
Ti -3.57919479 -2.94813114 2.24060919
Ti -3.70800914 -2.12768815 -0.40712807
Ti -0.45800657 -2.89122174 2.25974265
Ti 1.99454594 -1.94510248 1.37475955
Ti -4.57179564 1.15141205 -0.22356021
Ti 1.83663199 1.27549794 -0.20694149
Ti -0.65422208 -1.94219739 -1.15423858
Ti -3.29343064 -0.10593181 2.53221172
O -2.23724010 0.60820241 3.93124501
O 2.95132681 1.81756337 1.16254810
O 1.25156536 -3.31514850 2.44891581
O -4.43343892 0.86866002 1.71407929
O -4.08298350 -1.61502350 3.31101528
O -2.29988562 -2.73513061 -1.36412711
O 2.84977093 -2.32359384 -0.05497156
O 0.99648096 1.20436855 3.51271184
O 0.70934535 -2.21828041 -2.19099471
O 3.03561200 -0.96279883 2.58247218
O -2.02104386 -3.82970842 2.56011783
O -5.83641657 2.00314605 -0.69638711
O 1.29588696 -0.04516181 1.08302567
O 2.42444244 0.29204748 -1.50797984
O -4.50393594 -3.33706019 0.73989318
O 3.57927456 -2.04796187 -2.96297958
O 0.28433955 2.18415649 -0.38687775
O -4.52105836 -0.67271200 -0.88404215
O -2.86079834 1.95236659 -0.63269285
O -1.04671710 -0.19478514 -1.17961917
O -2.80075368 -1.57435340 1.19645466
O -0.00257652 -2.28075576 0.57959009
O -1.51993896 0.69795097 1.56176479
O -0.49188633 -1.35532406 3.19709514

Ti12O24 (2)

36
Total DFT energy = -328788.453637826
O 2.20464357 -0.40139362 2.62252926
Ti 2.09866948 1.28246669 1.90384612
Ti -0.66531893 1.73347114 1.67361141
O 3.61798260 1.77989086 1.23121713
O 4.23669746 -0.65455210 -0.69538950
O 0.92954610 1.33555043 0.40776719
Ti 4.31508866 1.28801981 -0.51704077
Ti 1.21560431 1.53844530 -1.45097388
O 0.75573098 2.27836445 2.67598577
O -2.22080709 2.67157028 1.89253158
O 2.87145716 1.98227745 -1.61997566
O 5.75164469 1.90041744 -0.84842610
Ti -3.27530697 2.08992020 0.51049429
O -3.26966911 2.87512909 -1.15970503
O -0.16532373 2.60369394 -2.05830405
Ti -1.84522293 1.97213490 -1.83943181
O -1.65305371 1.33644793 -0.11654344
O -0.92954690 -1.33555122 -0.40777131
Ti 0.66531796 -1.73347180 -1.67361550
Ti 3.27530618 -2.08992105 -0.51049845
O 2.22080616 -2.67157093 -1.89253568
O 0.95508782 -0.07650733 -2.23907187
O -0.75573188 -2.27836511 -2.67598991
O -2.20464443 0.40139296 -2.62253307
O -4.23669805 0.65455115 0.69538558
O -3.61798348 -1.77989169 -1.23122114
Ti -2.09867037 -1.28246746 -1.90385015
O -2.87145773 -1.98227862 1.61997159
O -0.95508901 0.07650663 2.23906789
Ti -4.31508928 -1.28802091 0.51703685
Ti -1.21560500 -1.53844603 1.45096992
O 1.65305316 -1.33644868 0.11653957
O 3.26966817 -2.87512996 1.15970088
Ti 1.84522222 -1.97213562 1.83942792
O -5.75164512 -1.90041888 0.84842227
O 0.16532305 -2.60369465 2.05830010

Ti13O26 (1)

39
Total DFT energy = -356187.963492444
O 2.52580893 1.05450287 -0.55449123
O -1.77995963 -0.42885145 -3.15288250
O -1.16772026 1.69386549 1.58377986
Ti 1.33308796 0.07971641 -1.53345172
O -3.15846252 0.67469128 -0.88157738
O -1.96163111 -4.70018110 -2.23115135
O 1.02122465 -4.35471055 -1.26248340
Ti -1.47518744 -2.68843070 1.35442917

Ti13O26 (2)

39
Total DFT energy = -356187.864652994
Ti 0.38246556 1.84846792 3.50454070
Ti 1.90027493 -2.69015789 1.16890291
Ti 1.85675568 3.33351337 1.06304262
Ti 0.27367806 0.29536665 0.27534581
Ti -1.19736228 -3.31931131 -0.49358599
Ti 3.01251081 1.95218199 -1.01772213
Ti 0.51759625 -1.24903947 -2.76724950
Ti -2.12818172 1.80424869 2.18775795

Ti13O26 (3)

39
Total DFT energy = -356187.821491511
O 0.00000472 0.00002180 -1.79096080
O 1.18130091 -3.65744069 -1.74706315
O 2.06467253 -1.05648189 -2.75775829
Ti -1.93928328 -0.62635955 -2.07979384
O -2.06466762 1.05655753 -2.75772000
O -1.05651841 -2.06463158 -2.75776974
O -3.65746157 -1.18127633 -1.74701919
Ti 0.62638874 -1.93925516 -2.07981799

O	-4.15246157	0.10869335	-3.74894691	Ti	0.81211783	-1.30787368	3.28515209	O	2.63104009	-3.05243591	0.89540254
O	-0.29645048	0.47300537	-0.88235836	Ti	0.04677879	1.93915997	-2.52738287	O	-0.86464185	-1.68938704	2.52411543
O	3.15672278	-3.23601838	0.84080887	Ti	3.02978853	-1.21078054	-1.45320477	O	-1.88661391	-0.60934371	-0.07979281
Ti	-1.70451874	0.58728488	0.21184429	Ti	-1.28863123	3.85990128	-0.54468344	Ti	-3.70377722	-1.19638729	0.06060495
Ti	-2.57296831	0.46363719	-4.82329445	Ti	-2.11655808	-1.39146379	1.70712022	Ti	-1.20774320	-2.36033746	1.03669657
O	-3.85220203	-2.20732087	-1.81235029	O	-0.64214073	-2.35098384	-2.13223143	O	-3.05241355	-2.63105056	0.89541944
O	1.08549163	-0.00286646	-3.33893598	O	3.23595078	-2.36677188	-0.08553144	O	-0.34806421	-4.01475499	0.89571181
O	1.87616132	2.03223594	2.34438387	O	-0.09630049	0.31016567	-3.44722196	O	0.60934645	-1.88662400	-0.07981287
Ti	3.67053819	-2.21280248	2.40673917	O	0.52272182	-3.41178579	0.45870673	Ti	1.19638740	-3.70378829	0.06055879
O	3.80843925	-0.36589042	1.82880866	O	-1.30913929	2.38481034	3.78022038	O	-4.01473124	0.34805110	0.89578466
Ti	-2.81431461	-3.52665004	-1.12379588	O	-1.93163362	5.31565874	-0.58434162	Ti	0.00001139	-0.00005504	3.23598877
O	4.96617286	-2.76981153	3.15652829	O	1.84662688	-2.77884980	3.02920744	O	0.00001711	-0.00007952	4.82501666
O	-2.28146833	2.02870951	-4.82205927	O	-2.29467406	2.88431177	0.85799683	O	1.68935246	-0.86469293	2.52412223
O	0.05584789	0.00356863	3.86802831	O	1.01712652	0.28879797	4.19751711	O	0.86465813	1.68930071	2.52416384
Ti	-3.42555035	-0.48220035	-2.27314771	O	0.47051081	4.00966869	0.32552113	Ti	-0.62638393	1.93931237	-2.07975694
Ti	1.69672576	-3.08438819	-0.08387751	O	2.30743912	-1.78673738	-2.99323324	Ti	-1.19637720	3.70377836	0.06067682
O	-2.77390336	-3.81307732	0.65792008	O	-2.57865327	-2.83070250	0.86305222	O	-1.18129577	3.65748519	-1.74694847
O	-1.10617788	-2.54762327	3.08140065	O	3.92037793	0.37388303	-1.34731535	O	0.34807499	4.01472084	0.89583408
Ti	-0.25582266	-0.99979578	-4.06177212	O	-2.99609875	0.22061323	2.09154486	Ti	1.20775535	2.36029722	1.03676519
O	-0.07437959	-2.79293233	-3.73659549	O	1.85770393	2.29729043	-2.31437299	O	-0.60933608	1.88661729	-0.07975469
Ti	-0.36480017	-3.81208992	-2.27135231	O	3.35290593	3.44578800	-0.04172172	Ti	-2.36031006	1.20772849	1.03675330
O	-1.19928870	-2.66667002	-1.08582668	O	-0.94705796	3.35445976	-2.44610211	O	-1.68933488	0.86460641	2.52415573
O	2.03557450	-2.21144144	3.48652170	O	-0.90183190	-1.70009116	3.07902713	O	-2.63102551	3.05240047	0.89550687
Ti	0.52067537	-1.58512555	2.97845426	O	-1.55817100	-4.79161073	-0.97979261	Ti	3.70378768	1.19637709	0.06063114
O	-1.95018604	-0.99367995	1.01691508	O	1.59412411	3.02775350	2.87954706	O	4.01474575	-0.34808734	0.89576146
O	-1.03018488	-0.46888456	-5.54259186	O	-0.47688940	1.45011125	-0.86045504	O	1.88662480	0.60933808	-0.07977865
Ti	2.63212496	0.76467041	1.24153863	O	-0.32248029	1.18629799	1.90659297	Ti	1.93928817	0.62641440	-2.07978050
O	0.40578066	-2.69585296	1.18028640	O	1.88220432	1.56318011	0.40118661	O	3.65746782	1.18132255	-1.74699247
O	1.75098880	-1.60384419	-1.11063286	O	1.32492859	-0.92894967	1.54290984	O	3.05242404	2.63101480	0.89549195
O	1.00451205	-0.17047707	1.59374997	O	-1.05739066	-0.89320174	0.32073119	O	1.05652181	2.06470757	-2.75770929
Ti	0.26342110	1.24124652	2.61016105	O	1.29826054	-0.58843197	-1.13144976	Ti	2.36032515	-1.20776900	1.03670745

Ti14O28 (1)

42
Total DFT energy = -383588.053217711

O	0.59785769	-1.44654723	-2.01183531
O	-2.35094093	0.97657427	1.73328667
O	-0.49691831	1.63902323	-0.33612274
Ti	-1.08144468	0.65430080	2.99797502
O	-2.89400950	0.38294326	-4.24820554
O	2.90880059	0.84411012	3.12820723
O	-1.04925163	-0.98649951	3.66863088
Ti	-2.00000597	0.70517988	-0.03763559
O	-1.71697721	3.19667353	-3.61853326
O	1.75150207	-1.80382245	3.76198861
Ti	-2.08612276	-1.33277512	-4.72047765
O	-0.39735224	1.12724325	-3.11772985
Ti	0.57779028	-3.83811873	0.75033736
O	-2.99437869	1.31649436	-1.43930404
O	2.15793788	0.81573338	-1.11658349
Ti	0.37212445	-1.80135386	2.75570507
Ti	2.22152663	-0.74009979	-2.03321260
O	1.71173607	2.66421059	1.02735626
Ti	1.16071542	2.21991633	-0.63039147
O	0.90338517	2.17908815	-4.96271023
O	0.98733544	3.36690661	-2.08371738
Ti	0.06268906	2.93672125	-3.56604614
O	-1.88014061	-2.26394977	-3.04937038
O	3.33681958	-1.87651568	-1.17172588
Ti	1.48003952	1.58989689	2.49759761
O	2.26932023	-0.26908178	-3.79896908
O	-1.72115026	-1.02617152	-0.36094534
Ti	-2.31390961	1.51958696	-3.10140044
O	2.33291460	-4.27756561	0.53106347
O	-0.13284229	-3.54864361	2.36112511
O	4.53737545	-1.15851969	4.61159961
O	0.04287161	1.96456074	3.58260406
O	-2.89102287	-2.15685611	-5.82624876
Ti	3.47926991	-0.98694298	3.42708624
O	0.38768402	0.12798715	1.96088352
O	-0.53999851	-3.75577703	-0.66042418
Ti	-0.98292299	-2.20728353	-1.55412027
Ti	3.02645123	-2.57625827	0.48658326

Ti14O28 (2)

42
Total DFT energy = -383587.417688194

Ti	1.38610394	4.42736552	-0.99406734
Ti	1.38610393	-4.42736556	-0.99406737
Ti	-1.38610396	4.42736552	-0.99406734
Ti	-1.38610393	-4.42736555	-0.99406737
Ti	-1.63137989	-2.55933967	1.31567638
Ti	-1.63137988	2.55933960	1.31567640
Ti	1.63137988	-2.55933967	1.31567637
Ti	1.63137987	2.55933961	1.31567639
Ti	-1.36820799	-0.00000003	3.04913016
Ti	1.36820798	-0.00000004	3.04913014
Ti	1.69377460	1.55887732	-1.88808293
Ti	1.69377460	-1.55887736	-1.88808294
Ti	-1.69377457	1.55887733	-1.88808293
Ti	-1.69377459	-1.55887736	-1.88808294
O	-1.79988404	1.44384164	-0.10178326
O	-1.79988405	-1.44384170	-0.10178327
O	1.79988405	1.44384164	-0.10178326
O	1.79988406	-1.44384170	-0.10178327
O	-2.20277220	-4.18169129	0.61055188
O	-2.20277220	4.18169123	0.61055191
O	2.20277220	-4.18169129	0.61055188
O	2.20277220	4.18169123	0.61055191
O	-2.47638598	-0.00000001	-2.44937756
O	2.47638600	-0.00000002	-2.44937756
O	2.16081247	-3.33484793	-2.21235241
O	2.16081247	3.33484790	-2.21235239
O	-2.16081247	-3.33484792	-2.21235241
O	-2.16081247	3.33484789	-2.21235239
O	0.00000000	-1.37097710	-2.44684414
O	0.00000001	1.37097709	-2.44684416
O	0.00000000	-2.86902064	1.99112328
O	-0.00000001	2.86902058	1.99112331
O	-0.00000001	-5.59952430	-1.36790401
O	0.00000000	5.59952426	-1.36790395
O	-2.28437761	1.53814523	2.68388264
O	-2.28437761	-1.53814530	2.68388263
O	2.28437760	1.53814523	2.68388262
O	2.28437760	-1.53814530	2.68388261

O -0.32692610 -0.71688452 -5.29720245
Ti 0.74443946 0.38368411 -4.51287295
O 1.23733634 -2.08199787 0.87149276
O 3.95224514 -1.91301047 1.79838189

Ti15O30 (1)

45
Total DFT energy = -410988.195944419
O 1.86173578 0.01101599 1.20481520
Ti 0.30068659 -2.64020151 2.39392677
O -3.40211159 -0.53224232 1.68627903
O -1.13878282 3.48976876 1.70084232
O 1.96190329 -2.12780480 2.94379138
O -0.70760557 0.24849553 1.63420326
O -1.74657478 1.20548866 3.59441477
O 1.16336988 2.15857240 3.20643235
O 3.07394929 2.70383564 0.61562135
O 3.87226582 -1.75361037 0.54273108
Ti 3.09903178 -1.02810172 2.02260546
O 3.66778891 0.53268964 2.70751546
O 0.71445563 1.98831394 0.68568948
Ti 2.40264274 1.68511129 1.94425509
O 0.29369928 -4.24208598 1.52038533
Ti -0.50449667 1.99714945 2.50568488
O -1.15155629 -1.97453338 3.21484353
Ti -2.03391796 -0.39406290 2.73488057
Ti -1.95539361 -2.18284298 -1.91426025
Ti -4.31182221 -0.51210652 -0.04947651
O -2.26649310 3.75155357 -1.11379067
Ti -2.68179219 2.02285349 -1.62613068
O 2.04006373 -3.58660988 -0.97895322
Ti 0.41116617 -3.60670053 -0.19195955
O -3.47719718 -1.87574549 -1.16777220
O 1.72510300 -0.88509169 -1.06886245
O 0.23487189 -1.96612911 0.67266536
O -5.86596262 -0.82124628 0.14296789
Ti 2.30224652 0.22729469 -2.56509290
O -1.39495545 1.59577719 -0.41074446
Ti -0.64693634 0.04050023 -3.07086199
O -4.05720877 1.12376398 -1.03854256
Ti 1.91429135 2.60435455 -0.83325009
O 1.02958362 -0.01790809 -3.83565067
O 0.74968182 1.14600755 -1.59965148
Ti 0.25569580 0.12279400 -0.04195121
O -1.59297940 -1.43996809 -3.54572647
O 2.98982464 1.85975185 -2.16765437
O -0.91726953 -0.75367602 -1.31431741
O 3.60736276 -1.16042615 -2.53696459
Ti -0.82696011 3.36569184 -0.09657546
O -1.81291862 1.39313218 -3.13795604
Ti 3.08008676 -2.06020417 -1.07844252
O 0.73226996 3.93059535 -0.98684430
O -0.99084220 -3.64321378 -1.30311854

Ti15O30 (2)

45
Total DFT energy = -410988.105396724
O 2.46469100 2.72105719 2.84416722
O -1.20403078 -0.02565090 0.00121605
O 2.08509358 0.05267604 1.13463697
O -0.14014633 2.09134732 -0.98902973
O 3.87741474 0.04515672 2.75047633
O 2.11458743 0.90482649 -1.45665389
O -2.83572982 2.03006270 -1.43699574
O 4.19934097 1.64727774 -2.49388611
O 4.34114306 2.03784870 0.44416469
O -1.51858795 -2.07141930 1.97551343
O -1.24054989 0.24424997 3.86409467
O 0.49650726 4.47350333 0.86285536
O -0.00950134 1.48139950 1.66679716
O 2.44146995 3.89382663 -1.50952858
O 1.44134982 -3.43159192 -1.70365663
O 1.33568228 -1.62223083 3.24631386
O 2.05688873 0.19722596 -4.17154523
O -0.97471345 -2.50398691 4.81866109
O -0.80431389 1.63360144 -3.66817660
O 0.90313049 -1.21991975 -0.75690249
O -0.29926485 -1.46500575 -3.34087316
O 3.05482147 -2.49090152 0.89000209
O -0.24330811 -0.12656293 -5.94324084
O -2.76327533 1.79102622 1.66313766
O 3.53799661 -1.41273798 -1.98722691
O -0.52027020 4.23127693 -2.03761890
O -3.59142547 -0.60543288 0.20564543
O -0.47263441 3.18698581 3.35496993
O 1.81976116 2.35134064 0.41321683
O -1.56453741 -2.75716031 -0.94587560
Ti 3.26258246 1.48007533 1.78182014
Ti -0.07087254 -2.39381291 -1.90552203
Ti 3.14341457 0.19711916 -2.81907466
Ti 0.77049868 3.81666783 -0.79768855
Ti -1.37937406 1.67455867 2.89215973
Ti -2.09464239 -1.66665540 0.40092593
Ti 3.32796363 2.36313003 -1.06097675
Ti -2.80385573 1.00574528 0.06008016
Ti 0.70504728 0.66856274 -0.03433540
Ti 0.14118156 0.09878254 -4.41118877
Ti 2.49179248 -2.26819010 -0.82023383
Ti -1.32133907 2.60497164 -2.32950243
Ti -0.58060072 -1.55335853 3.59934416
Ti 0.85493134 3.15982091 2.10524430
Ti 2.71735803 -1.28926462 2.25487616

Ti16O32 (1)

48
Total DFT energy = -438387.315367218
Ti -4.82070783 -0.59263026 -1.01953005
Ti 2.35297647 -2.17946098 0.25116308
Ti 1.47812974 -0.62748330 3.24783934
Ti -0.04935350 -3.74573434 0.16227419
Ti -3.61806569 1.81580925 -1.68939399
Ti -1.89848344 2.22841377 0.75236248
Ti 4.47148180 -0.01996811 4.62679271
Ti -3.35152399 -0.59481839 1.58256214
Ti -2.15191434 -1.91781379 -1.26318141
Ti 4.58898069 -0.94501667 1.53753253
Ti -0.76619794 0.89413321 -2.16273039
Ti 2.24605745 1.01081021 -1.27204615
Ti -1.12484550 -2.30448607 2.24049809
Ti 4.13204025 2.48363588 2.47918828

Ti16O32 (2)

48
Total DFT energy = -438386.420614522
Ti -0.00000001 -1.39279790 5.56891869
Ti -0.00000000 1.39279791 5.56891868
Ti 1.39279790 0.00000001 -5.56891869
Ti -1.39279791 0.00000000 -5.56891868
Ti 1.67950771 1.62485729 3.06827770
Ti 1.67950770 -1.62485731 3.06827771
Ti -1.67950770 1.62485729 3.06827771
Ti -1.67950771 -1.62485730 3.06827772
Ti 1.62485730 1.67950771 -3.06827772
Ti -1.62485730 1.67950771 -3.06827771
Ti 1.62485731 -1.67950770 -3.06827771
Ti -1.62485729 -1.67950770 -3.06827770
Ti 1.77313147 1.77313146 -0.00000001
Ti -1.77313146 -1.77313147 0.00000001

Ti 5.08287163 1.45147331 0.07655334
Ti 1.07022401 2.46109068 1.68748195
O 2.15708691 -0.73520396 -0.85705654
O -2.71280454 1.07534498 1.88278777
O -5.01948548 -0.81186284 0.75635282
O -0.97110046 -4.02700754 1.75258985
O -2.11036704 -1.55175418 0.58551298
O 0.95144993 1.25660715 -2.56802657
O 3.84109590 0.92721327 1.41143217
O 0.27564459 -2.10314825 0.79073596
O 5.15216294 -0.29777868 6.04687070
O 4.12759569 -2.32952639 0.38400014
O -2.77973233 -1.62232806 2.90239020
O -0.61852698 3.21095585 1.54306363
O 1.69275088 2.09448088 0.04036497
O 5.87678304 -0.07436057 0.43622917
O 5.34024767 2.89865305 1.15442372
O -3.21566866 0.25703019 -0.76233677
O 0.81884203 0.92769310 2.55643547
O -3.92991843 -2.00177603 -1.74370142
O 4.01099207 1.47163189 -1.40177665
O -2.25401264 1.76483547 -2.85953565
O -1.11372312 -0.87064658 -2.29137111
O 2.48435320 3.27312237 2.48295108
O -3.21189679 2.94507857 -0.34994974
O 4.67400171 1.79824096 3.97039860
O 1.69887371 -3.87464314 -0.21195212
O 2.56427078 -0.33702838 4.56773208
O -5.23800908 0.95729929 -1.92428996
O 5.14508282 -1.11677371 3.16069336
O 2.58735213 -1.31325468 1.94449577
O 0.05919900 -1.77662076 3.46964181
O -1.27660718 -3.47589120 -1.18863287
O -0.86923912 1.30416159 -0.41383150
Ti 1.77313147 -1.77313147 0.00000000
Ti -1.77313146 1.77313146 -0.00000001
O -1.45858903 2.18750530 4.83228583
O -1.45858904 -2.18750529 4.83228585
O 1.45858903 2.18750529 4.83228583
O 1.45858902 -2.18750529 4.83228585
O -2.18750530 1.45858903 -4.83228584
O -2.18750529 -1.45858903 -4.83228583
O 2.18750529 1.45858904 -4.83228584
O 2.18750529 -1.45858902 -4.83228584
O -2.44721415 -0.00000000 3.10502133
O 2.44721415 -0.00000001 3.10502132
O 0.00000001 -2.44721414 -3.10502132
O 0.00000000 2.44721416 -3.10502133
O -2.46937278 2.35631626 -1.59962543
O 2.46937278 2.35631626 -1.59962543
O 2.46937278 -2.35631625 -1.59962543
O -2.46937277 -2.35631626 -1.59962542
O -2.35631626 -2.46937278 1.59962544
O 2.35631626 -2.46937278 1.59962543
O 2.35631626 2.46937277 1.59962542
O -2.35631625 2.46937277 1.59962542
O 0.00000000 -2.03080879 -0.22290418
O 0.00000000 2.03080877 -0.22290420
O 2.03080879 -0.00000001 0.22290419
O -2.03080878 -0.00000001 0.22290419
O -0.00000001 -1.53326551 2.43404287
O 0.00000001 1.53326550 2.43404286
O -1.53326551 0.00000000 -2.43404287
O 1.53326551 0.00000001 -2.43404287
O -0.00000000 0.00000001 -4.40698808
O -0.00000001 -0.00000000 4.40698807
O -0.00000000 0.00000001 6.80426961
O -0.00000001 0.00000000 -6.80426961

Ti17O34

51
Total DFT energy = -465787.571636384
Ti 2.36840633 -1.04086499 2.91355597
Ti 0.55442158 -0.23760063 -0.27731658
Ti 0.48703799 -1.29967637 5.08856237
Ti -2.45867472 -1.38644743 1.31754912
Ti -0.71987871 2.67487850 -1.48017446
Ti 2.37553064 1.81054042 2.24509195
Ti -1.10516388 -2.98123708 3.61211916
Ti 2.29683255 2.79399195 -0.39795971
Ti -0.26407732 -4.40736726 1.18480414
Ti 2.64898120 -2.87529420 0.74346831
Ti -2.07144599 1.41413935 1.26567115
Ti 0.07830722 1.55070720 3.80763515
Ti -0.21148907 -2.03989528 -3.10144110
Ti 2.87783897 0.79419565 -2.86230272
Ti 2.90540040 -1.93831753 -2.40179361
Ti -1.62871191 -3.11849239 -0.89873898
Ti -0.25776906 1.28249903 -4.29015216
O 3.85973382 -0.71755532 -3.31840607
O 2.25853622 -1.22513076 4.75149177
O 3.35916320 -2.48557518 2.34921627
O -3.37889030 0.20508608 1.47339196
O -0.64744443 -0.58805054 -3.91965821
O 1.67818455 -1.36260449 0.90665919
O -0.87497539 -2.73467884 1.05628287
O 1.46009031 2.68703166 3.60717338
O -3.05026521 -2.24330361 -0.16490908
O -2.01128549 2.52902051 -0.13400659
O 3.44757450 0.42016752 2.66362545
O -0.08183373 0.97351628 -1.42748068
O 3.47371841 -2.78571191 -0.89255314
O 2.03863516 -0.45628382 -1.68934790
O -0.54693959 1.58844001 -5.82880378
O 0.31499364 -1.83805160 3.32706625
O -1.20760150 -4.80088072 -0.31490867
O 1.61492792 1.32116202 0.47743773

O -0.76518810 -4.63207200 2.93296043
O 3.34756533 2.13251729 -1.72036505
O -0.22382326 -1.77049710 -1.22657641
O -1.07877615 2.66551462 -3.17556485
O -0.14560580 0.38120417 5.22308021
O 1.66433867 1.29573740 -3.96349151
O -0.73646643 -2.65706724 5.36688843
O -1.01851337 -0.08997473 0.86122356
O -1.38906915 2.02017183 2.83048733
O -2.58148828 -2.13311596 2.97130140
O 0.96238413 0.47406406 2.70888368
O 1.53011337 -2.65276424 -3.30713524
O 0.78915776 3.60540968 -0.98302832
O -1.56895969 -3.19163018 -2.71747691
O 3.04942562 3.18639302 1.18114534
O 1.51443020 -4.28034918 0.87728590

Ti18O36

54
Total DFT energy = -493186.658878693
O -3.12068630 -0.88236079 0.31843349
O -0.57644956 -0.11365056 2.36669624
Ti -3.86544708 -1.94105287 -1.07475601
O -0.43128438 -1.77963768 0.00890751
O 2.69890498 0.26276264 -2.20031142
Ti 5.58612153 -2.04531819 -1.97799272
O -4.97828775 1.33646710 0.93237380
Ti 2.43941331 -1.49689072 -2.00773377
O 4.27216930 1.37487603 0.02797286
O -5.84552109 1.33091772 3.81667441
Ti 1.18986388 3.23953114 1.77337672
O 1.21050744 4.59598291 0.56250039
Ti -0.74814806 -1.44473937 -1.71619073
O -0.89966057 0.34414627 -1.90803006
O -0.35709015 2.84380259 2.61037894
Ti 2.75492449 -1.90233868 1.51170966
O -4.80933583 -0.48407854 -1.43396773
O 1.12980152 2.15470019 0.30393340
Ti -1.48292666 1.45261838 2.21995029
O 4.32636233 -2.84385525 1.67704004
Ti -3.60646107 -2.13014502 1.68590189
O 5.16911124 1.73205149 -2.65419031
Ti 6.13013330 0.36378240 0.62501247
O -4.59651632 -1.15106981 2.71278793
O 2.67496778 3.21301136 -1.81714500
Ti 1.15107487 3.52454295 -0.90550202
O 6.87199778 -1.17122929 1.40928264
O -2.05798634 1.54109264 0.43197703
Ti 6.92126600 0.95389489 -2.46170403
O -2.37653231 -2.22618263 -2.06407955
O 0.76397098 -1.94161766 -2.57727718
Ti 5.83750292 -2.45574667 0.75917021
O 6.64547810 -0.93975879 -2.78351599
O -1.97384347 -2.64419034 2.29261716
Ti -0.43107226 -1.80693750 1.80781867
O 6.25486200 -3.29020046 -0.79658147
O -2.94810707 1.38656892 3.13560127
Ti -1.56316793 1.91257860 -1.31547448
O -3.28854744 1.90946876 -1.70320533
O 5.50896990 1.20690287 2.18449254
O 2.80133489 2.79106244 2.47165562
Ti -3.97413427 0.80077739 -0.35076017
O 5.17340253 -1.08249755 -0.37627460
O 1.20787212 -2.46927967 2.25997310
O 2.42883106 -1.84706047 -0.24306919
Ti -4.74587300 0.78184623 2.79660467
O -4.34716780 -3.05350839 0.27467873
O 3.92764814 -2.31273551 -2.66780844
Ti 3.70500930 1.70059785 -1.73490769
O -0.48121342 3.33832097 -1.67129996
O 7.17618369 1.08953852 -0.52422339
Ti 3.79026660 1.40385204 1.81784587
O 3.02151706 -0.20715675 2.07309378

O 8.06157413 1.63152138 -3.35152618

Ti19O38

57
Total DFT energy = -520587.335504025
Ti 0.60598134 -1.95222157 3.11604987
Ti 1.28212621 -4.72662213 -1.30199290
Ti -2.33299233 -2.88369648 2.00748623
Ti 3.38246940 -1.66470727 -1.82602410
Ti 0.75503672 2.94596937 -0.84533624
Ti 1.65180630 1.70209332 -5.07855421
Ti -1.34797599 -3.84137340 -0.52583112
Ti -3.29802362 1.88606005 0.65390194
Ti 2.83283069 1.05209997 -2.59683275
Ti -3.27722390 -0.08893886 3.10408539
Ti 2.77590667 -3.85625341 -3.50125271
Ti 1.95987898 -3.01126328 0.84498201
Ti -0.35097340 2.77782459 1.77384628
Ti -0.64745355 -0.31848647 0.42104780
Ti -2.47053234 1.70921832 -2.10079715
Ti -0.27205285 2.95832150 -3.48273501
Ti -0.78989956 0.68994266 4.07558938
Ti 1.27248439 -1.34645294 -4.56858817
Ti -1.38836138 -1.31638228 -2.56683475
O 0.87827432 1.37196363 -3.48548988
O -0.25253597 -0.71387282 -1.25326552
O -2.59214803 0.00693654 -2.75458771
O -0.90149109 -2.94101643 3.11342953
O -3.76107289 2.45379589 -1.01129773
O 0.51536956 3.09289787 -5.18330488
O 1.97001096 -3.05396830 2.68788381
O 1.46362059 -0.00232020 -5.76682722
O -1.51585832 0.08838612 2.47333631
O -2.00772009 -2.88243638 -1.93481435
O -0.43579074 -1.55620317 -4.09112316
O -4.19549762 1.03097262 2.04375088
O 4.20909465 -2.92626026 -2.84083939
O -2.27896044 0.64306040 -0.07132893
O 3.24818391 1.82497017 -4.18890889
O 0.37393153 -3.27242290 -0.13512907
O -2.09343767 2.74378025 -3.55720130
O 4.12923410 -0.00172450 -1.86630758
O 2.23480088 -5.40879378 -2.77068369
O -0.47625554 -5.25299756 -1.28802684
O 2.05692618 -2.93715429 -4.93388761
O 3.12422546 -1.97327133 -0.05342352
O 0.43645186 -0.59287018 4.37059133
O 0.17438555 1.42381677 0.71428084
O -2.38714255 -4.33840759 0.91637219
O -3.61573901 -1.83420953 2.85678737
O 1.77669020 -3.07043331 -2.22486109
O 0.56010450 3.91616513 0.71001622
O 2.30075880 2.09796547 -1.20861316
O -0.14621204 2.28669782 3.55355080
O 0.59268836 4.04224874 -2.32386730
O -2.51670535 0.50718587 4.66261992
O 0.71297727 -1.23839509 1.46952616
O 2.17231738 -0.73100486 -3.04090786
O -1.76255989 -1.90944133 0.65291692
O -0.70887656 2.08215760 -1.65462961
O 2.35617053 -4.67707145 0.15047961
O -2.10490824 3.00715243 1.42536562

Ti20O40 (1)

60
Total DFT energy = -547986.822287173
O -3.97052262 1.99681881 -0.75213991
O -7.86400523 -0.69247877 5.94042509
O -0.20137990 1.02685197 4.88597895
O -1.09660557 -2.69936178 4.28126165
Ti -4.59155524 2.19721890 4.62348074
Ti -6.21366639 0.00161966 5.42687987

Ti20O40 (2)

60
Total DFT energy = -547986.365685410
O -1.70463691 -3.37845249 1.81170382
O -2.78431813 0.09769126 -3.24304278
O 1.25388717 -2.87605412 1.05541801
O -1.19732046 2.60443787 -3.79580019
O -5.39148546 3.80154761 -2.24777918
O 3.33304344 2.48096208 2.28558787

Ti20O40 (3)

60
Total DFT energy = -547986.091979391
Ti 0.68215922 2.44842817 1.93365589
O 4.91079113 -1.91174741 0.31684537
Ti 4.73432956 -0.21485866 0.47751452
O 3.06237956 -3.32807941 2.16511826
Ti 2.24220617 -2.31861213 3.28392677
Ti -2.61012311 2.56778497 2.18244529

Ti	-7.85490937	-2.35063160	5.20346500	O	-5.37860970	0.90923197	-2.17899003	Ti	3.99231567	-3.64357670	0.44882868
O	0.81718957	-1.82527481	5.62326487	O	-3.98502934	1.52584784	0.31060219	O	-0.93004812	-3.49496610	1.55164529
O	-2.04316314	-2.40137638	1.79928883	O	0.54408759	1.31258158	3.61193395	O	-1.87171083	-1.44601448	3.43204705
Ti	-3.93973304	2.41146378	1.02888615	O	0.94167517	1.20734886	-4.96641683	O	0.78008433	-3.04503986	4.09073948
Ti	-1.53937137	1.85869239	3.98810649	O	-3.52535033	-1.18668401	-1.34544273	O	-4.62219410	-1.05029916	4.29858327
O	-3.50069670	4.18033955	1.41303592	O	2.09886945	4.00636774	-0.36982932	O	-0.85450632	2.92226678	2.72000194
O	-4.84543134	-1.80334786	2.00939132	O	2.80838562	-0.18254183	-2.92633843	O	-2.18306570	1.88552235	0.51678732
Ti	-6.81366071	-2.46277581	2.53005420	O	-3.24406873	2.81059852	-1.58681476	Ti	-3.61635489	-0.65324790	3.12401997
Ti	-5.28248462	-3.51733676	5.05520386	O	-1.94069102	1.08514968	-6.00518069	O	0.26247435	0.99057663	0.84182442
Ti	0.34493995	-3.51020752	5.12757345	O	-0.16892044	-0.54879748	-2.91557649	O	-3.35577048	1.26289017	3.02726504
Ti	-3.30524291	-0.54761843	5.22050255	O	-4.70150807	-0.26880364	-4.73307682	O	2.12457231	1.92192112	2.92794518
Ti	-3.38978381	-2.20435583	-2.14797519	O	-6.37155121	2.10242894	0.26238242	O	5.10151395	-4.74241073	0.75313059
Ti	-0.18582547	-2.81004777	2.43900610	O	-2.60375577	4.99892575	-3.61590818	Ti	3.40608050	0.61405349	2.82820159
Ti	-3.10622320	4.12609511	3.18329011	O	1.82627803	-0.50952488	-0.32557290	O	3.16676377	-0.80534288	3.87140393
Ti	-0.44344016	-0.76829916	4.80465542	O	-0.41935478	3.90885136	-5.71663953	Ti	-0.52613054	-2.42993934	2.95941699
Ti	-3.71431571	-3.36036911	2.39846859	O	-1.70917072	1.93405016	1.73182077	O	-4.26477827	-1.30579025	1.41624787
Ti	-2.48289520	-4.02699552	5.01370771	O	-4.50457935	-3.35881036	0.56193074	O	5.05381649	0.67743569	2.09497190
Ti	-1.36993800	-2.32504132	-0.10303661	O	-1.34105288	0.71214893	-0.73554369	O	-3.72665318	3.62126248	1.17868588
Ti	-5.49519869	0.04681910	1.91830201	O	-3.98326950	2.52166394	-4.43231832	O	0.91822673	-1.40847491	2.24516216
Ti	-1.49169474	-0.07756900	1.82919435	O	-5.16796464	0.55501130	2.95144264	O	2.94790830	-0.08462512	1.15264173
Ti	-5.20947141	-2.56656792	0.04325710	O	1.46165997	1.64296707	0.98796794	Ti	-1.09980278	-2.99201299	-0.16378306
Ti	-3.94662131	0.19135325	-0.75115581	O	-5.86940830	-0.74773931	0.39814782	O	1.82955358	-2.28365977	-0.17393036
O	-6.04877606	1.81299534	5.61812207	O	-4.05830420	-2.39721449	3.60310158	O	-2.83209282	-3.00376391	-0.58022932
O	0.94295438	-3.86570534	3.47845965	O	-1.03419880	-2.04845312	-0.69928816	O	-3.23120917	0.32170453	-3.76765755
O	-2.15790289	-0.16588705	3.67398568	O	0.34339966	4.73832820	-2.81112043	O	3.08410464	-4.20836219	-1.22266170
O	-7.07644655	-0.60364169	2.23701496	O	-0.42968709	-0.73692235	1.89130557	O	0.22805029	4.68756828	-2.11043010
O	-4.16117732	-3.94648395	0.82303355	Ti	-0.93753644	4.39825982	-4.02904770	O	-0.15481465	0.00985134	-4.65354111
O	-3.09289835	1.51351884	5.38190239	Ti	1.19084618	0.57428790	-3.26577614	Ti	-1.19737279	3.52430288	-2.39337629
O	-3.65514732	-2.43559135	4.60019433	Ti	-1.58800315	-0.68480567	-1.77724646	O	-2.61941596	4.27439771	-1.53096627
O	-0.93887377	-0.61948608	0.12559805	Ti	-0.47030517	-2.30410908	0.98879613	O	-2.28334671	1.79560559	-1.91114355
O	-0.92212045	-4.57695289	5.86858628	Ti	2.07087153	1.19098240	2.61654147	O	2.70521524	2.88779281	-1.66967301
O	-1.84042857	-0.90960087	6.08542752	Ti	-0.98095060	0.70899169	2.82811625	O	-4.73137449	2.02035528	-1.30447576
O	-5.01959293	0.39754536	3.84766418	Ti	-3.43167931	-2.89178681	1.95423226	Ti	-3.98285336	0.53642341	-2.09277923
O	0.04510618	-3.17392006	0.68547918	Ti	3.36441248	-0.16222388	-1.18646901	Ti	1.02349851	-0.41559009	-3.30810388
O	-5.49937496	-0.47577043	-0.09341430	Ti	0.68034122	3.58745930	-1.42659055	Ti	1.25316543	-0.72328121	0.42894972
O	-8.32436287	-2.82466389	3.51151146	Ti	2.54168564	-1.58761877	0.92084987	O	-1.18496711	2.70427887	-4.01000002
O	-3.61761024	-0.45769510	-2.46561631	Ti	-4.67250935	-0.57530242	-2.90777283	Ti	3.06951780	1.13830050	-1.98119452
O	-3.31994668	-1.72854795	-0.35346716	Ti	-0.54869109	2.10419540	-5.42942794	Ti	-1.11274707	0.73574540	-0.60432777
O	-0.92811908	1.52065453	2.22096068	Ti	-3.82042157	-0.59782961	3.35483121	Ti	1.64794167	-3.33655558	-1.66297711
O	-5.49775990	-3.92838203	3.30223773	Ti	-3.30704737	0.89155293	-4.79223151	O	4.59896184	0.62380166	-1.12292301
O	-2.70869339	-4.61530428	3.35537583	Ti	-4.96088819	-1.97489176	-0.55711894	O	-0.04469636	-3.93920674	-1.26109497
O	-6.24816920	-1.80432945	4.44749518	O	4.01516020	-1.54546865	-0.17165489	O	-0.57051980	-1.15116689	-0.08516942
O	-1.71933157	-2.84984205	-1.85566542	O	-5.68181728	-1.96769237	-2.22290115	O	1.20880731	3.75559042	0.80901355
O	-1.52014283	3.69584341	3.96257414	Ti	2.89376789	2.61643588	0.50930569	Ti	-3.97931369	-1.59999237	-0.26838531
O	-3.34130914	2.29328522	2.99087186	Ti	-5.16810312	2.34893560	-1.12231064	O	-2.82699141	-0.24226519	-0.76606429
O	-4.97862357	-2.98509754	-1.73096433	O	-3.32938316	-1.09028307	1.66483605	O	1.48314866	-2.13482091	-3.06909197
O	-5.55046814	1.88049750	1.54904429	O	1.14760996	1.99565213	-2.14771103	O	-0.56467921	0.11445080	-2.33261112
O	-4.80753952	-0.58502124	6.33564410	Ti	-3.78232759	3.69494975	-3.08074895	Ti	-3.42000024	2.99650658	-0.52444212
O	-4.03225917	-4.57519688	5.81590890	Ti	-2.06943743	2.15677983	-0.04270740	Ti	1.21738374	3.66713502	-1.01328673
O	-6.89764849	-3.65268125	5.97280269	Ti	-5.43584173	0.82835434	1.15444293	Ti	-1.50633349	0.91091162	-3.78254567
O	0.08402915	-1.04871003	2.77549329	O	-2.30301341	0.15217677	3.96706485	O	2.53225861	0.60206274	-3.60640846
O	-4.43372173	4.03704470	4.38056347	O	3.84320931	1.46822885	-0.53552582	O	1.74906785	0.13297429	-1.26926842
O	-3.28898126	0.50215198	1.11848586	O	-0.84351046	3.43345617	-0.48470407	O	-0.09304791	2.43980320	-1.23815033
O	-6.80160042	-2.99656462	0.79720638	O	2.71055463	-0.49397265	2.36546094	O	-5.01938258	-0.87800185	-1.59632727

Ti21O42

63
Total DFT energy = -575386.034583528

O	0.41149866	-3.54971760	-5.02622591
O	-4.10245668	0.43920180	-3.30149767
O	2.12678527	1.18836288	-0.15965552
O	-0.46521979	-2.62434118	3.46453371
Ti	2.75342486	1.91656851	4.23758392
Ti	-3.65466742	1.50079535	-1.90899086
Ti	-2.36333933	-2.24479374	-0.57161278
O	2.44176490	-2.29429454	3.24874923
O	2.11698590	0.15097409	-3.32256471
Ti	0.34878308	0.32307484	-3.70034396
Ti	0.10500208	1.15109776	4.95331706
O	-1.98558870	-0.36162157	2.62105580
O	-3.31599212	-2.32985355	0.97447693
Ti	-1.16532671	2.31237542	2.16012229

Ti -0.67943339 -2.09742586 -4.69158776
Ti -1.58301716 -1.35931877 4.12120770
Ti 0.92328641 -2.59757049 2.30183120
Ti 3.75691297 3.14417612 1.93273894
Ti -0.47855835 2.48785705 -2.16106337
Ti 0.58820717 -0.07095477 -0.06290282
Ti -3.09862075 -1.10786150 -3.56012194
Ti 2.92119664 -1.05493993 -2.29413979
Ti 1.47020095 -3.46470046 -3.53593352
Ti 0.36694026 -3.11335456 -0.87882217
Ti 1.18155092 2.95536183 0.61706722
Ti -3.58861400 -1.18572230 2.33821198
Ti 3.87694090 0.66419537 0.11885077
Ti 2.71158588 -0.54834276 2.88761082
O -2.87836838 2.51420049 1.58563851
O -3.32055239 -1.90117824 3.99497339
O -1.46593142 -0.50256243 -3.39548001
O 2.60964489 4.06679390 0.90064513
O 4.74744767 2.12337585 0.78994506
O 0.30248915 -2.16944272 -2.99132259
O 1.50405956 2.18210780 5.56580142
O -3.07568820 0.49465007 -0.47332856
O 1.19677239 0.42546501 3.79545646
O -0.16942849 1.33133343 0.93984884
O -4.85586149 2.17245617 -0.71133418
O -0.03692702 0.78687025 -1.72673525
O 3.91367760 3.26907195 3.75176176
O 3.67000008 0.38434556 4.17335802
O -0.94676937 -0.30513420 5.44434993
O 0.52728895 3.44122604 -0.99656506
O -3.37820240 -2.04505324 -2.05174942
O 3.83027790 -0.50394052 1.45750002
O -0.74308697 -1.38035106 -0.30408063
O 2.41548687 1.96034626 2.30264135
O 1.18631986 -4.32406572 -1.98243106
O 0.04713925 2.09431512 -3.85309076
O 0.18060146 -0.64399198 -5.27450139
O -0.08346750 3.66574656 1.74981756
O 4.28996787 -0.23496556 -1.41233080
O 3.03946367 -2.55781136 -3.32600100
O -1.00413012 2.14979224 3.95123768
O 1.72479135 -1.44874777 -0.94165136
O -1.38074405 -3.68975095 -0.91385063
O -2.28204184 2.65568891 -2.15992444
O 0.86711976 -3.59287865 0.79084493
O 1.11351918 -0.92452821 1.63720098
Ti -4.05141286 1.43328133 0.74981270
O -2.50590495 -2.22680752 -4.89877439
O -4.72244110 0.16399352 1.87324268

Ti22O44

66
Total DFT energy = -602785.895974887
Ti -2.34876639 -3.38915109 0.13302623
O 4.71604552 1.05686632 3.03106005
O -2.40239128 -1.01681119 4.15848870
O 0.72899179 1.42422790 0.42992306
O 0.23788991 -3.99612421 1.71164114
Ti -2.22940476 3.24899271 -0.82505938
Ti -1.05999202 -5.08430521 2.29811174
O 2.41378857 3.81417278 0.03110231
O -2.22812367 2.70335141 -2.52788319
O -1.16000241 1.73351346 4.29847699
O -1.60689014 -4.13092994 3.76017852
O -2.14525800 1.61023672 0.05118908
O 4.77081069 -0.61510337 -2.18934732
O -0.70501093 3.96262348 -0.18845209
O 5.01379529 -3.17680061 -0.24389621
O -2.26289705 -5.04047498 0.87519760
O 0.47909294 3.91933916 5.26374501
O -4.57606417 0.23678072 -0.11951204
O 1.97847556 -4.18091282 4.02418216
O 5.92839638 -0.23319126 0.56417375

O -3.15271923 -0.23395525 -2.71717355
O 3.35260712 -1.33554419 0.05454979
Ti -3.88818343 1.64818689 0.76587700
Ti 0.85040594 -0.00882655 -3.13277831
Ti -1.79178256 0.95072952 -2.99827065
Ti 0.59612332 -2.58018685 -1.20640280
Ti 0.76915311 3.27532741 0.69896938
Ti -0.80241382 0.15895009 0.27049498
Ti -3.64964348 -1.01022236 -1.12713242
Ti 1.66353697 -4.96866518 2.39524544
Ti 2.10447378 -0.00449738 0.47304514
O -0.91235214 -3.46480175 -1.02543480
O -3.86674956 3.31586068 -0.00812565
Ti -2.16953195 0.63044777 3.42590492
Ti 3.54986003 0.67312296 -2.64796948
O 5.44670123 2.88735895 0.57639225
O -2.04442920 -1.05016060 -0.38014725
O 4.06110765 2.38743651 -2.12065291
O 0.33636578 -6.21582384 2.65695158
O -3.85521201 -2.77829483 -0.79411437
O 2.58818854 -2.89470771 1.93756006
O -3.61185994 1.41999193 2.49840188
O -2.09064438 -2.51465192 1.69100234
O 2.12507071 0.38329037 -1.60801808
O 3.59742072 1.32035829 0.42605840
O 0.61588305 -1.15125462 0.06898598
O 2.43733900 0.43140638 -4.02742008
Ti 5.02484852 -1.39785756 -0.55704633
Ti 2.00235590 -2.41423554 3.60936308
Ti 3.30113046 -3.59930059 0.39584832
Ti -1.43740749 -2.35720056 3.37054249
Ti 3.91701560 2.94643476 -0.42832665
O -0.54620913 0.57865729 -4.22917824
O -1.12823049 0.10689898 2.00775477
Ti 0.49909294 2.72034473 4.20950067
O 0.64910818 3.44700161 2.39867385
O 2.98644818 -5.23055233 1.11099594
Ti 3.09363287 0.43205567 3.76247013
O -0.50913122 0.58359846 -1.79465826
O 2.06953399 1.62458437 4.48371676
O 2.04541182 -3.56456917 -0.92688527
O 0.70943467 -1.75917154 -2.83533268
O 2.19440200 -0.09311486 2.24625710
O 0.29279143 -1.89091675 3.67694483
Ti 5.23689740 1.23582443 1.34894234
O 3.06462550 -1.21908277 4.50981605

Ti23O46

69
Total DFT energy = -630185.540673243
Ti 1.41558917 -1.73469641 -1.61373539
O -3.35914144 2.50378294 -0.55247510
O 1.79427182 -3.21470643 -0.56459504
O -0.46302682 1.72081007 -0.54297430
O 2.96765406 -1.52449768 -2.69240088
Ti -1.77851463 -2.44703908 -0.30804105
Ti -2.34713678 -0.45650679 2.33449488
O 4.90187362 -2.61282198 -1.14477241
O -3.94743189 0.25206234 1.67135089
O -2.19997291 -1.95348469 1.35058526
O -1.26103531 4.33690123 -2.32323867
O -3.22000593 -2.57612761 -1.39938143
O 0.52905322 -2.12886437 -6.87146563
O 0.14050700 0.79643455 -7.49131825
O -1.40181830 -2.51809923 -4.98501871
O 0.71383454 -1.85210635 1.90941307
O 3.54494770 1.68380852 2.14654106
O -1.44232799 1.90092439 -2.72091589
O 2.95202229 -0.13274278 -6.37676098
O 4.75149510 -1.81855568 -4.38893304
O -0.98175706 -4.05519708 -0.25188135
O -2.49567823 0.26539273 -5.99015388
Ti -0.24144258 2.25552956 1.34641902

Ti 3.31991660 -0.69388062 -4.68073260
Ti -3.88887140 0.83325469 -0.05839001
Ti 1.14224933 -0.44915675 -6.51543373
Ti 1.92927542 1.52616685 2.90877448
Ti -0.96933819 1.29869245 -6.16447003
Ti 0.71998817 -4.64866633 -0.25437836
Ti -1.69915597 3.16206992 -0.97003171
Ti 1.80796544 -3.27143737 2.25982080
O 3.29757969 0.93625252 -3.79983192
O 2.52618903 -0.85054930 -0.21428926
Ti 0.37901740 -2.83350956 -5.18186217
Ti -0.84041538 0.35998387 -1.76379033
O -0.96052909 2.98231292 -5.33498202
O 1.22635877 -4.83914284 1.47705735
O 3.36330011 -4.23920391 -3.18902750
O -4.88328212 -0.00227779 -1.31938905
O 0.70619803 2.84247424 2.81436972
O 0.02136627 0.31014567 -5.10849708
O -2.46625209 -0.12753049 -0.70879509
O -1.40548147 -1.04196258 3.79257676
O 0.95630588 -4.55868578 -4.91987336
O 1.33940533 -2.91758335 3.99000352
O -0.36788372 -1.42031252 -1.01646908
O 1.19665359 2.91923500 -3.18605675
O 3.48972661 -2.80556265 1.75476191
Ti 4.29088169 -2.71981143 -2.86242263
Ti -3.66507967 -1.04779347 -2.23179615
Ti 2.21218823 1.56232792 -2.56632450
Ti 3.22011173 0.85442557 0.50598026
Ti -0.55511343 3.21775403 -3.59200529
O 4.69454274 -0.28168785 0.70367815
O -1.37056221 0.99577377 1.93274459
Ti 4.01599216 -1.85763535 0.27912517
O 1.44091314 0.08612574 3.93344924
O -4.05473034 -1.42467382 -3.97906415
O 1.36594832 1.02919437 1.24171059
Ti 0.41573880 -1.37481686 3.62290488
O 0.96982695 0.18257427 -2.27075769
O -1.09665048 3.71787371 0.64889249
Ti 1.57953826 -4.58037459 -3.21165149
O 3.10265486 1.85034428 -0.99418375
O 0.75907969 -2.98659442 -2.95630785
O -1.98359162 -0.51640953 -3.08342606
O 1.06118037 -5.60914632 -1.77324826
O 1.65713433 -1.49562555 -4.81980129
Ti -2.45990759 -1.06969503 -4.77735183

Ti24O48

72
Total DFT energy = -657585.884263940
Ti 0.17659534 3.82910409 -3.15519257
O 3.87713477 -0.43766271 -1.43160963
O 1.45096551 -1.23204332 4.22347588
O 2.60637404 -0.00543378 1.51674799
O 0.27442391 3.37254154 3.55846112
Ti -2.10187690 -2.48921757 -2.73374071
Ti -4.46294274 -2.04073340 1.99321841
O 4.12017502 -0.73865810 3.29096928
O 3.34581596 4.59340059 -1.29714468
O -1.58122102 -1.12654898 2.95628494
O 0.92660663 0.04449671 -0.91062924
O -2.81234977 -0.76066353 -1.66194996
O 2.26432104 2.86992108 -3.30076515
O -1.07496081 -2.30025331 5.03495674
O -5.18717147 -0.41075229 -1.32520552
O -0.83248102 0.78237980 5.16120679
O 5.28996565 2.21924834 -2.02789850
O -2.45113010 1.03518038 -4.64378035
O 2.09315249 2.33288414 -5.83205397
O -3.66235514 1.24115342 0.35284627
O -1.80412974 1.46889902 -1.74866261
O -1.62018912 4.00501653 -3.29253425
Ti 4.01878436 0.78476241 2.33786560

Ti -0.32366212 -0.76497002 4.36174190
Ti 3.93198883 3.40114838 -2.48060779
Ti 4.51012326 1.15141204 -0.80557215
Ti 2.01159674 3.70401568 -0.34718456
Ti 1.68148059 3.10044230 2.42935351
Ti 1.17976764 1.15591985 -4.76912037
Ti -2.90531413 0.33656985 1.70690926
Ti -3.86696108 0.85132694 -1.39997389
O -2.31011451 1.71460321 2.77883970
O 0.59177586 4.04853938 -1.37488571
Ti 2.52520024 3.80206141 -4.83784318
Ti 0.34450971 -3.33232869 -1.58607854
O -3.62883456 -3.14967649 3.18088760
O 5.10973381 1.10853267 0.91770506
O -4.36913305 -0.33248968 2.58385010
O -0.85840069 -2.11473169 -1.06026687
O 1.05571394 4.79480561 -4.44005976
O -0.10258846 2.08488594 -3.78232237
O 0.77885141 -4.20435866 -0.04166386
O 0.25720490 0.74184835 2.88135352
O -3.62890031 -3.12174528 -1.98276915
O -2.36678289 -1.95742627 -4.46298487
O -0.66167643 -3.84300437 2.57478297
O -0.84533384 -3.83808005 -2.84379791
O 3.02627356 2.15945272 -0.91913369
Ti 0.68570773 0.32335627 1.03895578
Ti 2.22842849 -0.67468799 -2.10761391
Ti -0.82614672 1.92586212 3.74035661
Ti -1.41516116 -0.41549421 -4.71560416
Ti 0.79808319 -3.42996929 1.58933633
O -3.19244651 -1.57297671 0.77784556
O 1.80146711 -2.41245055 -2.17679932
Ti -0.98591066 -0.13409183 -1.30334616
O -0.62730612 -0.66571580 -3.11255768
O 2.13211454 4.44163647 1.33290091
O -4.01017724 2.15291304 -2.66433201
Ti -1.86012635 -2.83964695 3.49887363
O 0.83902492 -1.60923197 1.51694455
O 2.39029076 -3.32662266 2.46576001
Ti -2.31532868 2.30837307 -3.31816169
O 2.20698648 0.07442542 -3.72031188
O -5.42429290 -2.57134977 0.55032482
O 1.15123681 2.19884879 0.90828897
O 4.15342697 4.19142602 -4.13754464
O -1.09476406 0.23331032 0.57590505
Ti -4.32217986 -1.91691817 -0.78373725
O 0.09214222 0.05395973 -5.67979496
Ti 2.49613814 -1.53623477 2.82042014
O 3.18056548 2.24634114 3.03072075

Ti28O56

84
Total DFT energy = -767184.776690152
O 1.61237190 0.26456052 -6.41569382
O -2.84411353 1.97720288 -1.91077199
Ti 3.82331885 1.04345707 2.20294307
O 1.03002007 2.91247108 2.93333775
O 3.12738986 -2.40826497 -1.12298925
Ti 0.04348501 -0.32213904 -5.75914595
Ti 1.10566555 0.92323085 5.96402838
O 4.33387401 -0.10734193 0.83283629
O 2.14883522 -2.40847764 3.07120790
O 0.58610644 -3.75002236 -2.42073447
O -5.32031056 2.17749833 -3.53395688
O -0.87344111 5.16152200 -4.91674775
Ti -3.24969959 -1.52194509 -2.82776310
Ti -1.58619262 4.91917091 -3.26987274
O 0.69760439 1.31947661 0.69422529
O 1.14887091 -1.44263927 0.43844505
O -2.01770909 -0.98591949 4.77020659
O -1.39232978 -0.15974714 -6.85199485
O -0.92104855 3.22671013 -3.47196694
Ti 2.28794044 1.61118052 -5.34004741

Ti -2.40900201 2.98808837 3.43800528
O 3.95987622 1.75560530 -4.65975867
O 3.32541863 2.68781749 -1.89577985
O 3.94078065 2.53458034 3.43052455
O 1.86331982 4.97446022 3.95490662
Ti -0.39602080 3.42003665 -5.31980743
Ti 1.40573489 -2.88930088 -0.95180316
Ti 0.23306645 -0.04919958 -0.62117505
Ti -1.58866826 0.61898999 5.43699722
O -1.78420258 3.58874872 0.13804341
O 2.00351201 2.47000071 5.69062657
O -0.27428178 -0.70985073 2.49404091
O 0.07413068 -1.86568635 -4.80536520
O 2.13239882 0.48004408 2.82367824
O -1.46822000 1.84472662 2.43387591
O -2.23193606 -2.98813873 -3.10316156
O 1.10314958 -3.85896635 0.59312712
Ti 2.47814088 3.24623434 4.10727208
Ti -1.70148729 -1.68128997 3.07232864
Ti 3.70380544 -0.69220944 -0.76283684
Ti -3.15969574 -0.55996197 0.35247884
O 2.30913977 0.46756503 -1.11783573
O 1.86983012 0.92272676 -3.76586974
O 2.12259732 -0.49468918 5.59420671
O -0.09814826 1.29898974 -1.82615046
O -0.57456124 1.21400586 -4.89909782
O -3.35429307 4.54099916 -3.16330095
O 1.34445824 3.18242265 -5.62873122
O -0.01529087 0.97979763 4.51062957
Ti 3.50522459 1.24766941 -2.93972442
O -0.77358489 -3.15471100 2.71992409
O 4.58386502 -0.06003224 -2.17829014
Ti 2.76285934 -0.91392106 3.90363108
Ti -1.43067053 1.36851331 -2.97087007
O 1.06109460 3.75889339 -0.58011681
O -1.59887943 2.90013710 -6.60485890
O -3.07609181 -1.47217687 1.93354676
O -3.83276473 -1.38965962 -1.11892270
Ti 2.22265473 2.34323596 -0.47150749
Ti -4.60663821 0.90800748 -4.66222433
O -4.14899875 1.04296506 -6.41948271
O 4.33954066 -0.31218962 3.50971558
O -3.68882515 3.40123606 2.23967667
O -4.62268247 3.50605055 -0.70737909
Ti -3.43175209 2.85386496 0.49652220
O -2.91882261 1.48850065 -4.41569764
O -4.46734987 -0.77051882 -3.99988469
Ti 0.21665481 1.11931447 2.38917162
O -1.25422824 4.35905805 3.78225288
Ti 0.80512986 -2.61151846 1.86503701
Ti -0.44957246 -2.48281241 -3.17531444
O 3.24946456 2.33773844 0.93788049
O -1.43582090 -0.36763293 -0.05178937
O -3.80187972 1.08042401 0.62598451
Ti -4.17406113 3.08760298 -2.42292763
Ti -2.31286800 1.29243126 -6.21959943
O -0.46709699 0.69952539 6.88349338
O -2.67896491 1.97986750 4.96482030
Ti 0.34181479 4.66420533 2.99278509
O -0.87674511 5.58740013 -1.74255607
O -1.78591289 -0.50030839 -3.02178400
Ti -0.39978044 4.66456337 -0.22349922
O 0.06940490 5.42802075 1.40949571
O 0.39952095 -1.44768139 -1.87491642

Ti35O70

105
Total DFT energy = -958982.552526297
O -2.53353312 5.74650706 0.03833930
O -3.79635690 -0.80397184 -4.29610852
Ti -1.35422526 3.44258324 -4.08669786
O -0.16587394 3.62430030 -5.47187388
O -3.27593656 -0.43478151 1.31075504

O -2.15318755 -0.68952213 3.83700286
O 0.72872052 2.79813225 2.10752752
O 0.35712900 -1.61860546 -5.53904445
Ti 4.15467291 -1.02830178 -4.22629002
O 1.78083252 -4.12971111 3.75892697
O -0.56034673 -2.55652044 5.29202080
O 0.12528710 2.21256192 -3.54406169
Ti 1.68787124 -0.37267629 -5.74613351
O 3.14063937 -4.31718651 -2.34952020
Ti -3.14057110 -2.35089755 -3.64172614
O 2.72197028 2.96830090 -4.62423224
O -0.86260982 0.55034481 1.93735899
Ti 2.06381120 -0.85231121 -1.56263239
O -0.55267442 1.62501590 4.55880529
O -2.33481218 -0.08575779 6.19449042
O -1.78805143 5.07310472 -3.34007392
Ti -1.45863844 -0.86763697 -1.50962283
Ti 4.23349205 -2.88268026 0.83586311
O -6.34064970 2.81822604 -0.23397894
O 5.25126030 -2.27014546 -3.49263730
O 2.66403915 0.82020588 -1.77292320
Ti -3.93472029 -3.38450525 3.39085229
Ti -3.35918475 0.91988316 -3.74059038
Ti 2.96305986 -0.06444539 1.56332798
O -1.89148006 0.44655694 -2.85046596
O 0.28469523 -0.21342008 -1.85609259
Ti 1.13198731 2.36500560 -5.18883934
Ti -2.29986602 1.56182751 1.02680436
Ti 3.36674682 1.80213913 -3.34555787
Ti 0.62458839 -2.46651547 0.58273444
Ti 2.77299734 2.53719604 -0.53107706
Ti 2.61775452 -4.71909814 2.28092278
Ti -0.38672774 1.68499473 -1.84349336
Ti -1.99740866 5.00515673 1.51800780
Ti -2.18213862 -4.83474491 1.62544688
Ti -3.87640616 3.17269416 3.59923207
Ti -0.52251677 -2.83837638 -4.55729423
Ti 0.24959984 -5.85214841 0.44064557
Ti 0.45691231 1.39120261 3.00195501
Ti 4.32147824 -2.94955623 -2.04479787
Ti 0.55378903 4.07037843 0.55604228
Ti -1.68516563 -1.18973547 1.99764075
Ti -2.23436421 1.12865472 4.78400114
Ti 0.08062684 -3.44469968 3.81170561
Ti -4.01274254 -3.18781209 -1.00895608
Ti -1.97777463 4.75565065 -1.56080746
Ti 1.35490720 -4.29198939 -2.25618466
Ti -5.76828218 2.01142923 1.24863575
Ti -4.76521653 2.77361368 -1.25863512
Ti -2.13120106 -1.68060920 5.37718773
Ti -4.99567475 -1.19510989 1.36750713
O -0.26851437 4.76762248 -0.93493785
O -1.72746878 2.93767200 -2.09856080
O -3.45745319 -2.89840674 5.07370354
O 1.16982644 1.14033308 -6.57861381
O 3.36750761 -1.11741894 -5.85928823
O -1.02580961 -4.63699640 3.25091370
O -1.38449955 -6.37478239 1.02914394
O -3.14302985 -1.68260814 -1.60274582
O 4.34003902 -4.31682513 2.03947959
O 2.83249400 -1.64911906 -3.09145962
O -2.22660568 -3.18880244 -5.01606580
O -5.22737301 -2.24803057 2.81193747
O -2.59505239 -2.82815668 2.28764553
O 0.71787690 -5.69605946 -1.31588949
O -4.09781918 2.02193729 0.38957797
O 0.55044514 -4.13176351 -3.86299445
O -3.69240146 -5.02675498 2.67359700
O -1.04899725 -1.63564230 0.20716073
O 0.02754835 -2.11894045 2.45243183
O 3.72952224 2.98631231 -1.99382082
O -0.26269121 -4.15472096 0.77518862
O 3.56128753 -1.81784459 -0.76303526
O -3.00751893 -4.23649139 0.00415798

O -4.60442910 1.55384260 -2.60145199
O -5.26651822 -2.31597969 -0.00478779
O -2.68347320 2.32998127 -4.67844074
O 1.98527653 0.36902291 3.00332329
O 1.71774818 -6.09717030 1.48372793
O -2.93211323 1.77380150 2.91649113
O 0.99187515 -2.74373303 -1.26713242
O 0.82576080 2.35106691 -0.65377141
O 4.68188704 0.67238503 -3.83173282
O 5.25766795 -3.48446002 -0.57089202
O 3.48887027 1.43299691 0.75589772
O 2.32208398 -3.36346576 1.05735464
O 2.33233247 4.11227355 0.27139459
O -1.67765973 3.24468116 0.84828479
O 1.95813294 0.59139283 -4.26832442
O -3.37398169 2.52126923 5.21267631
O 4.26478574 -1.33049908 1.78343547
O -6.09768800 0.23183166 1.39506728
O -0.25403739 5.30228545 1.69362178
O -5.52296759 2.89189737 2.80070765
O -4.19154669 -3.59029044 -2.78329653
O -1.65800304 0.82587280 -0.50995934
O -3.94541606 4.22523512 -1.54413172
O -3.11760025 4.66399697 2.98333025
O 1.63659312 -0.80543458 0.44233703
O -1.25439057 -2.10156758 -3.05739609

Ti38O76

114
Total DFT energy = -1041181.399680686
Ti 1.73138783 3.21768453 4.63380981
Ti -1.95695352 0.93282925 -0.77079828
Ti 0.71928355 -4.59791671 0.26127334
Ti -1.61273961 3.64799452 4.40750105
Ti 0.29678267 2.59905476 -4.96294196
Ti 5.10355629 0.74539415 1.92216432
Ti -2.35589787 3.24585881 -3.17194963
Ti -1.01331415 -4.63868072 -2.55782462
Ti -4.00017301 -3.43311237 1.12896496
Ti 2.89056022 3.20272507 -4.18542836
Ti -1.11547857 4.24567892 -0.42482865
Ti 4.69414570 0.50367888 -3.70057563
Ti -5.03890796 2.02605013 -2.15868497
Ti 0.33454845 -1.78999298 -1.61171051
Ti 2.61163660 -1.40499404 0.66497320
Ti 2.13455231 3.80618338 -1.04951491
Ti 4.99588290 -3.13975162 -1.30336496
Ti 0.87274466 -3.20038905 -4.49682587
Ti 5.52916089 0.16231436 -0.99811665
O 5.88786831 -1.62914278 -0.99980788
O -1.83622224 5.23416714 0.93124328
O 1.72286816 3.58090686 -5.54785886
O 3.00153767 4.15336818 -2.66436388
O -2.43245595 0.32319251 1.19667903
O 1.40317120 1.25189407 5.02685624
O -2.12699566 4.47087896 -1.90714445
O 1.22229484 -0.51042972 1.64150130
O -1.13006273 3.56920134 -4.50537858
O 2.48757946 -3.00866269 -5.30049568
O 2.18590455 -4.00772075 4.73839860
O 4.91262848 -1.05261449 -4.64925588
O 0.12805867 4.02564408 4.71142174
O 1.38708775 -1.37654341 4.31784073
O 1.54735051 -2.58581299 -2.94599040
O -4.98160228 -4.31423230 -0.13789020
O 4.35197130 -3.20259175 -2.97806792
O -0.99483997 -2.82421103 -2.30486259
O -1.80233838 1.67706967 -2.51627610
O -2.06222716 2.14229693 5.28293474
O 4.35043794 -4.71417719 2.70686251
O -4.43855997 -2.58695406 -2.63970223
O 2.89066914 4.29934516 3.69308143
O -2.84714102 -3.15945871 -0.22244584

O 4.01659040 0.36512412 6.01951840
O 6.19626167 0.55816796 -2.63444357
O -1.86428749 3.08960632 2.71014103
O -2.58627699 -0.62487926 -4.17786023
O 5.24135371 -4.55021610 -0.16689853
O 2.86340718 -0.32694179 -3.64577814
O 1.75024262 2.04816499 -1.04428363
O 2.51107094 3.03260842 6.27771321
O -2.76843893 -5.05244699 -2.41618939
O -1.24910750 2.51291195 -0.03932588
O -0.74670387 -3.60185455 4.43378227
O -0.08052695 -5.33012758 -1.17276965
O 3.41419168 0.05478617 3.23339881
O 3.51461643 -2.81329625 -0.31143426
Ti -0.72402917 -0.53456104 1.53541886
Ti -1.35405400 -3.80347851 2.77700628
Ti 2.02102407 0.63453499 -2.16555457
Ti 4.60163563 -0.45320944 4.50964521
Ti -1.78880685 0.45673531 4.66431802
Ti 2.47746219 1.22742561 6.54888688
Ti 3.06263789 3.36527950 2.18235048
Ti 3.83600476 -4.31789363 0.98253978
Ti -0.81065834 -0.39219851 -4.37740217
Ti -3.87023365 -3.88771886 -1.53156706
Ti -3.93522688 -0.16907726 2.15082089
Ti -0.03008440 -0.83602268 7.51589914
Ti -5.08038516 2.47751473 0.58036195
Ti 3.48856184 -2.05790150 -4.10243906
Ti 3.51061304 -3.45297616 3.67089327
Ti -2.87793346 4.48378285 2.18706087
Ti 1.49616202 0.18915330 3.45123897
Ti 0.79493985 -2.90660104 5.18530184
Ti -3.86423367 -0.87463728 -2.88966450
O -0.20208749 -1.88921673 -5.12863502
O 6.21957383 0.93303549 0.48209595
O -4.18080253 3.08926209 -3.32890675
O 3.93665799 0.79277174 -1.86068431
O 1.41826974 0.43851576 7.68360662
O 5.93363782 0.13814888 3.42484660
O 1.93924750 -0.76024402 -0.98966686
O -0.24260242 -4.79235254 1.76874953
O 0.23424743 -0.25045193 -2.82348329
O -3.32123851 -0.14228596 3.82915312
O -0.50421400 0.37054532 3.23640499
O -0.08212715 -4.73222157 -4.10422300
O -2.74090735 5.01625475 3.92127846
O 4.26363037 2.10055502 -4.51652146
O -6.19466580 2.61824497 -0.85877464
O 4.56775777 -2.25348826 4.51788682
O 0.81112075 -2.79939872 -0.06358250
O -5.17711594 1.08990118 1.71804555
O 2.90806889 4.14410575 0.52869295
O -1.26814626 -2.11567066 2.04870110
O 2.38079604 -5.25860915 0.52387959
O -3.05760956 -0.45596436 -1.41707056
O 4.03038533 -0.31763995 0.68959877
O 1.79896837 2.23502933 2.81520589
O 0.56572142 4.65808454 -0.93960185
O 0.67527783 -2.50568166 6.86006936
O -5.20446978 0.40817433 -2.87671740
O -3.07363824 -4.27371680 2.45403283
O -1.18887699 -0.47876270 5.97445739
O 1.49889499 2.08600178 -3.62432651
O -0.85282015 -1.00034418 8.87615118
O -3.85040904 1.93245254 -0.69336901
O -0.33315183 0.99018408 -5.46443513
O -0.62252546 -0.35861087 -0.36583629
O -4.55139708 -1.79376521 1.68802818
O 2.92563959 -2.78039241 2.04188012
O 4.59535379 2.42227647 2.18983069
O -4.46820276 3.92014179 1.44584151

Top-down generated nanocrystals

Ti28O56

84
Total DFT energy = -767174.873300945
O 9.24622799 8.29828746 18.93344925
O 9.78646416 10.57592416 17.12961496
Ti 5.74011689 6.60854409 23.19128423
O 5.24266028 6.09408870 24.92430386
O 5.45774823 5.71503028 21.76083770
Ti 9.42422179 6.18333333 23.27601161
Ti 7.36210358 5.11293882 21.30548422
O 7.32112496 3.52610437 21.42346214
O 9.46990245 5.60200585 25.03788328
O 7.50651949 6.13382797 23.10529059
O 7.28308697 5.89199282 19.43708589
O 9.39166015 5.59179537 21.50425248
Ti 13.09964079 6.60442914 23.12007907
Ti 11.43312381 5.22657075 21.17783333
O 11.50753239 3.63777811 21.15561865
O 13.60802251 6.09620103 24.86016245
O 11.33369145 6.14385485 23.03061520
O 11.37262320 6.16268966 19.37175448
O 13.35003112 5.77988045 21.63969918
Ti 5.75052623 10.04221867 23.45017343
Ti 5.77898782 6.93640517 26.39960278
O 5.22919217 8.60323868 26.65697768
O 6.05339480 6.09002711 28.02565300
O 5.15385107 8.39022540 23.22305453
O 6.02674393 10.85781852 21.79084968
Ti 7.46879384 7.56703246 19.30482514
Ti 9.40796929 9.84516699 23.90204245
Ti 7.58819527 10.14383822 21.34300802
Ti 9.47200897 7.14683210 25.89948059
O 7.24597619 8.40774412 20.88083060
O 9.43248126 9.14754891 25.86606424
O 7.55628941 9.70999308 23.38937548
O 9.48252083 6.50338806 27.86821719
O 9.44749546 7.84443957 23.93552953
O 7.02344677 8.75585452 17.89651057
O 9.39747455 10.48861963 21.93327908
O 7.60013023 7.20314437 26.43444346
Ti 11.07466842 7.81156330 19.23992817
Ti 13.10097233 10.05565101 23.40187984
Ti 11.19980163 10.25042872 21.38119994
Ti 13.12947026 6.94989546 26.35129827
O 11.39928909 8.54372276 20.84785747
O 13.72611937 8.60192834 26.57829055
O 11.27984300 9.78880986 23.36704642
O 12.85331553 6.13434195 28.01064632
O 13.65088635 8.38885833 23.14443200
O 11.91639487 8.92704506 17.93927128
O 12.82653199 10.90204471 21.77585324
O 11.32368010 7.28201456 26.41211167
Ti 5.78038199 10.38767544 26.68137020
O 5.52997759 11.21213430 28.16180518
O 5.27191975 10.89588081 24.94132244
Ti 8.38533439 9.86358216 18.18105616
Ti 9.45577525 10.80864855 26.52553229
O 7.98161029 10.79600683 19.58424936
O 9.48833537 11.40002350 28.29732696
O 9.41007984 11.38995379 24.76360346
O 7.54630063 10.84830501 26.77082899
Ti 11.37985067 10.58737475 17.89776290
Ti 13.13984980 10.38360107 26.61013997
O 11.09831320 10.99800650 19.53703811
O 13.42223782 11.27702979 28.04064395
O 13.63728061 10.89807595 24.87712113
O 11.37345330 10.85830324 26.69615812
Ti 7.50021931 6.40446577 31.90364911
O 7.78169318 5.99380610 30.26439764
O 9.09359722 6.41598515 32.67182124

Ti 10.49478468 7.12831654 31.62044913
O 10.89846420 6.19594582 30.21721440
Ti 7.68015634 6.74155494 28.42028919
Ti 7.80536809 9.18033401 30.56163951
O 6.96358596 8.06476962 31.86218139
O 7.48077152 8.44823624 28.95367553
O 9.63379356 8.69361988 30.86812261
Ti 11.29179280 6.84822394 28.45846092
Ti 11.41116168 9.42496400 30.49667599
O 11.85664448 8.23610419 31.90492701
O 11.63391331 8.58435667 28.92061642
Ti 7.44687792 11.76536634 28.62376514
O 7.50740759 10.82920464 30.42984110
O 7.37256901 13.35415533 28.64611304
Ti 11.51788574 11.87901250 28.49608184
O 11.59689606 11.10000434 30.36446082
O 11.55876363 13.46585548 28.37820354

Ti33O66

99
Total DFT energy = -904174.233260810
Ti -1.73214779 -1.96852543 -4.66119274
Ti -1.96122086 -3.70086337 -2.38398175
Ti -3.60373921 -3.60304084 -0.00515310
Ti -3.70262650 -1.95986710 2.37283184
Ti -1.97005030 -1.73074626 4.65045456
Ti -1.73164188 1.97266713 -4.66122078
Ti -1.99564900 0.00220573 -2.32996034
Ti -3.64452741 0.00088454 -0.07195698
Ti -3.70257471 1.96056502 2.37349366
Ti -1.96995233 1.72985289 4.65113225
Ti -1.34630942 -0.00098729 7.04244433
Ti -1.96133699 3.70438602 -2.38240186
Ti -3.60403175 3.60457393 -0.00409491
Ti -0.00221101 -1.34438556 -7.05261306
Ti 1.72890827 -1.96844874 -4.66208316
Ti 1.95908441 -3.70079203 -2.38498443
Ti -0.00046281 -3.64376736 0.06066440
Ti 0.00007761 -1.99492077 2.31887371
Ti 1.97134918 -1.73066221 4.64948024
Ti -0.00226665 1.35067687 -7.05400392
Ti 1.72820847 1.97263696 -4.66214210
Ti 1.99349622 0.00226124 -2.33091278
Ti -0.00054264 0.00052260 -0.00546986
Ti 0.00003099 1.99481351 2.31952210
Ti 1.97120062 1.72990787 4.65014709
Ti 1.34877815 -0.00093197 7.04183470
Ti 1.95904539 3.70439428 -2.38338922
Ti -0.00050511 3.64477195 0.06233408
Ti 3.60284768 -3.60292347 -0.00692366
Ti 3.70282633 -1.95981851 2.37103648
Ti 3.64338007 0.00092551 -0.07369344
Ti 3.70268047 1.96064994 2.37171113
Ti 3.60282385 3.60476392 -0.00574922
O -2.16724360 -3.68374771 -4.18859655
O -1.60062050 -2.04283005 -6.48152248
O -1.94036978 -1.91866559 -2.47247216
O -1.84952181 -3.90869188 -0.19675621
O -3.69003445 -4.10534127 -1.77892211
O -4.10898937 -3.68803489 1.76820261
O -3.68473037 -2.16641017 4.17754847
O -1.92023951 -1.93946149 2.46078941
O -2.04560809 -1.59874389 6.47086655
O -3.90629250 -1.84843453 0.18573770
O -2.15743803 0.00250784 -4.22427620
O -1.59966050 2.05012821 -6.48161732
O -1.94061549 1.92209578 -2.47060595
O -1.89030650 0.00125975 -0.25942918
O -3.78869777 0.00127077 -1.85417207
O -4.09772673 0.00024321 1.94574486
O -3.68459114 2.16609821 4.17824798
O -2.05194742 -0.00035959 4.30561534

O -1.92030943 1.93936863 2.46146456
O -2.04545156 1.59710468 6.47147838
O 0.00151698 -0.00110990 8.28863044
O -3.90812108 1.85010276 0.18648065
O -2.16859773 3.68669019 -4.18699264
O -1.84966544 3.90835223 -0.19485222
O -3.68949563 4.10979305 -1.77744733
O -4.10770375 3.68936013 1.76951580
O -0.00152395 -2.04926561 -4.31818011
O 2.16426419 -3.68366271 -4.18972785
O 1.59653143 -2.04281347 -6.48236829
O 1.93820428 -1.91859202 -2.47346976
O 1.84853162 -3.90841181 -0.19771576
O -0.00091825 -4.09549801 -1.95717437
O 0.00003205 -3.78757567 1.84317890
O 0.00056662 -2.15639205 4.21304631
O 1.92049164 -1.93937831 2.45977832
O 2.04779560 -1.59864465 6.46985215
O -0.00057210 -1.88952949 0.24792701
O -0.00182943 0.00403462 -5.88957389
O -0.00162111 2.05512685 -4.31521094
O 2.15438607 0.00263551 -4.22528399
O 1.59538735 2.05029019 -6.48245989
O 1.93811232 1.92214084 -2.47138357
O 1.88908955 0.00086603 -0.26033772
O -0.00250703 0.00208939 -8.29979756
O -0.00102326 0.00135584 -1.92208745
O -0.00005018 0.00021401 1.91060983
O 0.00046582 2.15562061 4.21389206
O 2.05300460 -0.00028993 4.30459202
O 1.92043400 1.93956380 2.46064853
O 2.04752377 1.59715249 6.47048127
O -0.00018642 1.89046163 0.24889609
O 0.00096963 -0.00083075 5.87843966
O 2.16547186 3.68662686 -4.18807331
O 1.84845598 3.90907885 -0.19574958
O -0.00106823 4.09918318 -1.95537067
O -0.00018190 3.78793817 1.84470282
O 3.68817880 -4.10530254 -1.78071341
O 4.10882533 -3.68798516 1.76622366
O 3.68581385 -2.16633213 4.17574954
O 3.90567822 -1.84834102 0.18381647
O 3.78672454 0.00150206 -1.85601490
O 4.09764829 0.00038170 1.94370626
O 3.68561767 2.16614778 4.17649940
O 3.90648011 1.85022156 0.18463531
O 3.68757058 4.10952066 -1.77923034
O 4.10774595 3.68936925 1.76755420

Ti35O70

105
Total DFT energy = -958971.845648739
O 18.99202066 18.99695202 37.39470746
Ti 17.22800996 17.02641743 43.84721550
Ti 17.07503335 15.29087803 46.15319162
O 17.09847393 17.08249619 46.01930370
O 17.15278340 15.09376136 48.36202285
O 16.96885953 15.26656370 44.35877220
O 17.26810049 16.84646258 42.07261817
O 15.33998629 14.89303847 46.73854652
Ti 20.76871150 17.02652400 43.84732832
Ti 18.99843654 17.21774592 41.45747073
Ti 20.92165058 15.29087835 46.15322108
O 20.89823927 17.08251521 46.01935528
O 18.99835733 17.22259380 43.92198062
O 20.84385899 15.09406988 48.36202984
O 21.02785986 15.26665341 44.35878186
O 18.99850413 17.23816611 39.68502465
O 20.72880056 16.84690355 42.07267139
O 18.99835673 14.89629573 46.60621951
O 22.65665391 14.89292568 46.73857275
Ti 17.22802337 20.96721068 43.84739024

Ti	17.02359928	18.99671629	46.16044644
O	17.09829046	20.91091737	46.01936664
O	17.11207044	18.99681675	48.23893469
O	16.82313687	18.99673992	44.26075487
O	17.26812750	21.14726386	42.07278474
O	15.22434921	18.99653490	46.62162091
Ti	18.99692074	18.99692148	38.98614519
Ti	20.76866831	20.96713677	43.84749573
Ti	18.99841338	20.77599993	41.45754558
Ti	20.97308557	18.99673678	46.16055641
O	18.99776183	18.99686527	41.58498607
O	20.89840874	20.91093735	46.01942601
O	18.99834286	20.77091333	43.92222347
O	20.88459507	18.99684099	48.23905155
O	21.17359384	18.99677008	44.26086644
O	18.99847575	20.75564803	39.68509836
O	20.72871763	21.14686674	42.07283038
O	18.99834609	18.99668342	46.59459502
O	22.77230696	18.99655397	46.62175110
Ti	17.07502446	22.70258284	46.15352761
O	17.15265131	22.89831336	48.36225041
O	16.96899897	22.72700855	44.35906038
O	15.34009937	23.10068749	46.73880224
Ti	20.92162026	22.70261712	46.15355334
O	20.84395017	22.89798861	48.36225742
O	21.02767284	22.72695581	44.35906450
O	18.99833269	23.09724427	46.60672384
O	22.65649073	23.10087442	46.73883405
Ti	15.39660317	15.39446029	48.51724312
Ti	17.02792084	17.22602142	53.18703927
Ti	15.29235253	17.07313823	50.88102568
O	14.89390208	15.33831708	50.29573687
O	16.84823653	17.26594862	54.96171839
O	15.26810151	16.96703165	52.67552544
O	15.09729601	17.15082736	48.67236633
O	17.08404376	17.09631490	51.01508132
Ti	18.99830711	15.35319035	48.63396301
Ti	20.96854539	17.22601929	53.18708063
Ti	18.99825229	17.02153872	50.87393764
O	18.99831331	15.22242380	50.41271036
O	21.14820624	17.26592693	54.96175657
O	18.99824637	16.82107842	52.77360942
O	18.99821500	17.11010255	48.79531465
O	20.91246200	17.09638266	51.01510196
Ti	22.60007203	15.39453500	48.51724380
Ti	22.70414181	17.07315079	50.88112314
O	23.10250152	15.33829786	50.29577764
O	22.72838312	16.96698891	52.67560275
O	22.89962932	17.15087044	48.67243835
Ti	15.35519548	18.99653909	48.40030398
Ti	17.02784268	20.76665403	53.18723211
Ti	15.29237614	20.91971584	50.88114629
Ti	17.21910639	18.99621657	55.57705152
O	14.89766529	18.99640870	50.42791395
O	16.84779959	20.72649984	54.96183313
O	15.26802318	21.02572309	52.67559951
O	17.23949554	18.99611270	57.34950443
O	17.22414812	18.99634842	53.11231031
O	15.09628153	20.84213714	48.67241321
O	17.08403621	20.89637173	51.01520600
Ti	18.99830893	18.99647645	48.51731109
Ti	20.96861726	20.76666611	53.18728002
Ti	18.99825084	20.97119475	50.87412457
Ti	20.77734567	18.99621128	55.57708022
O	18.99826347	18.99637218	50.43987506
O	21.14865212	20.72650907	54.96187694
O	18.99825567	21.17160203	52.77382062
O	20.75693701	18.99610293	57.34952934
O	20.77236994	18.99635161	53.11237285
O	18.99819803	20.88277792	48.79564691
O	20.91246875	20.89632082	51.01521108
O	18.99822870	18.99690714	55.44953653
Ti	22.64148931	18.99655681	48.40044771
Ti	22.70411041	20.91974334	50.88124606

O 23.09882672 18.99642626 50.42807401
O 22.72845448 21.02580031 52.67567888
O 22.90064180 20.84213243 48.67248022
Ti 15.39636625 22.59840149 48.51736447
O 14.89434206 22.65471340 50.29596918
Ti 18.99828466 22.63963873 48.63430251
O 18.99829934 22.77042258 50.41301262
Ti 22.60027257 22.59835712 48.51736191
O 23.10203640 22.65477659 50.29600330
Ti 18.99820675 18.99769010 58.04846730
O 18.99818104 19.00265932 59.63990520

Ti38O76

114
Total DFT energy = -1041173.491255814
O 11.17844037 14.72258018 20.94637996
Ti 10.26913258 14.66221373 19.34576137
O 6.36754323 14.04766499 21.22315685
Ti 6.91987613 14.16551702 19.52340834
O 10.70651235 15.13134612 17.66174176
O 7.91513088 15.30192057 16.20669596
O 10.25620941 14.58565836 14.54384317
O 8.50376567 15.04610744 19.50463337
Ti 9.64439786 14.64786135 16.21846164
O 5.44041592 14.50127060 14.68273417
O 5.85297434 14.56418736 18.09448273
Ti 6.31824335 14.51145640 16.31508595
Ti 5.31560413 2.94305801 13.95114184
O 5.20710206 2.69203060 15.71916134
O 5.45164755 2.02214388 12.34267366
Ti 8.98439387 2.69282950 13.81968552
Ti 7.07163664 2.63921572 11.78831058
O 9.28503574 2.41070244 15.55650153
O 7.15956553 3.31670428 13.62523903
O 8.55584833 1.73974379 12.26362856
Ti 5.36227404 6.11281728 13.47255659
Ti 5.75393032 4.07494211 16.84571626
O 5.66790333 5.81182421 16.12455198
O 5.45922859 3.82486643 18.58580056
O 4.52043868 4.47210794 13.75689889
O 5.43844255 6.11369899 11.76433650
Ti 9.20197056 5.85631851 13.61879670
Ti 7.35556752 6.03634352 11.44349254
Ti 9.38715369 3.87649483 16.70368254
O 7.24129387 4.18837566 10.93759570
O 9.27323080 5.32934379 15.72038830
O 7.27183020 6.06278151 13.45222364
O 9.24050531 4.00738945 18.73304361
O 9.88001367 4.08977059 13.39030979
O 9.13903075 6.10942199 11.84723729
O 7.45677799 3.72543932 17.13404877
O 11.19684043 3.84469194 17.24241071
Ti 5.36697527 9.32436169 13.69614085
Ti 6.29691220 7.51102984 16.63449017
O 5.75824454 9.06897192 15.71633970
O 6.02219870 7.87133572 18.31379989
O 4.57905383 7.68909458 13.87862869
O 5.18963213 9.62905003 11.88449778
Ti 6.89738487 9.25283599 11.46702154
Ti 9.83347677 7.43049820 16.09967388
O 7.26715074 7.68104713 10.63626853
O 10.23700347 9.21148883 16.10119289
O 7.08469188 8.99740280 13.25709720
O 9.26974209 7.52035386 19.52071017
O 10.10593679 7.21870664 14.27925532
O 8.07581320 7.54588838 16.58667930
O 10.99821029 7.01320352 17.45669987
Ti 5.99970013 12.89550074 14.00383461
Ti 6.26373947 10.84332263 16.21445361
O 6.56979929 12.78037206 15.96805744
O 5.86356887 10.96638984 17.91042001
O 5.27095306 11.20562905 14.38710418

O 6.26779327 13.17210705 12.22192022
Ti 9.72237350 12.87143482 14.06312272
Ti 7.89440526 12.36336327 11.96360992
Ti 10.08033204 10.94037654 16.33629838
O 7.79345878 10.80288264 11.07850028
O 9.33842914 12.91092030 16.17892953
O 7.86186934 12.23159587 13.83029619
O 9.50044023 10.85192127 18.33441497
O 10.58962137 11.44641958 14.56825195
O 9.51979882 13.04901327 12.19986923
O 7.96022600 10.58480526 16.59897979
O 11.67124846 11.33811053 17.28717683
Ti 9.73675877 2.81515514 23.84407988
Ti 7.94078960 2.82631306 21.64376121
O 8.12843943 2.17389489 23.44845435
O 7.78258372 2.19787863 20.02442861
O 9.79244414 3.39619088 22.00776781
Ti 11.56831270 2.78703614 21.75435582
O 11.24597534 1.91843068 23.37803700
O 11.50730173 2.53212626 19.97149368
Ti 7.19729905 3.92736494 19.25541381
Ti 10.41186164 6.09593206 24.20826241
O 7.06853729 4.22932098 21.20092603
O 9.91104314 4.37658738 24.74260727
O 7.29628341 5.73526837 19.15439494
O 10.02397452 6.09501296 22.44183434
Ti 10.99924104 4.01098541 18.98310509
Ti 11.72397181 6.02580726 21.87409483
O 12.46509174 4.25156720 21.93108064
O 12.09904941 6.20363383 23.68521915
O 11.42719606 5.63367197 19.84096388
Ti 7.37120600 7.45563426 19.57371692
Ti 9.68824199 9.24239817 23.86389244
Ti 7.58016336 9.30271202 21.86266254
O 6.92102734 7.71462601 21.30739371
O 7.86116981 9.05779204 23.59635195
O 9.92077218 7.73535197 24.83921213
O 7.59697906 9.56143891 19.76460324
O 9.53831554 9.38041936 21.84526035
Ti 10.95548425 7.44197256 19.20655203
Ti 11.36868960 9.48114004 21.54491515
O 11.96328911 7.71168902 21.14440731
O 11.55356349 9.46479022 23.26217983
O 11.42339540 9.32692815 19.41844478
Ti 7.61006586 10.86558822 18.62186967
Ti 9.42088264 12.50765761 23.78263862
Ti 7.29944202 12.60109461 21.91121270
O 6.67555292 10.96371897 21.94859354
O 7.71580124 13.09765852 23.63708649
O 9.60477876 10.94845620 24.58257025
O 7.52627115 12.45081060 19.63858543
O 9.24074016 12.30053770 21.89230209
Ti 11.14029264 11.10259797 18.94856639
Ti 11.00660622 12.98095326 21.49814993
O 11.78687607 11.32801849 20.97677082
O 11.02088786 13.23456953 23.30731362
O 10.46628324 12.89211199 19.50436959

Ti74O122

234
Total DFT energy = -2137163.03091586
Ti 17.08659134 15.47502495 46.07041047
O 17.13883739 17.25733471 45.88539269
O 17.17968250 15.42323679 48.27665734
O 16.97531943 15.46116093 44.28385335
O 15.34772253 15.21863409 46.64573500
Ti 20.93677921 15.47545234 46.08074150
O 20.88476915 17.25712592 45.89620624
O 19.02059386 17.06736751 43.35046422
O 20.83163077 15.42576165 48.29046001
O 21.06117532 15.46177713 44.29520729
O 19.01145554 15.03016313 46.58388377

O	22.67215821	15.21634374	46.66872657
Ti	17.17908129	19.17116043	46.44949520
O	17.43663537	20.95311412	46.35922654
O	17.10433277	19.04888460	48.46377848
O	17.70926060	19.13693793	44.55980048
O	15.33624350	19.17947519	46.75111351
Ti	20.83888546	19.17227108	46.45890027
O	20.58152545	20.95353666	46.36600923
O	19.02193445	20.14410085	42.30193708
O	20.90376986	19.05238105	48.47485165
O	20.32901452	19.13600941	44.56555416
O	19.00858832	18.84000484	46.98079539
O	22.68124205	19.18016211	46.77079667
Ti	17.26039112	22.35370105	45.31664486
O	17.41692374	22.95385385	48.23194702
O	16.80046807	21.55600829	43.72432718
O	15.76446098	23.02129005	46.22474622
Ti	20.76583734	22.35455016	45.32542167
O	20.59776292	22.94439269	48.25172699
O	21.23516865	21.55728790	43.73546178
O	19.01371517	22.98971671	45.23514188
O	22.25403145	23.02377822	46.24632339
Ti	13.85593878	13.61291082	53.47505441
O	12.89543078	13.67018998	55.07215447
O	13.74334778	13.29315855	51.65169080
Ti	17.20375549	13.46361406	53.50242974
Ti	15.28398722	13.62871619	50.72373947
O	17.45292420	13.41044116	55.27609780
O	15.45838001	12.85480811	53.59608721
O	15.05046055	13.60403319	48.95526672
O	17.05087481	13.20130202	51.32734044
Ti	20.77890523	13.45472016	53.49602750
Ti	18.99263982	13.45057376	50.92325479
O	20.51381535	13.40117116	55.27319041
O	18.99085061	13.00852204	52.89235786
O	19.00539992	13.33456006	49.08976808
O	20.94703443	13.20191248	51.34522402
Ti	24.12589904	13.62631584	53.51470077
Ti	22.71853940	13.63036230	50.75005826
O	25.05404855	13.68867819	55.13230081
O	22.52920350	12.85802413	53.61930703
O	22.95868192	13.60295042	48.98276411
O	24.25587041	13.30903754	51.69213436
Ti	13.58871129	17.24403169	53.32531659
Ti	13.47099984	15.25197198	55.82381123
O	13.01176390	17.08479957	55.31330430
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Ti84O168

252
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O	13.24953469	15.53449472	46.97254430
O	13.22911421	15.14824313	42.99197183
O	11.23165781	17.01887737	38.25190089
O	13.21818083	16.74351709	40.73398894
O	11.39813595	15.06001638	45.25178715
Ti	15.00838555	15.06075439	37.93643743
Ti	17.04719777	16.85930945	42.71979062
Ti	15.02685193	17.08714820	40.34917713
Ti	16.85129241	15.15955580	45.07386347
O	15.16549358	15.12260116	39.86492436
O	17.15743011	16.89601649	44.52744263

O 15.08992457 17.28616208 42.30993638
O 16.89594079 15.24321031 46.86905553
O 16.90451053 15.09100824 42.87088721
O 15.15295051 17.02074883 38.24121045
O 16.92021211 17.08666471 40.62642500
O 15.08430281 15.07628256 45.23501194
Ti 18.60228457 15.03935145 37.86575610
Ti 18.72214147 17.00348337 40.36551985
O 19.15932929 15.16633608 39.87218487
O 18.79553375 17.08971856 42.17236777
O 18.25673005 16.89713932 38.21738402
Ti 8.06641860 18.65751793 38.09928989
O 7.12744673 18.57141374 39.70076135
Ti 11.41434148 18.79937861 38.13301876
O 11.69833177 18.81063185 39.89838175
Ti 14.97215129 18.79781861 38.11191059
O 14.72085640 18.82423836 39.88547916
Ti 18.33026862 18.68178025 38.06299145
O 19.28033811 18.61101071 39.66190936
Ti 11.33187516 11.49486105 47.47459647
Ti 13.28448433 12.73650395 51.95850138
Ti 11.46387744 13.27764117 49.84499795
O 11.00897035 11.56769048 49.21497912
O 13.28271111 11.22454171 52.45427195
O 11.47126696 13.31335454 51.58561513
O 11.64825296 13.25843549 47.43520129
O 13.27240930 12.93028810 49.92362212
Ti 15.18831245 11.48970724 47.44042030
Ti 15.08071608 13.26822086 49.82293906
O 15.52674940 11.56216504 49.17832307
O 15.09692013 13.30140722 51.56335186
O 14.86766332 13.25303064 47.39837836
Ti 11.37432687 15.02613508 47.43359694
O 11.23121974 15.02155749 49.21132650
Ti 15.13284292 15.02103610 47.40976900
O 15.29707206 15.01126279 49.18625040