

## Electronic supplementary information (ESI)

### **Understanding the interplay between size, morphology and energy gap in photoactive TiO<sub>2</sub> nanoparticles**

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## Fitting parameters of the Spherical Cluster Approximation (SCA)

The simplest SCA is defined by:  $G(n) = G_{\text{bulk}} + a_1 n^{-\alpha}$ , where  $G(n)$  is an arbitrary generic property (e.g. total energies, ionization energies) of a system with a size  $n$  and  $\alpha$  is a fitting parameter. Here  $\alpha = 1/3$  is typically employed, as derived from the  $n^{-1/3}$  dependency of the ratio of surface area to “bulk” in an ideal rigid cluster of fixed shape (typically spherical). Realistic nanoparticles are composed of bonded aggregates of atoms/ions and higher order terms (e.g.  $a_2 \cdot (n^{-1/3})^2$ ,  $a_3 \cdot (n^{-1/3})^3$ , ...) can become more significant contributions to  $G(n)$ . When  $G(n)$  is the system energy, for example, higher order terms can be thought of as reflecting various energetic contributions to the total energy (e.g. surface stress, edge and corner energies, internal stresses). For fitting the size dependent total energies,  $E(n)$ , of our TiO<sub>2</sub> NPs (see Figure 2) we employ the more general SCA expression:  $E(n) = E_{\text{bulk}} + a_1 \cdot n^{-1/3} + a_2 \cdot n^{-2/3} + a_3 \cdot n^{-3/3} + a_4 \cdot n^{-4/3}$ . Table S1 compiles  $a_n$  fitting parameters along with the coefficient of determination ( $R^2$ ). Note that in each case our fits yield  $R^2 > 0.999$ .

**TABLE S1.** Fitting parameters for fit lines for data relating to: Total energy *versus*  $n$  for faceted, relaxed as-cut spherical, annealed core-shell, and global optimised TiO<sub>2</sub> NPs. These fittings are depicted with solid lines in Figure 2 in the main text. Note that we take  $E_{\text{bulk}}$  to be that of the bulk anatase crystal in all cases and set it to be the zero baseline for our relative NP energies.

	$E_{\text{bulk}}$	$a_1$	$a_2$	$a_3$	$a_4$	$R^2$
Faceted	0	1.068	11.185	-27.204	20.721	0.9998
Relaxed spherical cuts	0	4.084	-8.493	10.179	-	0.9998
Core-shell	0	3.325	-5.171	7.616	-	0.9999
Amorphous	0	3.532	-12.633	26.843	-11.971	0.9991

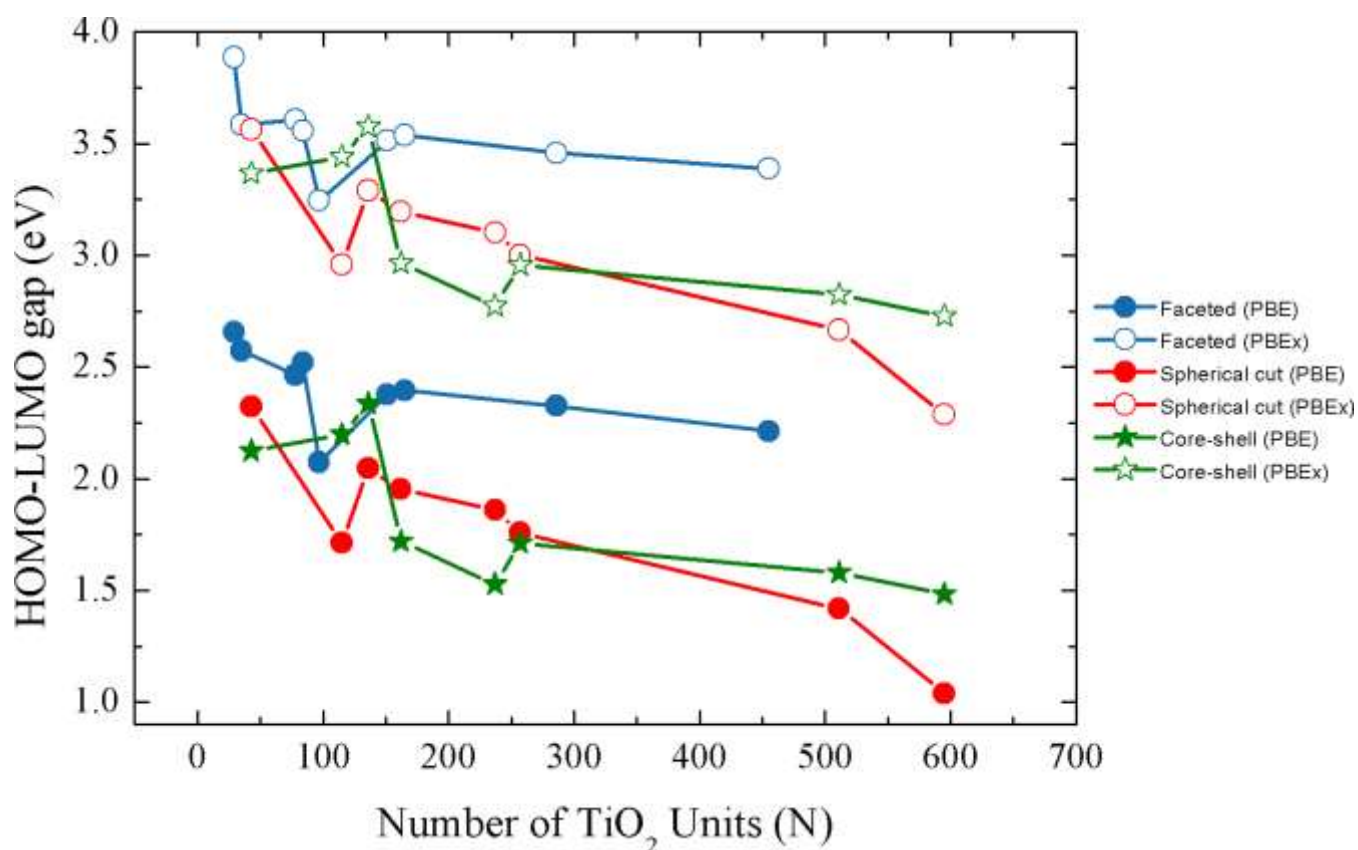
## Comparison of MA and NanoTiO interatomic potentials

**Table S2.** DFT calculated energetic stabilities and  $O_{\text{gap}}$  values of spherical  $(\text{TiO}_2)_n$  NPs with  $n=43, 115$  and  $136$  as annealed using NanoTiO and MA IPs. The relatively increased energetic stability of the NanoTiO-annealed NPs relative to those of the MA-annealed NPs is indicated by arrows in Fig. 2 in the main text.

	NanoTiO IP			MA IP		
	Energy w.r.t. Anatase (eV/TiO <sub>2</sub> )	$O_{\text{gap}}$ (eV) PBE	$O_{\text{gap}}$ (eV) PBE <sub>Ex</sub>	Energy w.r.t. Anatase (eV/TiO <sub>2</sub> )	$O_{\text{gap}}$ (eV) PBE	$O_{\text{gap}}$ (eV) PBE <sub>Ex</sub>
<b>(TiO<sub>2</sub>)<sub>43</sub></b>	0.590	1.383	2.629	0.696	2.125	3.367
<b>(TiO<sub>2</sub>)<sub>115</sub></b>	0.512	0.704	1.954	0.547	2.197	3.439
<b>(TiO<sub>2</sub>)<sub>136</sub></b>	0.492	1.079	2.327	0.533	2.335	3.576

## Optical energy gap ( $O_{\text{gap}}$ ) as function of exchange correlation functional

**Figure S1.** HOMO-LUMO gap ( $O_{\text{gap}}$ ) of faceted, spherical cut and core-shell  $\text{TiO}_2$  NPs calculated using PBE and hybrid PBE<sub>x</sub> (12.5 % Fock exchange) exchange correlation functionals. Note that the hybrid calculations for the faceted NPs were calculated and the values of spherical cuts and core-shell ones were predicted according to the recently reported correlation between  $O_{\text{gap}}(\text{PBE})$  and  $O_{\text{gap}}(\text{PBE}_x)$ .<sup>1</sup>



## XYZ files of faceted and annealed spherical TiO<sub>2</sub> NPs

### FACETED TiO<sub>2</sub> NPs

(TiO<sub>2</sub>)<sub>29</sub>

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PBE – Cuboctahedral shape

Ti	17.07749127	15.66160262	45.80279625
O	16.73997291	17.62235004	45.75094289
O	17.10730752	15.88577198	47.87547657
O	17.22526106	15.96829685	43.99117233
O	15.49956672	14.90360196	46.32397863
Ti	21.05395217	15.46082203	45.91003699
O	21.41732736	17.38244078	45.81587812
O	19.34587135	17.73118589	43.74036090
O	20.85449936	15.45432027	48.01037383
O	21.18334732	15.63204159	44.05968698
O	18.97886124	15.12606058	46.25440292
O	22.54458489	14.62555584	46.44909687
Ti	15.78916943	18.80824225	47.11938442
O	15.91876783	20.47802914	46.23799218
O	17.13414114	18.74673299	48.19991772
O	17.97514674	19.85247462	44.61766596
O	14.82088130	20.00527902	48.55865301
Ti	21.53152889	19.30287217	46.72825545
O	21.25033123	21.21340106	47.19665247
O	19.49484325	20.56928278	42.35867230
O	21.20649529	18.77691124	48.57715829
O	21.13962666	20.05340937	44.92803649
O	19.53360863	19.09203469	46.64943380
O	23.25206957	19.21202667	47.27042422
Ti	17.42597901	21.55164009	45.41903979
O	17.01164034	22.65654963	47.00272746
O	16.93746919	21.92178568	43.71804285
O	13.95621532	22.61537245	47.19537337
Ti	20.99908135	22.10890287	45.40836228
O	19.55569791	23.56957981	48.47904998
O	21.68183762	22.08098431	43.63934952
O	19.20875652	22.17656931	45.38728686
O	21.58132218	23.54052000	46.48132634
Ti	15.30510584	15.74411373	48.06057459
Ti	15.50511428	16.63067120	51.24142685
O	14.98842103	15.42560169	49.87570263
O	16.21822691	16.47912544	53.00994314

O	14.66916877	17.35685823	47.62792778
O	16.95690748	17.28248299	50.49610070
Ti	18.96426606	15.48304436	48.27501605
Ti	18.81732790	17.05675744	50.58022716
O	18.72022182	15.19398239	50.02878840
O	18.67541599	17.74664658	52.44566307
O	19.16965567	17.21046872	48.68512383
O	20.54031842	16.65149814	51.38570247
Ti	22.65978457	15.23723471	48.32148512
Ti	22.33474187	16.14534071	51.39811355
O	22.69914545	14.80634880	50.14319804
O	22.02760087	16.16376323	53.27546306
O	23.40503247	16.79177207	48.29140639
Ti	15.11348055	19.68181253	50.35497917
Ti	16.31524720	21.99066116	51.24475840
O	14.46720058	18.12945359	51.11662931
O	16.80781470	22.00283151	53.09311646
O	17.29550148	19.19263340	54.35060408
O	14.59302475	21.18859849	51.16512067
O	16.86756652	20.27466285	50.81847397
Ti	18.96227174	19.07256051	48.26032491
Ti	19.00087914	20.79074895	50.56975875
O	19.20526191	18.99815598	50.27964525
O	19.18970947	20.53582309	52.49695448
O	21.04463467	18.83695281	53.75763786
O	18.51063664	20.97959193	48.64277137
O	20.68872208	21.32514955	50.06291939
Ti	22.93520168	18.59760709	49.04304333
Ti	22.37426117	21.58517385	50.65742980
O	23.07991130	17.59644920	50.76710831
O	21.98300295	21.50299143	52.54246602
O	23.29801072	20.20644849	50.00786433
Ti	15.26933633	21.82628556	47.72980300
O	16.06464509	22.69601906	49.39734883
Ti	17.94726135	22.73447853	48.68721226
O	18.15596603	22.52501875	50.69346390
Ti	21.24647328	22.86129904	48.14081737
O	22.54603934	23.00348516	49.46703553
Ti	17.95319030	20.83285564	53.90426311
Ti	20.45276211	17.11424786	53.35568154
Ti	21.16199273	20.38968508	43.12564286
Ti	17.53359293	17.79214328	43.98474312
Ti	20.75290096	20.60476223	53.55386477
Ti	17.60325011	17.40093374	53.82379791
Ti	17.75035080	20.41800196	42.92520622
Ti	21.09890328	17.45834216	43.94657051
O	19.11532552	16.60374948	54.57293692
O	19.52688383	21.26082548	54.80208404
O	21.91219393	18.70236075	42.80415008
O	16.92543389	18.80430474	42.55580830

(TiO<sub>2</sub>)<sub>35</sub>  
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## PBE – Octahedral shape

O	11.39837812	14.76112310	30.24641893
O	6.23831189	14.73982313	30.11789886
O	10.47314733	13.17413905	28.37281762
O	10.50563317	13.18390954	32.64152102
O	10.75558031	11.42119911	30.25121238
O	8.74887730	13.65120686	30.87198263
O	6.98443850	13.10533839	28.26037192
O	6.91459234	13.12667955	32.54944069
O	8.65494195	15.35608558	33.43365826
O	6.74409240	11.35949743	30.17131459
O	10.79398637	15.27962433	26.55088503
O	12.27951610	17.07958585	21.86385273
O	10.94680814	16.80109366	19.11946674
O	12.06723744	14.94523012	23.89777434
O	12.93608330	14.64377479	27.72500547
O	10.70302477	17.52176552	24.00620676
O	13.24018975	16.54044506	25.34460226
O	10.48857118	15.05170985	20.85506625
O	6.79622377	14.83831500	26.00867966
O	8.98007144	17.31746415	21.69287035
O	7.10993376	16.99615697	19.34465484
O	9.34076535	15.04406512	23.87182923
O	8.37638125	15.43247711	27.97898653
O	7.11263235	16.51690073	23.29094477
O	8.56406842	16.85726810	25.58030856
O	6.78143168	15.07862859	20.86194065
O	5.43033690	17.51973867	21.77517026
O	4.63341155	14.96546701	23.67445391
O	4.85341450	15.21731770	27.65509010
O	4.98365588	16.90141733	25.23724097
O	10.69999748	11.39186412	26.17906870
O	12.52952550	13.52185284	21.58883938
O	11.06374753	13.17440643	19.10950576
O	13.22579625	11.36767969	23.09845786
O	12.44120353	11.01639099	27.95544358
O	10.71119768	12.71380132	23.17619166
O	12.94489205	13.02700010	25.38169434
O	10.90598279	11.26399065	20.80587404
O	6.90381219	11.11491541	26.23657801
O	8.82711839	13.15812162	21.59797628
O	6.60100769	13.04082538	19.22695067
O	8.47986037	11.32418970	23.91416600
O	8.81058231	10.89493766	27.94040307
O	7.00300269	13.55597691	23.25755785
O	8.85140717	13.19302503	25.55616038
O	7.07194957	11.20422314	21.07939842
O	5.07060990	12.96509632	21.68395550
O	5.57277302	11.29875934	23.83896888
O	5.01509429	11.11471695	27.81668417
O	4.60554507	13.06783090	25.43776535
O	12.35277742	8.77323633	21.75808517
O	10.81150934	9.37739428	19.23288198

O	10.73290494	9.92469738	23.25916209
O	12.87115315	9.73054907	25.22521818
O	8.92960452	9.01437928	21.62353145
O	6.76808588	9.33725576	19.41026804
O	7.10009814	8.90593906	23.42594878
O	9.03901760	9.39054319	25.42913255
O	5.14932207	9.24305488	21.85070272
O	4.47847289	9.60338918	25.29999691
O	10.44608557	15.17079676	16.81908778
O	6.96656091	15.47492207	16.99269941
O	8.58367684	14.91784068	14.52128564
O	8.77366363	14.77624588	18.70893162
O	10.52407255	11.06951548	16.89526184
O	7.09427965	10.76019035	17.05078643
O	6.46552798	13.02379365	13.78902658
O	8.70362929	11.27829804	14.54695565
O	8.83463831	11.40550773	18.85731880
O	8.31338332	13.10176345	16.24573181
Ti	11.30794896	14.77309971	28.42381665
Ti	6.56769577	14.88350410	28.35197603
Ti	10.56623051	13.19452048	30.87512920
Ti	10.64844689	11.36193985	28.44975542
Ti	6.93900663	13.12116405	30.78132890
Ti	8.68905709	13.81094564	32.93943311
Ti	6.78229147	11.33432816	28.34319376
Ti	12.54397237	14.94198679	25.88464312
Ti	10.70299556	16.81316142	20.91569807
Ti	12.26116374	16.75928614	23.69801309
Ti	10.57808015	15.01295391	18.60895034
Ti	8.73621488	15.13689581	26.22273366
Ti	7.06247621	16.88901936	21.18747221
Ti	8.96159312	16.76208762	23.81296400
Ti	7.04459789	15.23598967	18.78912302
Ti	5.05145823	15.06777067	25.86332481
Ti	5.31327152	16.65619287	23.47510116
Ti	12.47946811	11.26253055	26.15818119
Ti	10.76660098	13.15051184	21.07412048
Ti	12.44625389	13.07185210	23.33103076
Ti	10.60682695	11.14829211	18.72076769
Ti	8.78562665	11.18049941	25.98086754
Ti	6.86046620	13.14598011	21.10315199
Ti	8.85697111	13.21041572	23.59218965
Ti	7.04875220	11.11157265	18.81318228
Ti	5.06189509	11.23743701	25.97534148
Ti	5.27088272	13.15133711	23.45995215
Ti	10.75131202	9.42883554	21.07927992
Ti	12.52514077	9.75637427	23.36850194
Ti	6.93405850	9.42766790	21.20154213
Ti	8.88638684	9.59729507	23.64868327
Ti	5.38865579	9.52218407	23.64152719
Ti	8.63637770	14.93349713	16.28966567
Ti	8.75649713	11.28842412	16.31249406
Ti	8.03261087	13.07791388	14.19744230



**(TiO<sub>2</sub>)<sub>78</sub>**

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PBE – cuboctahedral shape

Ti	17.07116584	15.43840332	45.97657092
O	17.12977488	17.23809636	45.80375963
O	17.16733276	15.38378532	48.23516016
O	16.94578759	15.42526160	44.17010702
O	15.31695547	15.17386168	46.56255436
Ti	20.94845445	15.43926070	45.98401808
O	20.88951567	17.23847026	45.81197528
O	19.01612469	17.04585696	43.22456626
O	20.84305502	15.38883001	48.24860956
O	21.08376454	15.42651550	44.17844758
O	19.01038528	14.96427101	46.49827448
O	22.69891889	15.17128676	46.58129200
Ti	17.15655706	19.17049671	46.38467062
O	17.41072225	20.96764462	46.27113045
O	17.08265977	19.05766614	48.42410117
O	17.69910368	19.14110472	44.46599766
O	15.29385930	19.16910209	46.67863897
Ti	20.85790008	19.17189332	46.39222115
O	20.60281196	20.96828192	46.27599484
O	19.01649646	20.15765737	42.18388560
O	20.92399580	19.06086076	48.43341113
O	20.33264829	19.14041232	44.47020950
O	19.00689516	18.83879104	46.91980306
O	22.71987959	19.17056633	46.69422694
Ti	17.23763844	22.39339450	45.22432530
O	17.40337912	22.98764481	48.18580995
O	16.76734479	21.58693841	43.61829542
O	15.73534380	23.07780126	46.14879435
Ti	20.78299144	22.39444475	45.23121640
O	20.61170977	22.97592851	48.20721829
O	21.26013915	21.58841124	43.62663489
O	19.01066533	23.03435424	45.14452282
O	22.27801851	23.08015781	46.16723657
Ti	13.81993953	13.55307495	53.47954290
O	12.83157174	13.61445001	55.08812611
O	13.70616350	13.21184451	51.63952310
Ti	17.18726483	13.40606770	53.51136125
Ti	15.25041771	13.57471833	50.69008985
O	17.44928313	13.34611555	55.30995702
O	15.43259725	12.77434168	53.63213542
O	14.99951813	13.55374441	48.89766398
O	17.02700334	13.12653084	51.30160322
Ti	20.80261771	13.39529134	53.49789901
Ti	18.99072085	13.38711315	50.90802897
O	20.51696103	13.33403563	55.30087004
O	18.99174437	12.93375444	52.89108701
O	19.00739392	13.25229990	49.04372979
O	20.97442193	13.12869153	51.32246496
Ti	24.16647712	13.56924522	53.51716228

Ti	22.75374488	13.57744930	50.71329340
O	25.12586525	13.63494883	55.14380898
O	22.56056700	12.77647195	53.65695243
O	23.00849712	13.55383469	48.92110550
O	24.29381072	13.22950079	51.67649353
Ti	13.53848678	17.22068988	53.32340441
Ti	13.41688569	15.20993377	55.84598993
O	12.94005199	17.05433220	55.32968878
O	13.36095142	15.08458303	57.68798566
O	13.92144233	15.34804991	53.63636298
O	13.29827680	17.09156211	51.52553158
Ti	15.37029282	15.33057139	48.38046843
Ti	17.15014284	17.19867082	53.38333700
Ti	15.07296868	17.25286655	50.92682703
Ti	17.13032599	15.09429725	55.80052207
O	15.32822616	15.37301786	50.60099860
O	16.97654122	17.10411608	55.30970923
O	15.25644383	17.56610234	52.97879076
O	17.07901157	14.89690437	57.77654050
O	16.98866058	15.18926381	53.64879663
O	14.88951994	17.19973561	48.87681156
O	17.07880686	17.17904174	51.38478829
O	15.22952839	15.10807447	56.07683332
Ti	19.00566517	15.00731265	48.50183881
Ti	20.83137012	17.18705819	53.36667906
Ti	18.98967153	17.09108209	51.01268616
Ti	20.81507429	15.07645968	55.78767908
O	18.99250536	15.13849713	50.66380987
O	20.98221522	17.09528737	55.28630228
O	18.99014454	16.92285475	53.00198847
O	20.86011677	14.81986376	57.78821720
O	20.99362032	15.17660494	53.64831957
O	18.99798044	17.11146051	49.09733982
O	20.91137309	17.16523435	51.38087523
O	18.98361115	15.42102975	56.13372302
Ti	22.63949278	15.33048210	48.39852207
Ti	24.44566253	17.23893795	53.35123678
Ti	22.92594896	17.25408510	50.94502785
Ti	24.53112114	15.23707711	55.88327959
O	22.67784670	15.37481135	50.61900663
O	25.01650691	17.07368289	55.38504044
O	22.72929590	17.57107711	52.98480571
O	24.58005809	15.14287197	57.72699989
O	24.05484552	15.36481921	53.68165831
O	23.11883123	17.20107561	48.89348286
O	24.69894442	17.09567975	51.55728815
O	22.71417814	15.14706374	56.12155795
Ti	13.53146432	20.86404432	53.34984914
Ti	13.26320803	19.02065084	55.79023752
O	12.93714177	20.98318882	55.37434062
O	13.05686015	18.97936248	57.65343156
O	12.96842010	19.03436771	53.77871295
O	13.31003183	21.03470988	51.55954042

Ti	15.29088108	19.13450465	48.49786763
Ti	17.15221770	20.89344601	53.45357172
Ti	15.11573826	20.96369136	50.99462651
Ti	17.05295874	18.99553961	55.80151987
O	15.05319342	19.10317425	50.47405405
O	16.98117706	20.90057312	55.37308623
O	15.25794450	20.54244196	53.02933631
O	17.12135765	18.98208007	57.64543432
O	17.37279186	19.02471118	53.75094902
O	15.09762578	21.11499881	48.86616212
O	17.10145764	20.84053658	51.45697509
O	15.01015961	19.00473938	56.00256043
Ti	19.00293622	18.98086245	48.80539581
Ti	20.83056741	20.90910378	53.44263026
Ti	18.99392993	20.85156696	51.09088944
Ti	20.89828691	18.99441383	55.73084773
O	19.00130964	18.98566595	50.76781583
O	20.97743782	20.91204398	55.34950076
O	18.99102732	21.11232622	53.09932599
O	20.95843990	18.98090091	57.59198159
O	20.61692016	19.02609826	53.71291255
O	18.99395399	20.97951030	49.21797572
O	20.88736722	20.85883450	51.44828415
O	19.00027353	18.99049077	55.99512054
Ti	22.71626243	19.13424859	48.51281248
Ti	24.45003297	20.84979337	53.37821739
Ti	22.88552436	20.96432457	51.00958493
Ti	24.66979332	19.02070124	55.86417350
O	22.94330054	19.10396164	50.49101676
O	25.01611471	20.96866135	55.42837240
O	22.72581490	20.53813348	53.03326941
O	24.73567525	18.98338817	57.71688218
O	25.01411949	19.03648248	53.81531260
O	22.91612759	21.11536588	48.88258058
O	24.68739001	21.03299064	51.59179522
O	22.91536519	19.00541918	55.97420951
Ti	13.83843626	24.52856776	53.56208722
Ti	13.41646996	22.82790369	55.90857901
O	12.84731791	24.44394875	55.17277073
O	13.35415173	22.90502118	57.75901547
O	13.90102701	22.72798101	53.71066723
O	13.82944044	24.96883210	51.71253059
Ti	15.64108094	22.82029665	47.97097610
Ti	17.17365261	24.68085466	53.70249823
Ti	15.31360994	24.50525923	50.73439443
Ti	17.12970241	22.90709841	55.91982197
O	15.41048434	22.78421388	51.06979601
O	17.43294301	24.67290490	55.50245169
O	15.42063305	25.30110123	53.86350802
O	17.06988237	23.04978787	57.89372359
O	17.01624588	22.88081223	53.77439924
O	15.04880297	24.28914297	48.88429019
O	17.01598758	25.01018086	51.50568340

O	15.22731060	22.87811937	56.16207531
Ti	19.00225589	23.01718660	49.01444677
Ti	20.81185159	24.69568847	53.68771776
Ti	18.98741864	24.74330830	51.18063727
Ti	20.81396701	22.93008470	55.90681655
O	18.98790455	22.92391073	50.93805593
O	20.52938578	24.68864891	55.49328890
O	18.98874995	25.20859581	53.15661097
O	20.86698414	23.13046541	57.90812111
O	20.96377526	22.89723857	53.77428370
O	19.00681401	24.89769710	49.40864611
O	20.97902100	25.00933732	51.52664502
O	18.98290796	22.57368901	56.24057930
Ti	22.37345455	22.82190126	47.98982866
Ti	24.14433633	24.51592976	53.59855846
Ti	22.68685708	24.50616981	50.75806626
Ti	24.52936070	22.80456355	55.94551564
O	22.59353962	22.78516185	51.08988291
O	25.10889104	24.42541710	55.22553904
O	22.56697112	25.30214821	53.88730620
O	24.58512720	22.85478092	57.79664955
O	24.07022398	22.71452401	53.75271550
O	22.95816593	24.29200603	48.90831465
O	24.16672446	24.96000185	51.74860185
O	22.71432104	22.84429780	56.20509727
Ti	15.10547703	15.43260398	58.23722718
Ti	15.51763242	17.11210818	60.89268436
O	14.98163671	15.54061763	60.12138714
O	16.14513430	16.86696222	62.63974202
O	15.19244002	17.17764501	58.07446855
O	17.06627817	17.33792180	60.14479122
Ti	18.98665279	15.22704322	58.15974225
Ti	18.88595407	17.07925486	60.22339075
O	18.90512686	15.22421467	59.97307170
O	18.73405291	17.64536474	62.11325187
O	19.07231750	17.04024820	58.26598721
O	20.73891930	17.01444899	60.91455840
Ti	22.81475325	15.36364440	58.27375574
Ti	22.55110665	17.00077707	60.80187983
O	22.93083739	15.31495646	60.12891197
O	22.44839709	16.86718928	62.60381399
O	22.60682143	17.13031650	58.42472473
Ti	14.76915729	18.97364799	58.24107306
Ti	15.51379853	20.77399097	60.93031222
O	14.79401785	18.94798472	60.30720446
O	16.14488688	20.97719556	62.68260244
O	17.54698896	18.90370884	64.32363671
O	15.17223401	20.77480385	58.12003655
O	17.06242824	20.56542885	60.17730397
Ti	19.01348806	18.97891921	57.93544239
Ti	18.88359491	20.81397271	60.27255441
O	19.26695306	18.95281964	59.80011090
O	18.73240811	20.19600683	62.14237484

O	20.75285839	18.91146750	63.49571742
O	19.07512769	20.90654482	58.31899462
O	20.74029550	20.86855123	60.95802158
Ti	22.96202346	18.97697389	58.22949354
Ti	22.55393712	20.88580540	60.84721215
O	22.98698075	18.95233045	60.25173722
O	22.44901060	20.97681473	62.65128888
O	22.62216245	20.81664042	58.45751359
Ti	15.08700739	22.51851724	58.31611693
O	14.96814735	22.36126684	60.19853441
Ti	18.98658959	22.72240208	58.26485566
O	18.90233211	22.67622568	60.07619529
Ti	22.83073043	22.58910337	58.35458455
O	22.94581245	22.58299135	60.21133801
Ti	20.68930024	19.97105221	42.91592958
Ti	17.31188670	17.25732375	43.78293438
Ti	20.56823357	20.62522104	62.94665991
Ti	17.74545617	20.56853882	63.58163947
Ti	20.56765835	17.21023044	62.91033825
Ti	17.74678875	17.25436031	63.54748532
Ti	20.71800202	17.25842449	43.78840864
Ti	17.34170259	19.96961333	42.91145398
O	19.36118832	16.40983170	64.09859055
O	19.36066500	21.40509953	64.14568432
O	16.51970144	18.33147977	42.47629647
O	21.51028302	18.33317839	42.48098319

**(TiO<sub>2</sub>)<sub>84</sub>**

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PBE – Octahedral shape

Ti	13.69147265	13.13529165	23.72431871
Ti	13.14969462	11.32791997	25.87918659
O	13.49996462	13.14997496	25.77877454
O	13.17122112	11.56808736	28.39239874
O	13.11445446	11.30787075	24.11399706
O	15.24064986	13.12666182	23.25524803
O	11.40400313	11.10583811	26.54857396
O	14.86108028	10.87759511	26.54816539
Ti	13.16025954	14.97450490	25.85462356
O	13.17701119	14.76454028	28.34112833
O	13.12752782	14.97057637	24.08860282
O	11.40642002	15.20158105	26.50491098
O	14.87553798	15.43867577	26.51275626
Ti	9.56412156	9.31932278	33.11988842
Ti	9.41961486	7.63780606	35.51068374
O	9.33406769	9.46426936	35.25122926
O	9.51850212	8.06183348	37.70671330
O	9.32318903	7.56266099	33.67331759
O	9.51206543	9.21099175	31.28438882
O	7.79280075	7.06027468	36.20228098
Ti	13.19980769	9.15941836	33.19534897
Ti	11.25620193	9.54543806	30.72497579
Ti	13.24779753	7.56694674	35.55594753

O	13.20239211	9.32957098	35.28151394
O	11.34696169	9.46894849	32.96339734
O	13.22102686	7.17875944	37.56490177
O	13.22421255	7.38749164	33.72221605
O	11.15365616	9.50975241	28.90127144
O	13.17017855	9.05363402	31.19916307
O	11.27510907	7.21536252	35.99746522
Ti	16.85335551	9.41753674	33.01007311
Ti	15.07293539	9.54903147	30.70367528
Ti	16.97649449	7.69042676	35.33797594
O	16.88849055	9.48573143	35.24061432
O	15.05310770	9.46289267	32.90514596
O	16.78621298	6.99948612	38.25432585
O	17.23139736	7.64893207	33.54973241
O	15.15317982	9.46684575	28.89207295
O	16.86519496	9.27053118	31.20291996
O	15.18593930	7.28090166	35.95926454
O	18.53745416	7.35340741	36.26912053
Ti	9.46809806	13.19699315	33.10864042
Ti	9.31966039	11.36780638	35.50777654
O	9.50518700	13.23621746	35.09525151
O	9.39949588	11.29347796	37.65677008
O	9.12489526	11.30605294	33.51652059
O	9.30321796	13.20823960	31.26835753
O	7.54378616	11.64320445	35.98146348
Ti	11.39054424	11.28224435	28.35135666
Ti	13.20498881	13.19551685	33.06633024
Ti	11.06833636	13.18857196	30.79114709
Ti	13.23500940	11.37280917	35.48861278
O	11.33825481	11.33292338	30.58469026
O	13.17039880	13.21226992	35.20506872
O	11.24121833	13.21897162	32.84368263
O	13.22365656	11.29899588	37.51112933
O	13.20893266	11.28900216	33.58701521
O	10.83891838	13.17191937	28.79043328
O	13.20571274	13.18128736	31.25270436
O	11.27504571	11.32300553	35.97769713
Ti	14.94535831	11.23504930	28.31026830
Ti	16.93228577	13.21702978	33.05245044
Ti	15.29231511	13.19275183	30.72621139
Ti	17.10890535	11.37445513	35.50874023
O	15.01615824	11.33060255	30.54600645
O	17.08946252	13.22153115	35.05500507
O	15.16535061	13.21046920	32.85518043
O	16.92586940	11.72987026	37.54835594
O	17.31719181	11.29811321	33.48046599
O	15.48786305	13.17761874	28.74864623
O	17.07104265	13.20208488	31.21996954
O	15.11951850	11.35091968	35.92281351
O	18.89861692	11.25913272	36.09939989
Ti	9.53052483	16.98134316	32.99698392
Ti	9.29913514	15.06024320	35.52534712
O	9.51762696	16.94029936	35.22454421

O	9.47490618	14.71295902	37.57149303
O	9.04162897	15.11192868	33.50028077
O	9.50796198	17.10359580	31.18029633
O	7.50970390	15.14879760	36.11299232
Ti	11.39577450	15.04703069	28.30880799
Ti	13.17322972	17.24952470	33.16060142
Ti	11.28264005	16.81882402	30.64875866
Ti	13.18814569	15.06052411	35.46749460
O	11.38487675	15.03556743	30.53765547
O	13.20021604	17.09065186	35.24043793
O	11.32870958	16.91707455	32.87996020
O	13.20114645	15.26938398	37.55191722
O	13.19933225	15.12816846	33.58143292
O	11.16768734	16.83242830	28.82796636
O	13.16646556	17.34652492	31.14368797
O	11.30187461	15.13102477	35.95866269
Ti	14.95062948	15.11049919	28.27979890
Ti	16.82394219	17.00642142	32.97819160
Ti	15.06134677	16.83309705	30.65789334
Ti	17.08982358	15.07069073	35.50300541
O	14.99786219	15.04757086	30.52389769
O	16.85354671	16.94937592	35.20568586
O	15.02496502	16.95350667	32.86318783
O	16.92895607	14.74185676	37.54102134
O	17.30033032	15.13139508	33.46417841
O	15.14905549	16.88574485	28.84412462
O	16.84579586	17.12661778	31.16643474
O	15.10125928	15.07459362	35.94010643
O	18.88644780	15.20758060	36.08006746
Ti	9.44614361	18.73644153	35.30909140
O	9.64017987	19.47695093	38.28994529
O	9.17400251	18.75540819	33.51568716
O	7.91387017	19.10054496	36.27431872
Ti	13.18356332	18.84718154	35.52708546
O	13.18958474	19.31852513	37.52018718
O	13.16452916	19.02333221	33.68898139
O	11.22004086	19.13991185	35.94030930
Ti	16.92553870	18.74824540	35.29609503
O	16.74603310	19.48770534	38.24941244
O	17.18522866	18.77897658	33.50471302
O	15.14958083	19.14918401	35.92796248
O	18.47289825	19.11355688	36.23893963
Ti	7.71638989	8.00586512	37.83714040
Ti	9.44475773	9.57448412	42.90073707
Ti	7.68850256	9.45404881	40.58558555
O	7.32855268	7.88814938	39.66398198
O	9.31803175	9.56637724	44.70814719
O	7.66974242	9.20183768	42.37442359
O	7.00640685	9.64424655	37.68782838
O	9.48367975	9.54268717	40.65708794
Ti	11.40628410	7.75808566	38.02823492
Ti	13.22939657	9.51434900	42.82116072
Ti	11.37076536	9.32667153	40.38453428

O	11.31191913	7.53088199	39.82766400
O	13.21804456	9.36366683	44.65471667
O	11.31326127	9.08745362	42.40579068
O	11.65594624	9.48698741	38.34271130
O	13.19271914	9.57077719	40.80583076
Ti	15.02077479	7.62291064	38.14632144
Ti	17.10709389	9.60484256	42.78999567
Ti	15.05463634	9.34421212	40.40802681
O	14.77872031	7.57921643	39.94710424
O	17.21749242	9.56869708	44.61946248
O	15.11717128	9.16380992	42.39676105
O	15.17950048	9.41390099	38.25831537
O	16.96121293	9.37166220	40.67042988
Ti	18.40958939	7.74402881	38.09489670
Ti	18.78946396	9.44996175	40.40653667
O	19.37874513	7.83019762	39.71033916
O	18.86812561	9.35220845	42.23867941
O	18.30554274	9.54406904	38.23400385
Ti	7.59908625	11.42290191	37.77676015
Ti	9.20497345	13.23104959	42.71592421
Ti	7.56918608	13.17814202	40.37672924
Ti	9.60111962	11.35890203	45.21180658
O	7.27212446	11.24751757	39.97215935
O	9.10343396	13.25874026	44.70883310
O	7.42078754	13.20772386	42.20699124
O	9.53785552	11.27448640	47.02306734
O	9.50076091	11.37448300	42.99855641
O	7.15051447	13.21544245	38.36277484
O	9.33457106	13.22966361	40.60500466
Ti	11.35857479	11.42495154	37.93452835
Ti	13.23423984	13.22583140	42.82028151
Ti	11.37715310	13.21357316	40.39532817
Ti	13.24203676	11.13721838	45.15327088
O	11.28421204	11.35014552	39.92369773
O	13.25053565	13.23316903	44.64219722
O	11.30367854	13.22400888	42.28923345
O	13.25444921	10.95122192	47.12971757
O	13.21345315	11.28270754	43.05202240
O	11.50727281	13.22663496	38.30957201
O	13.22280454	13.26533680	40.70003142
O	11.38111252	11.43027509	45.35501577
Ti	15.01603696	11.39624798	37.95353428
Ti	17.25770324	13.25344679	42.68352362
Ti	15.05880008	13.25285523	40.37636948
Ti	16.89251421	11.33022606	45.14525706
O	15.13230287	11.32649536	39.89882482
O	17.36362716	13.26000681	44.65984285
O	15.15120921	13.22888189	42.27426479
O	16.97401391	11.26285065	46.95969137
O	16.97479829	11.39198241	42.92714945
O	14.85460248	13.24301886	38.33652491
O	17.11846476	13.23082735	40.56557828
O	15.10811622	11.38288560	45.31511299



Ti	18.65229693	11.42660939	37.88360556
Ti	18.88782987	13.24851047	40.34197451
O	19.24031740	11.29881330	39.90258105
O	19.04058954	13.26122974	42.16922967
O	19.20558448	13.24286747	38.30869386
Ti	7.75293352	15.02476706	37.90675861
Ti	9.34608286	16.86932138	42.79579933
Ti	7.64448299	17.00415567	40.42560663
Ti	9.59561173	15.17473905	45.19293572
O	7.21291113	15.16180002	39.92957339
O	9.25813851	16.91789409	44.63415231
O	7.57853433	17.10370602	42.26158198
O	9.57883988	15.27593069	47.01615418
O	9.50137555	15.08683167	42.94482808
O	8.11103536	16.90712252	38.22555967
O	9.46756023	17.10372497	40.67636584
Ti	11.38306866	15.10267684	37.94648021
Ti	13.22224259	16.94646442	42.76899302
Ti	11.37776831	17.10994394	40.39720343
Ti	13.23877569	15.35363721	45.08816919
O	11.25668141	15.13474815	39.88787186
O	13.22815493	17.12019938	44.60336056
O	11.32865863	17.32147171	42.37431268
O	13.25150753	15.57914727	47.08347161
O	13.22932381	15.17272179	43.04817753
O	11.20167460	17.05967655	38.24588328
O	13.21705479	16.77059137	40.76526228
O	11.38154833	15.08378855	45.31751307
Ti	15.02321629	15.07527605	37.93614806
Ti	17.09368323	16.89298701	42.76918332
Ti	15.04403117	17.13347460	40.38304322
Ti	16.88618212	15.18013085	45.15495082
O	15.19004855	15.14129739	39.88953611
O	17.21075210	16.92958301	44.60414713
O	15.10925580	17.34045629	42.36434548
O	16.92773583	15.27277802	46.97681725
O	16.94663771	15.10790518	42.90712054
O	15.18231536	17.06160445	38.23761782
O	16.95830648	17.13172881	40.65136970
O	15.10246419	15.10078360	45.29971557
Ti	18.65351036	15.05859249	37.86751652
Ti	18.77872776	17.04693749	40.38927734
O	19.23014268	15.19422999	39.89072971
O	18.85817258	17.14002010	42.22307142
O	18.29048645	16.93749063	38.21039179
Ti	8.02426802	18.70922690	38.10404361
O	7.04996728	18.62186971	39.71242572
Ti	11.39235447	18.85365276	38.13791234
O	11.69342628	18.86903640	39.92846867
Ti	14.99290047	18.85215956	38.11577281
O	14.72044224	18.88452618	39.91505408
Ti	18.36861094	18.73884219	38.06977326
O	19.35426035	18.66643634	39.67566880

Ti	11.31616674	11.48510662	47.58614835
Ti	13.28818579	12.73794264	52.13403916
Ti	11.45151706	13.28286809	50.00470323
O	10.98324421	11.56831895	49.35298743
O	13.28527398	11.18859482	52.60359457
O	11.45809481	13.31752513	51.77086311
O	11.64514974	13.26061956	47.51204356
O	13.27634067	12.93276951	50.07839996
Ti	15.20886446	11.47828758	47.54874037
Ti	15.10090503	13.27178439	49.98308386
O	15.55919237	11.56248800	49.31230382
O	15.11869907	13.30356023	51.74889912
O	14.87733724	13.25333011	47.46724057
Ti	11.36202912	15.04177606	47.54370558
O	11.21065561	15.03232227	49.34879879
Ti	15.14912954	15.03461674	47.51699449
O	15.32332044	15.01854798	49.32094072

**(TiO<sub>2</sub>)<sub>97</sub>**

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PBE – Cuboctahedral shape

Ti	13.97898706	13.06019497	43.97646546
Ti	13.50836571	11.42682049	46.22997323
O	13.84843454	13.26885330	45.82274283
O	13.45676971	12.12436438	48.28592839
O	13.38686865	11.35843976	44.36705063
O	11.83135548	10.92994860	46.82387247
Ti	17.30996633	12.97327362	44.12808194
Ti	17.19011955	11.36288155	46.44381533
O	17.18261193	13.17652467	46.07732352
O	15.63433972	12.95920057	43.31601662
O	17.13865811	11.15666764	48.55942463
O	17.22294589	11.13571403	44.67790783
O	15.23998598	10.91297825	46.87723719
Ti	20.64376441	12.98315472	44.07463263
Ti	20.86037382	11.40479473	46.41593725
O	20.77388504	13.19897583	46.02394516
O	18.97356931	12.91061031	43.34532714
O	20.88867981	11.13377620	48.51714929
O	20.80209972	11.15957715	44.64513312
O	19.01482526	11.02936078	46.88536750
Ti	24.44201770	11.48508230	45.92846521
O	24.06011910	13.29321197	45.72063828
O	22.29685925	13.05484452	43.19476749
O	24.49802781	10.90698420	49.01279786
O	24.60734224	11.50733727	44.10792633
O	22.80237124	11.04577482	46.76982561
O	26.02691525	11.29557371	46.79501550
Ti	13.42849802	15.35838220	45.84714013
O	13.67344690	17.07336816	45.31416964
O	13.32155069	15.20030118	48.09212630
O	13.48331812	14.90021342	43.92894279
O	11.62968610	15.48746375	46.20357658

Ti	17.31801178	17.03284305	43.66928184
Ti	17.14918087	15.28185849	46.13304824
O	17.09162984	17.11186775	45.62672330
O	15.85111377	16.81812519	42.71223977
O	17.13842103	15.37452259	48.20611741
O	17.30146315	14.99185214	44.29908587
O	15.29071666	15.27964023	46.58192685
Ti	20.67313343	17.04281271	43.67402213
Ti	20.82165761	15.26505081	46.09980217
O	20.78066880	17.10785163	45.62577702
O	18.98910484	16.94949586	42.90810420
O	20.84657314	15.14093100	48.18681555
O	20.66976251	15.00762056	44.26432315
O	18.98240093	15.27984479	46.64100811
Ti	24.09261706	17.07260972	43.27592287
Ti	24.58100093	15.35450259	45.90818844
O	24.61415163	17.08445405	45.40190692
O	22.20775301	16.92937164	42.81402969
O	24.55135299	15.62269448	47.99463812
O	24.45045138	15.02959947	43.92221452
O	22.67462644	15.30610316	46.50007877
O	26.37879372	15.03052263	46.39809329
Ti	14.12370286	20.51805905	42.79907044
Ti	13.55559249	18.99904623	45.37711351
O	13.78248091	20.92777092	44.72536665
O	13.31157862	18.98740332	48.50383010
O	13.71424758	18.72730219	43.47446220
O	11.94589427	19.11525357	46.23033046
Ti	17.33364570	21.03107911	43.63505720
Ti	17.11284033	19.02397799	45.99126869
O	17.11922191	20.92166229	45.61864961
O	15.96970793	21.00749322	42.51934683
O	17.08711516	18.95232256	48.02706565
O	17.24767090	19.00749917	44.05913720
O	15.13178590	19.09755231	46.44431401
Ti	20.68722378	21.01392217	43.68194441
Ti	20.82814322	19.01756409	45.97967017
O	20.80394365	20.92243172	45.62949279
O	19.00210948	21.08959718	42.90908132
O	20.82644902	19.10606078	48.02836359
O	20.68394584	19.02337316	44.05303152
O	18.95064313	19.00925803	46.49540172
Ti	24.58451834	19.02698492	45.71425600
O	24.40330840	20.92021977	45.44463410
O	22.20329085	21.11679669	42.79303706
O	24.63211751	18.97398375	48.01381835
O	24.21904007	19.01662877	43.86483073
O	22.70582166	18.94466539	46.41387889
O	26.41231710	19.07136955	46.22180155
Ti	13.54714791	22.67880640	45.38540108
O	13.97642820	24.82505334	45.71247267
O	13.31450843	22.91529766	48.59610566
O	13.28130084	23.47327177	43.72608351

O	12.00211247	22.45368855	46.23956268
Ti	17.27502291	25.05625350	44.10237290
Ti	17.05543029	22.74159539	46.14094864
O	17.09913630	24.83260436	46.05977386
O	15.67028153	25.16586868	43.21070841
O	17.07998747	22.66253710	48.14152452
O	17.16736761	23.01255638	44.26852670
O	15.13505506	22.65817396	46.55480366
Ti	20.63616009	25.04164946	44.11130931
Ti	20.78250037	22.75772652	46.13929263
O	20.78768321	24.83951013	46.06282753
O	18.96141122	25.07846324	43.37011888
O	20.79237358	22.61216697	48.18494686
O	20.67366400	23.01692843	44.28443030
O	18.93284871	22.80127031	46.60734558
Ti	23.96396396	24.88689800	43.96928972
Ti	24.55551865	22.69029434	45.88645472
O	24.09114650	24.73357655	45.82890578
O	22.31687754	25.03687994	43.29863195
O	24.63853664	22.84017252	48.07782583
O	24.44047721	23.04788468	43.97485222
O	22.65350781	22.71088983	46.56318575
O	26.36439957	22.62490493	46.22113514
Ti	13.53150755	26.60952914	46.23369544
O	13.48444365	25.84218371	48.26374587
O	13.38902358	26.83928924	44.40541554
O	11.81601284	27.02658448	46.84736217
Ti	17.14443561	26.64578417	46.44661621
O	17.12296719	26.82513070	48.57780946
O	17.22499302	26.89288950	44.69208948
O	15.24529620	27.14102040	46.91085329
Ti	20.79943175	26.65531033	46.42682392
O	20.85847369	26.83032316	48.53922165
O	20.73409194	26.87690322	44.66015428
O	18.97868140	26.99632359	46.90644945
Ti	24.46658236	26.57805547	46.18995247
O	24.52092158	25.89927799	48.26565614
O	24.59665895	26.59026509	44.33111078
O	22.73660621	27.09789785	46.84203971
O	26.12952645	27.10527253	46.79503575
Ti	11.65575005	12.01270565	48.35916964
Ti	11.46267462	13.60441994	51.09467533
O	11.24256260	12.03622328	50.20570669
O	11.46896337	13.41463449	52.91451237
O	10.91282682	13.57505874	47.97149261
O	13.27938518	13.92986044	51.32083248
Ti	15.31532300	11.69836937	48.86573371
Ti	17.06763192	13.89009470	53.77421150
Ti	15.34811434	13.39669706	51.15035503
O	15.01568361	11.60235011	50.64590455
O	15.01235461	13.52501987	53.12369786
O	15.61411402	13.43627236	49.06034018
O	17.07998728	13.36319628	51.65332908

Ti	19.00948923	11.57218377	49.01885473
Ti	19.02588049	13.39926650	51.33956309
O	19.06726293	11.56955327	50.82222397
O	19.01505898	13.77918882	53.18387745
O	18.96488174	13.34214962	49.02084642
O	20.92355192	13.55600310	51.61528803
Ti	22.69762304	11.53800687	48.99813079
Ti	24.90977718	13.99046000	53.05335520
Ti	22.69111277	13.40575833	51.16367068
O	22.62570313	11.60030806	50.80877753
O	23.06613299	13.52392902	53.06191277
O	22.84682059	13.32551514	48.94608266
O	24.74063013	13.87412663	51.19701265
Ti	26.05123673	11.67518605	48.65228844
Ti	26.58668956	13.51763745	50.81652231
O	27.11437095	11.85743521	50.20410391
O	26.61365112	13.37274133	52.67600082
O	25.89400178	13.46916833	48.75078074
Ti	11.54071305	15.37315434	48.01681913
Ti	12.99981543	17.33264120	52.99576590
Ti	11.42000949	17.18654789	50.64318887
O	11.05632986	15.24703924	50.24875695
O	11.17385869	17.19164409	52.40950776
O	13.05314769	15.67254067	53.85746195
O	11.10282357	17.17667017	48.49696027
O	13.22179011	17.24869975	51.04798718
Ti	15.27944948	15.33426315	48.53914484
Ti	17.06196711	17.30702899	53.42646707
Ti	15.28493078	17.15294095	50.98534567
O	15.29761843	15.30282236	50.56354376
O	15.01639764	17.31368677	52.81770883
O	16.93583264	15.76590806	54.27582332
O	15.17893710	17.13381598	48.89073303
O	17.12037646	17.13837304	51.47693884
Ti	18.96729610	15.28632102	48.66678831
Ti	21.02189066	17.31508188	53.40072681
Ti	19.01896183	17.14943070	51.09606565
O	18.96134304	15.26206866	50.63149766
O	19.03563537	17.30626344	53.02549405
O	21.13227774	15.78542812	54.27516479
O	19.08577520	17.14379785	49.01771030
O	20.92300666	17.15890390	51.44659116
Ti	22.64501296	15.28403406	48.52210842
Ti	25.05257011	17.31338573	52.92442027
Ti	22.74662181	17.15752014	50.91795021
O	22.70114624	15.29814542	50.47582468
O	23.03610150	17.29244935	52.76238802
O	25.06098221	15.63630284	53.73053007
O	22.59417828	17.14526248	48.84837507
O	24.83786194	17.18355982	50.97315958
Ti	26.29122851	15.32747696	48.17868912
Ti	26.65209316	17.19786554	50.59884578
O	27.09650951	15.25280975	50.16926173

O	26.88609895	17.23308933	52.36402321
O	26.83265758	17.14999309	48.48339897
Ti	11.63919396	19.02625737	48.07766265
Ti	13.00910231	20.64832671	53.02373159
Ti	11.41544537	20.83366193	50.68347213
O	11.01447329	19.01277949	50.21327272
O	11.18102454	20.78026865	52.44861961
O	12.92202113	18.98033382	53.77835452
O	11.13182947	20.86572005	48.51872419
O	13.22423540	20.76420672	51.07664287
Ti	15.22219647	19.01129347	48.47314579
Ti	17.06622625	20.66452759	53.44592510
Ti	15.28235045	20.83625214	51.00480717
O	15.40162038	18.99724588	50.45151922
O	15.01959562	20.65743354	52.83904627
O	16.96594147	18.97873346	54.21119716
O	15.19506042	20.86701816	48.90741640
O	17.11905995	20.83898193	51.50404414
Ti	18.95688835	19.00152454	48.53029778
Ti	21.00312337	20.66379282	53.39601379
Ti	19.00139553	20.85265137	51.09196160
O	18.97669780	18.99209314	50.56040035
O	19.03087669	20.67139443	53.03436785
O	21.11392347	18.98695870	54.17710940
O	18.90101329	20.85010797	49.04279770
O	20.90874491	20.81294984	51.43414160
Ti	22.68527282	18.97565271	48.38346435
Ti	25.03531207	20.65068092	52.96166406
Ti	22.74581518	20.83662769	50.93790237
O	22.75243429	18.99140880	50.40462596
O	23.01796550	20.66805064	52.77480913
O	25.11289510	18.98170791	53.69753644
O	22.81294253	20.85270372	48.85388739
O	24.81231542	20.79327774	51.01065821
Ti	26.40520338	19.01678614	48.02656625
Ti	26.60375922	20.87375200	50.61595757
O	26.97338610	19.02439687	50.14864442
O	26.85683500	20.80933237	52.38546260
O	26.84331666	20.89375024	48.51447334
Ti	11.66336921	22.63562490	48.05008559
Ti	13.23630570	23.94949848	53.25627018
Ti	11.47842847	24.37402160	51.13899552
O	11.00105310	22.75275296	50.34244649
O	11.50224387	24.59570843	52.96318678
O	13.05983456	22.29733414	53.89891334
O	10.91522561	24.34851108	47.89486990
O	13.29698625	24.02561112	51.37284412
Ti	15.19406897	22.68337107	48.58845865
Ti	15.33968983	24.59478884	51.17882830
O	15.35531377	22.68330146	50.59849654
O	15.02572900	24.45954493	53.16320783
O	16.93683290	22.20418821	54.29670518
O	15.63231806	24.56256025	49.10545972

O	17.07757825	24.64621952	51.68336880
Ti	18.91683595	22.70791726	48.63487684
Ti	20.95929486	24.07443046	53.76380328
Ti	18.99961036	24.59317492	51.33555726
O	18.98263581	22.73997057	50.63170985
O	19.01429430	24.16907582	53.17126059
O	21.12440112	22.19907098	54.25431102
O	18.97025495	24.63261706	49.02261179
O	20.92943984	24.60842417	51.64018459
Ti	22.64803972	22.65223100	48.50253283
Ti	22.66122873	24.58616746	51.12111572
O	22.70192903	22.68489565	50.53412015
O	22.99066220	24.45525044	53.10881606
O	24.96814201	22.30833221	53.83402820
O	22.36598936	24.55519069	49.03962031
O	24.71682029	24.07304613	51.30316107
Ti	26.42615827	22.69975988	48.03105431
Ti	26.52361287	24.45812719	51.08602062
O	26.95685221	22.81363847	50.25220138
O	26.50988587	24.62251211	52.90693747
O	27.06853531	24.49684734	48.00528121
Ti	11.67653670	25.90958976	48.33174437
O	11.24876687	25.89613363	50.17267367
Ti	15.30502238	26.29624649	48.89577847
O	14.98886622	26.38498784	50.67536473
Ti	18.98672800	26.41057224	49.02191942
O	19.01283990	26.42473780	50.82089579
Ti	22.66986664	26.29478743	48.84716761
O	22.97628764	26.38249188	50.62743110
Ti	26.31453951	26.05667141	48.35709914
O	26.70582712	26.04070680	50.21381116
Ti	24.77720677	23.95508318	53.19333902
Ti	17.07377120	24.08123326	53.79150939
Ti	13.22059554	14.02786768	53.20874260
Ti	20.97791145	13.92466500	53.74997732
Ti	13.95655833	16.76667798	43.06459243
Ti	13.98566220	25.16381624	43.87951275
Ti	24.07155396	20.97569871	43.29766671
Ti	23.94553912	13.24367843	43.83129643
O	21.00541882	25.04836297	55.05770773
O	17.04997710	25.06094014	55.08098576
O	17.00997667	12.90895098	55.06186656
O	21.05957484	12.91200787	55.01184973
O	13.08207663	21.07192750	41.68284772
O	13.13956612	16.59652067	41.67146369
O	25.05024568	17.00982217	41.97027870
O	25.07458363	21.05606914	42.02748934

**(TiO<sub>2</sub>)<sub>151</sub>**

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PBE – Cuboctahedral Shape

Ti	3.29201212	1.41011597	12.47810042
Ti	-3.29143771	-1.41012949	12.47861662

Ti	0.00043701	-1.91328764	11.88063562
Ti	-3.29152443	1.41008036	12.47855717
Ti	0.00035125	1.91336951	11.88063421
Ti	3.29210463	-1.40995371	12.47819313
Ti	3.74562481	3.46721299	9.85747975
Ti	3.85686122	0.00005297	9.25235730
Ti	-0.00004330	-3.72128452	9.64982391
Ti	3.74560646	-3.46705595	9.85745859
Ti	-3.85684710	-0.00006890	9.25246923
Ti	-3.74545497	3.46702827	9.85806742
Ti	-3.74542859	-3.46699015	9.85790721
Ti	0.00009198	0.00005608	9.37863534
Ti	-0.00004367	3.72137032	9.64983221
Ti	1.82834388	0.00003679	6.99391915
Ti	-5.44977014	-3.83460384	7.30629049
Ti	5.44989287	-3.83433285	7.30614452
Ti	-5.63768395	-0.00005465	7.13615153
Ti	-1.82867864	-0.00002357	6.99420065
Ti	5.63761915	0.00003853	7.13607014
Ti	-5.44978184	3.83444428	7.30648420
Ti	1.84824184	-4.01952042	7.16333634
Ti	-1.84825248	4.01955749	7.16319374
Ti	5.44989576	3.83441085	7.30609202
Ti	-1.84824439	-4.01973146	7.16316926
Ti	1.84824770	4.01964707	7.16333807
Ti	-1.94327214	1.88854189	4.75775627
Ti	5.74317561	5.50549319	4.87209100
Ti	1.88154847	5.62862994	4.82014919
Ti	-1.88140872	-5.62873908	4.82025296
Ti	-5.74291140	-5.50561333	4.87223068
Ti	-1.94324579	-1.88855625	4.75778647
Ti	-5.94803803	1.87493736	4.77117261
Ti	5.74310804	-5.50548027	4.87218626
Ti	5.94804366	1.87496707	4.77097426
Ti	-5.94806444	-1.87496509	4.77116790
Ti	-5.74283002	5.50556331	4.87236654
Ti	-1.88144014	5.62869356	4.82030404
Ti	1.94315565	1.88872575	4.75779833
Ti	1.94315020	-1.88867075	4.75779577
Ti	1.88157651	-5.62859818	4.82020178
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O	3.73690926	5.62935958	-4.99903819
O	-3.86863091	-1.80475693	-5.08634341
O	-3.73688196	-5.62919422	-4.99936375
O	-3.73689802	5.62918455	-4.99915054
O	3.73692155	-5.62946747	-4.99925071
O	3.86853962	1.80476481	-5.08598480
O	-3.86856453	1.80474731	-5.08615537
O	-0.00002779	1.89066212	-5.01390045
O	-0.00004893	5.79918488	-5.12848287
O	-0.00002219	-1.89085033	-5.01389533
O	-1.92055251	-1.85248259	-6.65473963
O	5.55883113	5.85037219	-6.70079753
O	-5.78340318	-1.84676523	-6.66581363
O	-5.55878743	-5.85020344	-6.70117773
O	-1.92759299	-6.01580943	-6.78587139
O	5.78329922	1.84684931	-6.66567787
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O	1.92068808	1.85230597	-6.65462659
O	-1.92062735	1.85236126	-6.65469434
O	5.78332180	-1.84694865	-6.66579332
O	1.92064158	-1.85246797	-6.65467704
O	1.92759517	-6.01584520	-6.78582956
O	-5.78336212	1.84671336	-6.66565131
O	5.55889332	-5.85031212	-6.70090659
O	-1.92765668	6.01585772	-6.78576450
O	1.92764707	6.01587777	-6.78574011
O	-3.76908585	3.69928399	-7.21490719
O	3.76902187	3.69935094	-7.21456998
O	0.00004841	-0.00003977	-7.32305079
O	0.00000777	3.84169441	-7.26844111
O	3.82050384	-0.00003157	-7.62787543
O	-3.82034369	0.00000359	-7.62800164
O	-3.76924286	-3.69923397	-7.21549774
O	3.76918528	-3.69938246	-7.21514351
O	0.00002320	-3.84175717	-7.26857411
O	3.98984168	5.37658351	-9.15846007
O	-0.00002145	-5.67963664	-8.97200238
O	4.10162877	1.93251851	-9.26123947
O	-3.98980859	5.37655693	-9.15864876
O	4.10143554	-1.93236473	-9.26155264
O	-4.10179596	1.93247436	-9.26142099

O	3.98973708	-5.37680905	-9.15867776
O	-0.00002454	5.67945664	-8.97200869
O	0.00002475	-1.82920297	-8.91032082
O	-3.98965172	-5.37677033	-9.15890208
O	-4.10160153	-1.93221143	-9.26173346
O	0.00000639	1.82916333	-8.91012525
O	-1.85336827	-3.61862704	-9.27709146
O	-1.85335498	3.61858457	-9.27721233
O	1.91500152	0.00026108	-9.85224803
O	1.85343836	-3.61874706	-9.27698633
O	1.85343641	3.61868484	-9.27713175
O	-1.91493136	0.00029467	-9.85233355
O	2.93517736	3.92848571	-11.66860459
O	3.75714628	0.00012866	-11.47000211
O	2.93521105	-3.92858735	-11.66856746
O	0.00010787	3.24334491	-11.20968757
O	0.00003527	-3.24382476	-11.21003808
O	0.00008652	-0.00008815	-11.32419692
O	-2.93523245	-3.92848404	-11.66851633
O	-3.75698010	0.00019996	-11.47016659
O	-2.93516070	3.92825015	-11.66872323
O	-1.75608761	1.56322649	-12.84111057
O	-1.75652265	-1.56310025	-12.84077625
O	1.75631167	1.56309012	-12.84108235
O	1.75672059	-1.56326084	-12.84065091
O	0.00014456	-3.90022213	-13.56151766
O	-0.00000140	3.90028575	-13.56092958

**(TiO<sub>2</sub>)<sub>165</sub>**

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PBE – Octahedral shape

O	16.94676742	19.04577622	29.05512501
Ti	17.24275536	17.09616578	34.09270403
Ti	17.11518123	15.38182759	36.47674558
O	17.17760101	17.16969386	36.33808665
O	17.17422617	15.32568611	38.68088562
O	17.01964963	15.32809570	34.66354964
O	17.32917620	16.75691703	32.32778182
O	15.34860554	15.05370036	37.01133457
Ti	20.79724802	17.15203224	34.12345232
Ti	19.03614993	17.21298679	31.65097815
Ti	20.93316788	15.38075325	36.46114636
O	20.86783695	17.16858182	36.35110244
O	19.01795364	17.43151422	34.18167480
O	20.87107438	15.33820013	38.68145145
O	21.03095155	15.36736682	34.64016222
O	19.06613725	17.20858495	29.88609559
O	20.78193851	16.99808643	32.31852911
O	19.02665263	14.89411672	36.94330013
O	22.69172986	15.04944616	37.00880817
Ti	17.24441653	20.95784599	34.10432808
Ti	16.87183328	19.01851545	36.53428035
O	17.17823974	20.86911724	36.34893689



O	17.04157989	19.01003922	38.64674960
O	16.68894952	19.02530852	34.55098918
O	17.33301885	21.30910565	32.34156236
O	15.11170570	19.01594414	37.05365337
Ti	18.49838957	19.04261104	29.51405860
Ti	20.79913609	20.90621615	34.13823329
Ti	19.03947271	20.85835730	31.66215424
Ti	21.13813734	19.02003461	36.60056416
O	18.69346539	19.03605865	31.56996637
O	20.87669220	20.87442878	36.36873461
O	19.02007358	20.62550141	34.19606057
O	20.98736697	19.01339479	38.67609473
O	21.36110960	19.02728640	34.60016731
O	19.07023666	20.87323675	29.89743794
O	20.78376778	21.07070374	32.33419888
O	19.03142372	19.01886091	37.04830895
O	22.91617938	19.01334431	37.08596584
Ti	17.11319899	22.65518000	36.49766604
O	17.16967765	22.70776136	38.69562572
O	17.01889794	22.72147462	34.68441630
O	15.34261481	22.96999680	37.02698917
Ti	20.93973573	22.66260861	36.48925209
O	20.87193240	22.70355545	38.71533120
O	21.03592302	22.68637679	34.66820150
O	19.02904595	23.14125795	36.96642636
O	22.69304626	23.00058899	37.04336761
Ti	13.50086389	13.33972298	43.56408003
Ti	13.37735818	11.59802045	45.88337130
O	13.44856782	13.39540245	45.79341250
O	13.57521565	10.87508086	48.81534553
O	13.14016737	11.56515481	44.08890549
O	13.43785008	13.25102088	41.74802738
O	11.82867574	11.22795023	46.81819146
Ti	17.16056125	13.07112512	43.72239238
Ti	15.21789007	13.50897616	41.21258634
Ti	17.10051790	11.48287073	46.08191117
O	17.12710855	13.24696692	45.79452009
O	15.28840069	13.38819477	43.41420483
O	17.15674805	11.03915973	48.10640101
O	17.07303319	11.30087017	44.25143095
O	15.10837213	13.42500437	39.39090102
O	17.12094649	12.99058870	41.69902374
O	15.15426204	11.18453029	46.52799477
Ti	20.87453063	13.07097381	43.72780645
Ti	19.02074401	13.40842665	41.29019934
Ti	20.93059981	11.48479222	46.08791998
O	20.89928604	13.24787712	45.79573896
O	19.01760171	13.21287831	43.34085319
O	20.86705446	11.04488036	48.11265418
O	20.96319789	11.30127664	44.25679155
O	19.02568596	13.24594685	39.45215578
O	20.91676016	12.98979754	41.70203954
O	19.01459982	11.17916408	46.44542690

Ti	24.53219226	13.35102033	43.57480523
Ti	22.81813333	13.51796768	41.21921763
Ti	24.64919290	11.61030770	45.89595111
O	24.56785676	13.40551400	45.80586286
O	22.74381162	13.39279306	43.42061893
O	24.44520495	10.87682139	48.84392086
O	24.89880555	11.57858681	44.10214629
O	22.93805333	13.43762039	39.39632197
O	24.59791278	13.26535833	41.75867677
O	22.87472627	11.18821179	46.53949916
O	26.19159287	11.25059388	46.84512451
Ti	13.40438224	17.11474131	43.64096556
Ti	13.21640423	15.28316587	46.09437324
O	13.28028258	17.13572751	45.67209001
O	13.39740634	15.58213100	48.13308202
O	13.02227614	15.22174626	44.06552279
O	13.24522342	17.10483344	41.80427883
O	11.42732146	15.16341152	46.67025937
Ti	15.38835379	15.18526239	38.82743903
Ti	17.16569654	17.06471853	43.66004903
Ti	15.01631680	17.15417515	41.30512027
Ti	17.09950486	15.26788019	46.04780525
O	15.34194158	15.28390689	41.03542203
O	17.08839051	17.10673003	45.69886820
O	15.16984909	17.12950222	43.37291541
O	17.13821542	15.17291358	48.10274751
O	17.14721508	15.16129924	44.12757533
O	14.88278271	17.09853270	39.29085010
O	17.09667874	17.13952951	41.75366487
O	15.21853670	15.23474446	46.52147845
Ti	19.02523871	15.01215622	38.94237679
Ti	20.86177009	17.07704717	43.66673006
Ti	19.01579530	17.17927406	41.28107613
Ti	20.92611197	15.27091752	46.04740427
O	19.02084796	15.16916869	41.02820644
O	20.91394356	17.10971975	45.71434367
O	19.01154049	17.09177702	43.35624111
O	20.88065556	15.13903268	48.10205373
O	20.88400728	15.16688603	44.13266910
O	19.01564904	17.11481145	39.38235565
O	20.92937610	17.14925360	41.76188559
O	19.00832408	15.22389571	46.49055623
Ti	22.65459455	15.19442730	38.82869503
Ti	24.62731119	17.12851645	43.65739762
Ti	23.01971283	17.15869596	41.31767162
Ti	24.80326545	15.29344836	46.10744205
O	22.68138692	15.29054891	41.04636480
O	24.74885359	17.14010607	45.68255685
O	22.85932496	17.14427197	43.38650135
O	24.61115774	15.61382860	48.14932743
O	25.00690801	15.23046253	44.07969469
O	23.16116269	17.10145213	39.30416263
O	24.78752728	17.10755607	41.81928911

O	22.80186360	15.24487286	46.52706400
O	26.58755309	15.16696912	46.69674109
Ti	13.39784831	20.87518791	43.64424599
Ti	13.12922161	18.99219850	46.12000143
O	13.26835124	20.84932982	45.67644982
O	13.29619825	18.98733539	48.21552605
O	12.96549606	18.99362351	44.05348291
O	13.24408410	20.89501908	41.80970946
O	11.35240078	18.98706282	46.66628747
Ti	15.27761342	19.00869216	38.88784284
Ti	17.16057828	20.93665617	43.66482779
Ti	15.01961756	20.85307890	41.31377047
Ti	17.07764979	18.99593781	46.07166352
O	15.17869275	19.00396201	40.92407657
O	17.10041990	20.88856310	45.71476323
O	15.16418035	20.86758102	43.38538256
O	17.12889602	18.95865834	48.07332885
O	17.09847716	19.00026232	44.10724708
O	14.88446034	20.91617652	39.29976703
O	17.08744983	20.87098403	41.76358802
O	15.15995236	19.00073880	46.55001445
Ti	19.00866849	19.01421495	38.85269921
Ti	20.85534849	20.95436638	43.66856552
Ti	19.02040721	20.83926318	41.28402149
Ti	20.93669243	19.00120529	46.07630087
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O	20.95997411	20.89372387	45.69514976
O	19.00692569	20.90710930	43.36249928
O	20.88215757	19.10492332	48.10588261
O	20.90876105	19.00022545	44.11627441
O	19.01236017	20.91000434	39.38565429
O	20.91424023	20.88285102	41.75169950
O	19.01336389	18.99721276	46.49489835
Ti	22.75998760	19.01671348	38.91146869
Ti	24.59833113	20.87953920	43.67191250
Ti	23.02468564	20.86035701	41.32115768
Ti	24.88038248	19.00098856	46.13230475
O	22.84966898	19.00569938	40.94002898
O	24.56053444	20.82363144	45.70059005
O	22.83362309	20.85054808	43.36241464
O	24.72541522	18.96047547	48.22627611
O	25.07890007	19.00200283	44.07159680
O	23.15312868	20.92390803	39.30730687
O	24.78109951	20.89021117	41.82944840
O	22.83534117	18.93091708	46.57272279
O	26.65578831	19.04633393	46.67133541
Ti	13.47973893	24.64782701	43.57752257
Ti	13.20237796	22.69831909	46.10567257
O	13.43789574	24.58666204	45.81292891
O	13.39690513	22.38664442	48.14101562
O	13.00717366	22.76723251	44.07628670
O	13.41898953	24.74737710	41.76332170
O	11.41954771	22.81466669	46.68779318

Ti	15.38225196	22.83322526	38.84233238
Ti	17.13979874	24.93080509	43.73522126
Ti	15.20247349	24.50028571	41.22984184
Ti	17.08069656	22.72691518	46.06053793
O	15.33263732	22.72672763	41.04779240
O	17.10654732	24.75160605	45.80881109
O	15.26841763	24.60807833	43.42956263
O	17.13501557	22.83736802	48.10827903
O	17.13360564	22.83689634	44.14109321
O	15.09244555	24.59062990	39.40892345
O	17.10470499	25.02129170	41.71685104
O	15.21329089	22.74682752	46.52681874
Ti	19.02290952	23.02056119	38.95997891
Ti	20.85555151	24.92764866	43.74609941
Ti	19.01197069	24.60848190	41.31529999
Ti	20.90570205	22.72592744	46.07924201
O	19.00055299	22.85067715	41.04320212
O	20.89611732	24.76080926	45.83316917
O	18.99610986	24.78713893	43.36209231
O	20.87580106	22.60501948	48.09802201
O	20.86172827	22.83945394	44.14327113
O	19.02336031	24.78403960	39.47881856
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O	22.71906700	22.73333294	41.07247291
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O	22.72878157	24.61406110	43.48400214
O	24.71189685	22.83606038	48.21517297
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O	22.94647932	24.60005011	39.44516310
O	24.59461797	24.80901029	41.83758111
O	22.81431554	22.79408046	46.55821140
O	26.55668531	22.41866277	46.54174989
Ti	13.34958567	26.38224235	45.90336456
O	13.55450572	27.10078661	48.84036352
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O	11.80298633	26.74156529	46.84461373
Ti	17.06018828	26.51264813	46.09740505
O	17.13323260	26.91964819	48.11943666
O	17.04479359	26.69966142	44.26660188
O	15.12668978	26.80700986	46.54369321
Ti	20.87759280	26.53436678	46.09064602
O	20.85077034	26.88710108	48.13775726
O	20.91899122	26.70147288	44.26335054
O	18.98780465	26.84040567	46.45981973
Ti	24.67189559	26.43302634	46.05815855
O	24.56773742	25.96271224	48.23396334
O	24.74299872	26.51100333	44.21914178
O	22.82723004	26.89297767	46.56587234

O	26.28714310	27.02454652	46.75386643
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Ti	13.26560942	13.47003723	53.35912694
Ti	11.57600823	13.29509693	50.97883808
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O	13.20071698	13.38394157	55.19509721
O	11.50245106	13.21599247	52.81413761
O	12.02326068	13.40668859	48.78752097
O	13.40174553	13.22638783	51.23410565
Ti	15.34406955	11.48623565	48.68355732
Ti	17.12949923	13.38480195	53.36256924
Ti	15.31623773	13.18143863	50.95820445
O	15.58765981	11.42500362	50.48925223
O	17.11393466	13.21416028	55.20294230
O	15.25378619	13.02704187	52.94371780
O	15.18765500	13.27815477	48.81934815
O	17.17589694	13.42557631	51.33294832
Ti	19.01045559	11.47605074	48.55110731
Ti	20.86873833	13.39185116	53.36611639
Ti	19.00283925	13.11450326	50.90683287
O	19.00895385	11.33442262	50.38046743
O	20.87601463	13.21540272	55.20844810
O	19.00055434	12.88729059	52.95530799
O	19.00257640	13.24883566	48.81236788
O	20.82760383	13.43727309	51.33813774
Ti	22.67830751	11.48819565	48.70099982
Ti	24.73792088	13.49035718	53.37490408
Ti	22.69200813	13.19626363	50.97115745
O	22.41891804	11.43710396	50.50281621
O	24.79070350	13.40219029	55.21279729
O	22.74543132	13.04318365	52.95504534
O	22.84267411	13.28073613	48.82776756
O	24.60487363	13.23516446	51.25838708
Ti	26.06392666	11.62859061	48.67661591
Ti	26.43162685	13.32323280	50.99901977
O	27.02391538	11.70721359	50.30091557
O	26.50311071	13.24806264	52.83615142
O	25.96987325	13.42776167	48.81425874
Ti	11.67115703	15.29705729	48.46125759
Ti	13.07419363	17.11935690	53.28826181
Ti	11.45892015	17.07757213	50.95029424
Ti	13.49281265	15.13604497	55.76005781
O	11.10295159	15.14105091	50.47089888
O	12.98832962	17.06430518	55.29115523
O	11.29672856	17.04924969	52.77701190
O	13.40449927	15.03125468	57.58585690
O	13.39093469	15.24714776	53.54578987
O	11.12775585	17.12151073	48.90396593
O	13.23036682	17.07933050	51.19788935
Ti	15.32726665	15.27038361	48.52011566
Ti	17.05898696	17.13538083	53.35804848
Ti	15.27201901	17.07429331	50.95301555
Ti	17.14247794	14.97562784	55.70525917

O	15.21371573	15.17888093	50.47503460
O	17.11908079	17.07374956	55.26596754
O	15.16357574	17.11494488	52.87818869
O	17.07493041	14.84152614	57.71977364
O	17.16119805	15.15332623	53.65618779
O	15.36157233	17.11895680	48.93028513
O	17.10539536	17.07303969	51.30820233
O	15.26731386	15.27584793	55.95370745
Ti	19.01159348	15.26694331	48.51699555
Ti	20.93071570	17.14046621	53.36314761
Ti	19.00062980	17.05646626	50.93861219
Ti	20.84102022	14.97275075	55.71418988
O	18.99585580	15.18059618	50.44401496
O	20.86113403	17.08234063	55.27633651
O	18.99542026	17.09623750	52.89717382
O	20.90102564	14.84028907	57.72873329
O	20.83124817	15.15926718	53.66844357
O	19.04316793	17.10631320	48.88398778
O	20.89092280	17.06186779	51.32501779
O	18.99122462	15.15573413	56.09378745
Ti	22.68641979	15.26297154	48.53049174
Ti	24.91474733	17.13976892	53.30207231
Ti	22.72449357	17.09342942	50.96549965
Ti	24.48898288	15.15120057	55.77797382
O	22.79568810	15.18388258	50.48004215
O	24.99066258	17.08097050	55.30894486
O	22.82929757	17.12748566	52.89130243
O	24.57075151	15.04713499	57.60463972
O	24.60522595	15.26648465	53.56261442
O	22.60414574	17.11975337	48.93384312
O	24.76151036	17.09713634	51.21155044
O	22.71309621	15.28509114	55.96632516
Ti	26.33482177	15.31679539	48.48496582
Ti	26.53504935	17.11645932	50.96578654
O	26.89647674	15.16651575	50.48902465
O	26.69296893	17.07823756	52.79238544
O	26.89792904	17.14339417	48.91567606
Ti	11.52087760	18.98349004	48.48725744
Ti	13.07099678	20.83510212	53.29531511
Ti	11.45622971	20.87923031	50.95646732
Ti	13.38770850	18.97354551	55.71016279
O	11.12610057	18.97983677	50.57932437
O	12.98754382	20.88548395	55.29642108
O	11.29399689	20.90289630	52.78330740
O	13.20702186	18.96733295	57.54462238
O	13.22114743	18.97708976	53.66294419
O	11.12678537	20.84412893	48.91059361
O	13.22795575	20.88498547	51.20199213
Ti	15.29463873	18.98766374	48.49856875
Ti	17.04683791	20.82818293	53.36508188
Ti	15.26870466	20.88939818	50.95533536
Ti	17.15612172	18.97956197	55.74759355
O	15.16397496	18.98808076	50.52665914

O	17.10937111	20.89099643	55.27468310
O	15.15741463	20.84541590	52.88408678
O	17.08373919	18.97917406	57.64462002
O	17.09070829	18.98408795	53.66304454
O	15.38557344	20.85510116	48.93095606
O	17.10177496	20.91569072	51.32477301
O	15.14354036	18.97428713	55.98396589
Ti	19.00362701	18.99687283	48.50453671
Ti	20.91797032	20.83510973	53.36694567
Ti	18.99563321	20.92139944	50.94646613
Ti	20.81682038	18.97624755	55.75037196
O	19.00047518	18.98497655	50.49366249
O	20.85030224	20.90683318	55.26527023
O	18.99614653	20.88823337	52.90550097
O	20.88252403	18.98240951	57.64853663
O	20.90240458	18.98897143	53.67031555
O	18.89596815	20.87983959	48.92139860
O	20.88800799	20.87131050	51.30582820
O	18.98687587	18.99196333	56.02080489
Ti	22.71701082	18.96751207	48.50578015
Ti	24.92073917	20.85464549	53.31341097
Ti	22.72585122	20.90840078	50.98275997
Ti	24.58623671	18.98276494	55.73479226
O	22.81205280	18.98386564	50.53449845
O	25.00454297	20.88753567	55.33246276
O	22.82783394	20.86726645	52.89468585
O	24.75416731	18.97098993	57.57065850
O	24.76903822	18.99871289	53.68372210
O	22.84608883	20.85999778	48.92450485
O	24.75296963	20.89122716	51.23704670
O	22.82754459	18.99442606	55.99905503
Ti	26.49882164	18.99607126	48.49730370
Ti	26.51419429	20.93536509	50.95816592
O	26.84205425	19.00692525	50.59318789
O	26.69293380	20.94708480	52.78911743
O	26.92919237	20.86191201	48.93443772
Ti	11.67196080	22.66994687	48.47822511
Ti	13.25331216	24.48624013	53.37344774
Ti	11.56455438	24.66385404	50.99546770
Ti	13.48344655	22.81651352	55.76826755
O	11.09774380	22.81898389	50.48318856
O	13.18791835	24.56962254	55.20968119
O	11.48948655	24.73506434	52.83109262
O	13.39135604	22.91033146	57.59311382
O	13.38310768	22.70932884	53.55696988
O	12.01945516	24.56086882	48.81008558
O	13.39115781	24.74090836	51.25440766
Ti	15.33293347	22.70747205	48.53045958
Ti	17.11743049	24.57424060	53.38049546
Ti	15.30504560	24.78254204	50.97358264
Ti	17.13731847	22.97846530	55.71911270
O	15.20535376	22.79131414	50.48181768
O	17.10905572	24.74351161	55.21902432

O	15.24525841	24.93078954	52.95839359
O	17.07137700	23.10342829	57.73345530
O	17.14887741	22.80837338	53.66988664
O	15.16482458	24.69740110	48.83547618
O	17.17181610	24.54165303	51.34297298
O	15.26022829	22.68928175	55.96581945
Ti	19.02689855	22.70745474	48.52981823
Ti	20.86551100	24.60276542	53.39380958
Ti	18.99401327	24.86431380	50.91864413
Ti	20.83381444	22.97597518	55.72329530
O	19.06422329	22.81511115	50.46866677
O	20.88228795	24.75116741	55.22888048
O	18.99257607	25.05903515	52.97451870
O	20.89318052	23.11259624	57.73725104
O	20.84829532	22.83433553	53.64635849
O	19.03110113	24.71533891	48.82155523
O	20.85466031	24.72697340	51.36200260
O	18.98934005	22.80803415	56.11007974
Ti	22.73446534	22.66196289	48.51512823
Ti	24.63912548	24.51421767	53.47570107
Ti	22.69939728	24.78931524	50.93987981
Ti	24.47965241	22.78836893	55.82156792
O	22.74878496	22.77976321	50.51044516
O	24.72964051	24.57334173	55.28901732
O	22.76312507	24.98858731	52.96831596
O	24.56221245	22.90158068	57.64177217
O	24.60079797	22.72516284	53.61999910
O	22.38437670	24.59878868	48.89913165
O	24.58720558	24.54837743	51.23612302
O	22.70661877	22.65394931	55.99242343
Ti	26.50430244	22.67055737	48.34350775
Ti	26.38111237	24.64280869	51.15393283
O	26.81351939	22.86869288	50.51140598
O	26.41033192	24.89179430	52.94579334
O	27.11713733	24.44026981	48.20929406
Ti	11.93175903	26.36054119	48.67588240
O	10.97722344	26.28346779	50.30331833
Ti	15.32418804	26.48797183	48.70799405
O	15.57379699	26.54240656	50.51140139
Ti	18.99792981	26.48895417	48.55840230
O	18.95008815	26.64151446	50.38341366
Ti	22.67807823	26.32138236	48.56771167
O	22.82602408	26.57283197	50.35688894
Ti	26.36715267	26.05893754	48.37683404
O	26.73873404	26.18867338	50.20730463
Ti	15.15349880	15.33321666	58.16545395
Ti	17.08923768	17.19708590	62.88548523
Ti	15.33461169	17.05386325	60.53585232
O	15.00409772	15.29708840	59.98677288
O	16.92583210	17.21344729	64.68994284
O	15.30907433	16.95897942	62.35745790
O	15.28781545	17.11863268	58.31474418
O	17.12172615	17.11922209	60.65800716



Ti	18.98663052	15.23567956	58.11687076
Ti	20.84885220	17.19581980	62.89739537
Ti	18.97744457	16.85462430	60.42751424
O	18.98016374	15.07788845	59.94359914
O	21.00140974	17.21080035	64.70247333
O	18.97096237	16.63590645	62.42580091
O	18.98526225	17.00816395	58.35398127
O	20.83092160	17.12033120	60.66863352
Ti	22.81879064	15.33963804	58.18062291
Ti	22.61940076	17.05666758	60.55666886
O	22.96227773	15.30376556	60.00275348
O	22.63279722	16.96007138	62.37796841
O	22.67080615	17.12365341	58.32914322
Ti	14.97122490	18.96884740	58.06658040
Ti	17.03219405	20.75200937	62.91643374
Ti	15.33518993	20.88611557	60.52062106
Ti	17.13686820	18.95820722	65.35961419
O	14.85444183	18.96710761	60.05706040
O	16.68233139	20.66374101	64.67950458
O	15.26909620	20.97878326	62.33422006
O	17.12218482	18.92716815	67.12452465
O	17.36577709	18.97655533	62.82563415
O	15.27397240	20.82440681	58.31630962
O	17.12193168	20.82399321	60.67117080
Ti	18.98170684	18.98617331	58.17790834
Ti	20.90009028	20.75071794	62.93118374
Ti	18.97476608	21.12325805	60.49357652
Ti	20.78213241	18.95623996	65.37020676
O	18.97662054	18.96406887	59.98186380
O	21.23984583	20.66327274	64.69641302
O	18.96752239	21.30321007	62.47493600
O	20.78591565	18.92474371	67.13514872
O	20.56788014	18.97500871	62.84102819
O	18.98226471	20.95240898	58.38274147
O	20.82534499	20.81625571	60.68922081
O	18.95923124	19.30402294	65.45123876
Ti	22.98715505	18.97186390	58.08396166
Ti	22.61208041	20.88014258	60.54848615
O	23.10115305	18.96567393	60.07975808
O	22.66826267	20.97398615	62.36216666
O	22.67469308	20.82427127	58.34924868
Ti	15.14356109	22.61225683	58.16775656
O	15.00825300	22.65101868	59.98540013
Ti	18.97841703	22.71636600	58.14133854
O	18.98076998	22.88308582	59.97617338
Ti	22.80196128	22.61168415	58.20378275
O	22.93258658	22.64998124	60.01959098
Ti	18.95331154	19.49573820	67.50786754
O	18.95266790	21.04498926	67.97541310

(TiO<sub>2</sub>)<sub>286</sub>

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PBE – Octahedral Shape

O	21.06399276	18.99749052	19.43842189
Ti	17.21571753	17.12259058	24.52191530
Ti	17.06667405	15.35821005	26.86376002
O	17.12863946	17.14536133	26.75232179
O	17.13078411	15.31088918	29.08465812
O	16.97581666	15.34039413	25.04296824
O	17.23354241	16.96579865	22.71705688
O	15.30856047	15.02860695	27.41224829
Ti	20.76974302	17.06825431	24.49077199
Ti	18.97577831	17.17548755	22.04211145
Ti	20.90864143	15.36438672	26.88188292
O	20.84109965	17.15092899	26.74062514
O	18.99432162	17.40062430	24.58952431
O	20.84526377	15.30015886	29.08416794
O	21.00197780	15.30482661	25.06875476
O	18.94563960	17.16437581	20.27784110
O	20.67949562	16.72261981	22.72785407
O	18.98466513	14.88783225	27.33875776
O	22.67510155	15.04381671	27.41797763
Ti	17.21584646	20.87323593	24.52230943
Ti	16.86476807	18.99804289	26.99282916
O	17.12899560	20.85068187	26.75262860
O	17.01761810	18.99824151	29.07129248
O	16.64853922	18.99796460	24.99283770
O	17.23388890	21.02942282	22.71752605
O	15.08645326	18.99825445	27.48362989
Ti	19.51294602	18.99740253	19.89764440
Ti	20.76950012	20.92808122	24.49132998
Ti	18.97580745	20.81961256	22.04211205
Ti	21.15782265	18.99816154	26.92513276
O	19.32113577	18.99752311	21.95549389
O	20.84086401	20.84541122	26.74124486
O	18.99435630	20.59479419	24.59073497
O	20.97123350	18.99832116	29.03638254
O	21.32975439	18.99812628	24.94253270
O	18.94526266	20.83070721	20.27823423
O	20.67940283	21.27282181	22.72834806
O	18.97096221	18.99788731	27.43203277
O	22.91037523	18.99832763	27.45309423
Ti	17.06674752	22.63782465	26.86411096
O	17.13080221	22.68520493	29.08536152
O	16.97578017	22.65555592	25.04341233
O	15.30864448	22.96754295	27.41296914
Ti	20.90840422	22.63197968	26.88264156
O	20.84500075	22.69612850	29.08524128
O	21.00173545	22.69149002	25.06945052
O	18.98457201	23.10858073	27.33958464
O	22.67471225	22.95295273	27.41908940
Ti	13.48765320	13.28036243	34.01947243
Ti	13.27282116	11.62109611	36.42372426
O	13.38800669	13.39497593	36.23493255
O	13.39340036	11.47634198	38.63938580
O	13.17862071	11.52944757	34.59849338

O	13.40563074	13.18702614	32.19540826
O	11.51836841	11.30795714	37.00881031
Ti	17.14111724	13.08721198	34.08955503
Ti	15.16155218	13.49303809	31.62585061
Ti	17.08668016	11.51125607	36.44514422
O	17.11183805	13.26916854	36.15720453
O	15.26606756	13.39730415	33.83182402
O	17.12120236	11.33222815	38.48062724
O	17.09228979	11.32531805	34.61107758
O	15.05255551	13.41671307	29.80054839
O	17.08217563	12.99528250	32.07855607
O	15.19189276	11.11566696	36.87097022
Ti	20.84346022	13.08789732	34.08700351
Ti	18.99021169	13.40130265	31.66677694
Ti	20.90303083	11.51167165	36.44290036
O	20.87672950	13.26949139	36.15539530
O	18.99198463	13.25934743	33.70652051
O	20.87065618	11.33240829	38.47859555
O	20.89366450	11.32594105	34.60885228
O	18.98606320	13.23359702	29.83088438
O	20.90010316	12.99768815	32.07645866
O	18.99501570	11.08664295	36.83561858
Ti	24.49794514	13.28103964	34.01463454
Ti	22.82210817	13.49309201	31.62381865
Ti	24.71703236	11.62230059	36.41835516
O	24.60187199	13.39641101	36.22860626
O	22.71905183	13.39650791	33.82804369
O	24.59862442	11.47777552	38.63417561
O	24.80828354	11.52991355	34.59337029
O	22.92929331	13.41482924	29.79984507
O	24.57894674	13.18777340	32.19089512
O	22.79845057	11.11692280	36.86726164
O	26.47215282	11.30961630	37.00195010
Ti	13.37688841	17.09264294	34.05754536
Ti	13.08450903	15.28132618	36.49419030
O	13.23837149	17.12501449	36.09474970
O	13.27652052	15.24026454	38.55585663
O	12.98686176	15.19958595	34.47712450
O	13.20048361	17.09386733	32.22419879
O	11.32481969	15.22542162	37.02420637
Ti	15.34682648	15.16966007	29.23292896
Ti	17.14175155	17.06470958	34.03107161
Ti	14.96580078	17.14232016	31.71007102
Ti	17.05804778	15.28631198	36.43419262
O	15.27853273	15.27110561	31.44695283
O	17.08333212	17.11053463	36.08843676
O	15.13937925	17.11433801	33.77525504
O	17.10747478	15.19523831	38.47781010
O	17.12088494	15.18197773	34.50932537
O	14.84437995	17.08817395	29.70154945
O	17.06739260	17.13155648	32.13270319
O	15.17729127	15.24547665	36.90963726
Ti	18.98626809	15.00007152	29.32391540

Ti	20.84236236	17.06428890	34.02970615
Ti	18.99123612	17.16767586	31.65982829
Ti	20.93114400	15.28606549	36.43274456
O	18.98821329	15.16106879	31.40880217
O	20.90542774	17.11033722	36.08628897
O	18.99218687	17.10340519	33.73013955
O	20.88355010	15.19547568	38.47574224
O	20.86509921	15.18183211	34.50733735
O	18.99571732	17.10150345	29.76121421
O	20.91511607	17.12839272	32.13074634
O	18.99458811	15.19847268	36.87502488
Ti	22.63299844	15.16955077	29.23514816
Ti	24.60704626	17.09412128	34.04930653
Ti	23.01397827	17.14478121	31.70296667
Ti	24.90426297	15.28284149	36.48760674
O	22.70697734	15.27257155	31.44283950
O	24.74823321	17.12591337	36.08704211
O	22.84431108	17.11800022	33.76889823
O	24.71440961	15.24155989	38.54945861
O	24.99755966	15.20133766	34.46934644
O	23.13280659	17.08974548	29.69243442
O	24.77967238	17.10003695	32.21490423
O	22.81195293	15.24550135	36.90574029
O	26.66431357	15.22762037	37.01611417
Ti	13.37709611	20.90402919	34.05827098
Ti	13.06300503	18.99787629	36.48552549
O	13.23861021	20.87086804	36.09553627
O	13.25189591	18.99772590	38.54303220
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O	13.20067854	20.90278828	32.22492292
O	11.30154837	18.99795776	37.01917583
Ti	15.24562097	18.99832560	29.30709367
Ti	17.14186232	20.93129835	34.03191421
Ti	14.96598377	20.85393407	31.71069868
Ti	17.04084412	18.99748195	36.44609400
O	15.12612808	18.99813677	31.34175748
O	17.08331293	20.88465601	36.08920523
O	15.13956678	20.88193769	33.77589297
O	17.09204496	18.99737769	38.46296807
O	17.06726507	18.99792008	34.48404428
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O	17.06751722	20.86424946	32.13339626
O	15.14590949	18.99751595	36.89786835
Ti	19.00037448	18.99813769	29.23028303
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Ti	18.99127667	20.82809917	31.66038256
Ti	20.94749503	18.99747098	36.44390193
O	18.99497089	18.99793119	31.39278540
O	20.90537999	20.88480061	36.08704306
O	18.99219588	20.89261485	33.73082295
O	20.89841350	18.99734287	38.46094724
O	20.91654747	18.99788349	34.48210488
O	18.99558917	20.89462545	29.76172186

O	20.91510202	20.86754532	32.13148863
O	18.99439742	18.99740525	36.86835056
Ti	22.73414485	18.99830984	29.28965759
Ti	24.60697782	20.90238916	34.05008723
Ti	23.01384869	20.85129250	31.70367599
Ti	24.92541257	18.99778258	36.47945229
O	22.84469719	18.99805327	31.32288281
O	24.74817386	20.86978388	36.08781333
O	22.84424272	20.87822970	33.76966670
O	24.73876174	18.99763410	38.53675501
O	25.03049535	18.99816865	34.44590094
O	23.13277459	20.90679758	29.69310649
O	24.77954928	20.89623192	32.21567985
O	22.84268112	18.99753777	36.89398232
O	26.68736293	18.99783843	37.01126003
Ti	13.48827970	24.71608414	34.02160726
Ti	13.08494663	22.71435365	36.49606884
O	13.38861838	24.60066093	36.23751423
O	13.27693744	22.75472101	38.55781466
O	12.98729909	22.79690916	34.47874920
O	13.40631668	24.80958315	32.19753551
O	11.32526544	22.77042781	37.02629082
Ti	15.34699235	22.82686481	29.23366756
Ti	17.14140752	24.90873123	34.09200741
Ti	15.16208090	24.50310243	31.62737470
Ti	17.05819533	22.70872699	36.43592559
O	15.27884849	22.72505888	31.44806235
O	17.11198259	24.72597885	36.15966522
O	15.26660559	24.59869160	33.83391021
O	17.10767201	22.79923311	38.47963486
O	17.12115986	22.81383555	34.51103689
O	15.05309044	24.57974584	29.80207832
O	17.08244201	25.00083948	32.08059919
O	15.17752709	22.74965736	36.91165919
Ti	18.98604496	22.99630006	29.32501308
Ti	20.84337385	24.90795332	34.08951744
Ti	18.99029390	24.59450833	31.66846553
Ti	20.93105249	22.70891207	36.43447475
O	18.98784675	22.83479031	31.40982257
O	20.87656166	24.72559927	36.15782861
O	18.99211047	24.73652227	33.70840676
O	20.88344907	22.79899920	38.47760518
O	20.86496738	22.81391772	34.50906485
O	18.98596978	24.76262905	29.83258909
O	20.90010935	24.99817120	32.07851689
O	18.99464687	22.79632221	36.87696599
Ti	22.63272161	22.82695338	29.23626860
Ti	24.49758616	24.71528490	34.01689603
Ti	22.82184676	24.50304424	31.62553339
Ti	24.90391321	22.71271152	36.48948170
O	22.70700960	22.72353901	31.44409140
O	24.60136039	24.59911544	36.23125364
O	22.71879813	24.59927961	33.83033634

O	24.71407858	22.75336063	38.55142820
O	24.99740664	22.79501638	34.47100165
O	22.92891910	24.58155154	29.80157539
O	24.57843861	24.80905248	32.19311818
O	22.81179800	22.74947778	36.90773821
O	26.66393707	22.76813280	37.01818402
Ti	13.27369390	26.37447378	36.42705725
O	13.39429026	26.51793308	38.64362791
O	13.17951903	26.46676348	34.60183433
O	11.51950288	26.68802737	37.01298676
Ti	17.08697191	26.48377948	36.44852040
O	17.12154353	26.66196286	38.48436791
O	17.09270713	26.67038209	34.61447687
O	15.19237566	26.87963011	36.87503040
Ti	20.90287188	26.48332861	36.44627038
O	20.87045659	26.66173330	38.48234405
O	20.89358554	26.66968818	34.61224264
O	18.99510091	26.90829151	36.83951150
Ti	24.71627053	26.37317983	36.42173144
O	24.59784828	26.51642705	38.63844669
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O	26.47110169	26.68632410	37.00610990
Ti	9.80599847	9.80278166	43.66665311
O	9.27112953	9.67721353	45.45938943
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Ti	13.46959730	9.67102054	43.73055665
Ti	11.39521813	9.66636718	41.21661457
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O	11.57354843	9.49373862	43.49996592
O	11.30141910	9.61070703	39.39337524
O	13.31630957	9.23819006	41.66016942
Ti	17.13631732	9.58483338	43.68142844
Ti	15.20310015	9.55980597	41.21474396
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O	15.27430030	9.17588838	43.26573638
O	15.22203506	9.39825579	39.38543733
O	17.11713587	9.20631419	41.60853113
Ti	20.86095525	9.58521100	43.67998685
Ti	18.99762507	9.54776694	41.19586676
O	20.88212857	9.41739283	45.50715132
O	18.99852436	9.19681304	43.26926693
O	18.99667888	9.37941079	39.36658620
O	20.87849996	9.20689591	41.60684276
Ti	24.52739381	9.67223030	43.72648514
Ti	22.79214224	9.56074628	41.21145354
O	24.55718162	9.48963922	45.54187850
O	22.72257420	9.17649925	43.26255820
O	22.77157657	9.39924879	39.38214884
O	24.67942596	9.23971679	41.65558791
Ti	28.19092532	9.80498209	43.65963087
Ti	26.59979312	9.66839135	41.21015398
O	28.72609103	9.67951194	45.45239722

O	26.42324596	9.49651160	43.49475347
O	26.69218907	9.61294886	39.38683888
O	28.31615468	9.27273231	41.86609321
Ti	9.67364517	13.46748080	43.60188883
Ti	9.66822969	11.39316154	46.11576123
O	9.23951609	13.31396527	45.67183692
O	9.61270099	11.29990264	47.93919839
O	9.50118671	11.57091549	43.83322065
O	9.49065867	13.43721223	41.78662401
Ti	11.62016303	11.36857192	38.83081142
Ti	13.42664501	13.42447064	43.66614412
Ti	11.27222731	13.38991090	41.27235706
Ti	13.39186881	11.27007690	46.05994934
O	11.44877747	11.46702494	41.07195258
O	13.34196440	13.30472645	45.63805793
O	11.44165703	13.49345911	43.35922202
O	13.30785453	11.15971671	48.04918162
O	13.49355470	11.43923703	43.97272010
O	11.16180615	13.30556703	39.28322714
O	13.30683515	13.34018864	41.69403766
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Ti	15.28160297	11.17213132	38.88810101
Ti	17.13939377	13.37242416	43.66969719
Ti	15.17991681	13.36956654	41.22404145
Ti	17.12669339	11.18985586	46.03929496
O	15.23412233	11.33688862	40.95792228
O	17.12527999	13.25347638	45.61540467
O	15.24971754	13.37083689	43.25723494
O	17.11498979	11.07357710	48.07253601
O	17.11265882	11.35770413	43.95474923
O	15.25050728	13.26937958	39.29604708
O	17.10852866	13.28789638	41.64846433
O	15.25521986	11.40240907	46.44970329
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Ti	20.85645717	13.37269091	43.66825547
Ti	18.99698232	13.34059061	41.20765536
Ti	20.87091551	11.19023419	46.03800940
O	18.99719922	11.32440113	40.91937684
O	20.87152276	13.25369195	45.61404834
O	18.99782158	13.29619305	43.24251772
O	20.88382839	11.07363378	48.07142009
O	20.88441366	11.35808008	43.95333887
O	18.99619199	13.23909562	39.26908785
O	20.88580453	13.28838025	41.64694788
O	18.99895251	11.34443154	46.43539052
Ti	22.71076213	11.17309583	38.88462998
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Ti	24.60547402	11.27101011	46.05625542
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O	24.65463275	13.30545587	45.63408655
O	22.74581992	13.37158526	43.25410724
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O	24.50261790	11.44035672	43.96888781
O	22.74165887	13.27003529	39.29275114
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O	22.74250190	11.40311020	46.44758320
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Ti	28.32203556	13.46896285	43.59467136
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O	28.49647808	11.57291745	43.82514515
O	26.83061594	13.30734869	39.27599453
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O	26.52814654	11.44734050	46.25590833
Ti	9.58679354	17.13410066	43.65079963
Ti	9.56153999	15.20098825	46.11747501
O	9.20811697	17.11489221	45.72373141
O	9.40011527	15.21974737	47.94676730
O	9.17787325	15.27210760	44.06646070
O	9.41889700	17.11398920	41.82364301
Ti	11.52133501	15.21041338	38.85940378
Ti	13.37435855	17.13734683	43.66244597
Ti	11.19175343	17.12476972	41.29290665
Ti	13.37145479	15.17794329	46.10802194
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O	13.28950644	17.10650896	45.68367517
O	11.35967344	17.11034951	43.37745409
O	13.27124287	15.24868800	48.03606956
O	13.37379382	15.24770389	44.07498528
O	11.07563371	17.11307008	39.25972266
O	13.25531813	17.12318453	41.71672982
O	11.33865853	15.23180154	46.37415670
Ti	15.28351676	15.14986203	38.84179233
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Ti	15.14343248	17.12321635	41.25238677
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O	15.19603268	15.21107614	40.86697156
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O	15.21184998	17.13011659	43.26712859
O	17.10097906	15.18817501	48.05593460
O	17.13168509	15.20992192	44.06494375
O	15.19003151	17.09918439	39.27622295
O	17.09299326	17.09983582	41.67105924
O	15.21291063	15.19397158	46.46522162
Ti	18.99558855	15.12343116	38.84134344
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O	20.89685067	15.18832897	48.05481962
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O	22.80139071	17.09941208	39.27275966
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Ti	11.49133393	18.99771619	38.85205449
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O	13.28997824	20.88386949	45.68515628
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O	13.24083721	18.99416479	48.06295704
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O	11.07568079	20.88205306	39.26088052
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Ti	24.62047530	20.85420500	43.65976610
Ti	22.84970109	20.86947732	41.25059278
Ti	24.65391194	18.99502998	46.12107107
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O	28.61595176	18.99449774	47.95985064
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O	9.24094302	24.67741969	45.67629378
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Ti	11.52175872	22.78479639	38.86150006
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O	11.33940517	22.75833304	46.37725029
Ti	15.28379516	22.84460978	38.84398950
Ti	17.13963551	24.61888518	43.67386106
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Ti	17.12529127	22.84799588	46.08275339
O	15.19624746	22.78217215	40.86916581
O	17.12568485	24.73631046	45.61972883
O	15.25023027	24.62062037	43.26098785
O	17.10116872	22.79949655	48.05924426
O	17.13205613	22.78112424	44.06803020
O	15.25114769	24.72474951	39.29959309
O	17.10878375	24.70460927	41.65240154
O	15.21330100	22.79559663	46.46863453
Ti	18.99562502	22.87069548	38.84351006
Ti	20.85624096	24.61859843	43.67242085
Ti	18.99700416	24.65214062	41.21116374
Ti	20.87133952	22.84780789	46.08155724
O	18.99655123	22.80447218	40.84581015
O	20.87117935	24.73608313	45.61837299
O	18.99783646	24.69553226	43.24629761
O	20.89669621	22.79930292	48.05812748
O	20.86392828	22.78090816	44.06680355
O	18.99622925	24.75478578	39.27252675
O	20.88558399	24.70411250	41.65088562
O	18.99849088	22.80917061	46.47390587
Ti	22.70776136	22.84409691	38.84061489
Ti	24.56856699	24.56654053	43.66605737
Ti	22.81367129	24.62270162	41.22464760
Ti	24.62463293	22.81167749	46.10749935
O	22.79721526	22.78162071	40.86557035
O	24.65374783	24.68479252	45.63843832
O	22.74533599	24.61981364	43.25785601
O	24.72602842	22.73916261	48.03581148
O	24.62165871	22.74328290	44.07429050
O	22.74112565	24.72406322	39.29629154
O	24.68678816	24.65169216	41.69364147
O	22.78354193	22.79528608	46.46653370
Ti	26.46964255	22.78348010	38.85387372
Ti	28.32125671	24.52381951	43.59856422
Ti	26.72095469	24.60196962	41.26966635
Ti	28.43398666	22.78919123	46.11480401
O	26.58755067	22.73940715	40.87739947
O	28.75523244	24.67620345	45.66975328
O	26.55301025	24.49842425	43.35709052
O	28.59653529	22.76869456	47.94395482
O	28.81748891	22.71936347	44.06288475
O	26.83011063	24.68750390	39.27942751

O	28.50255924	24.55305294	41.78297754
O	26.65709314	22.75751908	46.37282982
Ti	9.80747832	28.18961494	43.67311049
Ti	9.66985579	26.59777285	46.12176871
O	9.27325478	28.31401790	45.46620876
O	9.61438907	26.68981998	47.94519314
O	9.50147575	26.42154017	43.83810125
O	9.68105059	28.72311986	41.88012169
Ti	11.62114809	26.62625330	38.83498996
Ti	13.47089127	28.32053997	43.73759869
Ti	11.39672797	28.32709763	41.22235121
Ti	13.39325191	26.71992774	46.06613045
O	11.44973443	26.52649191	41.07673617
O	13.44243166	28.50158962	45.55323958
O	11.57508909	28.49768592	43.50747460
O	13.30909090	26.82863534	48.05594771
O	13.49521884	26.55217805	43.97872782
O	11.30284679	28.38374229	39.39915684
O	13.31728676	28.75459255	41.66684067
O	11.47071333	26.54422606	46.26670626
Ti	15.28219141	26.82203257	38.89268998
Ti	17.13670531	28.40634481	43.68836282
Ti	15.20387530	28.43297082	41.22062321
Ti	17.12718780	26.79954879	46.04538106
O	15.23475108	26.65606464	40.96253609
O	17.11654939	28.57273773	45.51569125
O	15.27522731	28.81614910	43.27239429
O	17.11552634	26.91472986	48.07957427
O	17.11270419	26.63323651	43.96070945
O	15.22276292	28.59561894	39.39144834
O	17.11754425	28.78590713	41.61491793
O	15.25627849	26.58636954	46.45664831
Ti	18.99628491	26.84297449	38.86676800
Ti	20.86060117	28.40595011	43.68692019
Ti	18.99764797	28.44471313	41.20154206
Ti	20.87047318	26.79915243	46.04409162
O	18.99724098	26.66826748	40.92377119
O	20.88155575	28.57232720	45.51422825
O	18.99853806	28.79454303	43.27593820
O	20.88335627	26.91463669	48.07845890
O	20.88437727	26.63284220	43.95929240
O	18.99673263	28.61416601	39.37241133
O	20.87812100	28.78534769	41.61322541
O	18.99898530	26.64418502	46.44214752
Ti	22.71027678	26.82102362	38.88923495
Ti	24.52613576	28.31928039	43.73350711
Ti	22.79139912	28.43201252	41.21732782
Ti	24.60414075	26.71895622	46.06241892
O	22.75959639	26.65512912	40.95921934
O	24.55522699	28.50054109	45.54910029
O	22.72167927	28.81548969	43.26920271
O	24.68966748	26.82802365	48.05249096
O	24.50095576	26.55101024	43.97488233

O	22.77094134	28.59458126	39.38814584
O	24.67846754	28.75305321	41.66223101
O	22.74150357	26.58565652	46.45452442
Ti	26.37132447	26.62427451	38.82812616
Ti	28.18948179	28.18734690	43.66602116
Ti	26.59829905	28.32503015	41.21586164
Ti	28.32729079	26.59608571	46.11606229
O	26.54474861	26.52434731	41.07035345
O	28.72400426	28.31165872	45.45914397
O	26.42173636	28.49483351	43.50221446
O	28.38372234	26.68860607	47.93935259
O	28.49625180	26.41947448	43.82993962
O	26.69084518	28.38142653	39.39258094
O	28.31396021	28.72137008	41.87277488
O	26.52657868	26.54275075	46.26168204
Ti	11.37055700	11.61817607	48.50153405
Ti	13.28226007	13.48622243	53.31309143
Ti	11.62300294	13.27091013	50.90871825
O	11.30993197	11.51652492	50.32363744
O	13.18882834	13.40442520	55.13713521
O	11.53138945	13.17698610	52.73396876
O	11.47865043	13.39141633	48.69284227
O	13.39689812	13.38625840	51.09753377
Ti	15.21236197	11.51945925	48.47287914
Ti	17.09434538	13.37551060	53.27491958
Ti	15.28309641	13.08271284	50.83805801
O	15.22742616	11.32304100	50.30814139
O	17.09546500	13.19922102	55.10833530
O	15.20142399	12.98542565	52.85542128
O	15.24216030	13.27471333	48.77659177
O	17.12673669	13.23688150	51.23770858
Ti	18.99952610	11.48942315	48.48027284
Ti	20.90547616	13.37561584	53.27418270
Ti	18.99949403	13.06119868	50.84676597
O	18.99961504	11.29973813	50.31318124
O	20.90417025	13.19932289	55.10761079
O	18.99985816	12.95431042	52.87910483
O	18.99944608	13.25003062	48.78932521
O	20.87238376	13.23695583	51.23695571
Ti	22.78649515	11.51979998	48.47085445
Ti	24.71740611	13.48659912	53.31092720
Ti	22.71586827	13.08303537	50.83626931
O	22.77184356	11.32337763	50.30612274
O	24.81105181	13.40487851	55.13498925
O	22.79830312	12.98565620	52.85379820
O	22.75638337	13.27502224	48.77467612
O	24.60206261	13.38669082	51.09495729
Ti	26.62786356	11.61905141	48.49746621
Ti	26.37591376	13.27166066	50.90547314
O	26.68955887	11.51753956	50.31954183
O	26.46807464	13.17760492	52.73068670
O	26.51927874	13.39218422	48.68869943
Ti	11.17403307	15.27946984	48.44406823

Ti	13.08885961	17.13957320	53.24264580
Ti	11.51295552	17.08472650	50.88697222
Ti	13.49476723	15.16042799	55.70668996
O	11.11741181	15.18987885	50.46122323
O	12.99684717	17.08084857	55.25362110
O	11.32699758	17.09066656	52.72106314
O	13.41844519	15.05165040	57.53197695
O	13.39916071	15.26469626	53.50055610
O	11.33400791	17.11913708	48.85150402
O	13.27085166	17.10992695	51.17495003
Ti	15.15164752	15.28164985	48.49041008
Ti	17.06632785	17.14048455	53.30111004
Ti	15.28798351	17.05624378	50.89793252
Ti	17.14384042	14.96452615	55.62229672
O	15.24715660	15.17558138	50.42256466
O	17.13309347	17.06623397	55.19953412
O	15.18366568	17.11947796	52.82283847
O	17.08981519	14.84318390	57.63113561
O	17.11631824	15.13805119	53.55734321
O	15.19708663	17.10565381	48.85434306
O	17.11219564	17.08147947	51.24376005
O	15.27286515	15.27738729	55.88555267
Ti	18.99905262	15.25572244	48.49865858
Ti	20.93288826	17.14052170	53.30034365
Ti	18.99915689	17.03906604	50.88608937
Ti	20.85546067	14.96461425	55.62167515
O	18.99921865	15.14417704	50.43435597
O	20.86595645	17.06624208	55.19884037
O	18.99954865	17.06604976	52.84813503
O	20.90991596	14.84329674	57.63058626
O	20.88317484	15.13812943	53.55664521
O	18.99908421	17.09023688	48.86924196
O	20.88629449	17.08146302	51.24302878
O	18.99969344	15.12515580	55.99111293
Ti	22.84630330	15.28185889	48.48831685
Ti	24.91030595	17.13969188	53.24027363
Ti	22.71034307	17.05632400	50.89630980
Ti	24.50454210	15.16069731	55.70506695
O	22.75124337	15.17571271	50.42064824
O	25.00230589	17.08089296	55.25161724
O	22.81540795	17.11963753	52.82121722
O	24.58113745	15.05191481	57.53036018
O	24.60004142	15.26497055	53.49840669
O	22.80092103	17.10575837	48.85260751
O	24.72758131	17.11008437	51.17260239
O	22.72646851	15.27747693	55.88436134
Ti	26.82365721	15.27997435	48.43961645
Ti	26.48537963	17.08490543	50.88374322
O	26.88116967	15.19023548	50.45732007
O	26.67195714	17.09080791	52.71780473
O	26.66370939	17.11936686	48.84794053
Ti	11.15265976	18.99416574	48.46974901
Ti	13.08952879	20.84195420	53.24493636

Ti	11.51328684	20.90113374	50.88907572
Ti	13.40288570	18.98898781	55.66532295
O	11.08833353	18.99306307	50.49642063
O	12.99931732	20.89878445	55.25552244
O	11.32753335	20.89209673	52.72308920
O	13.23511142	18.98450778	57.50120848
O	13.26100081	18.99057523	53.62558907
O	11.33415527	20.86864302	48.85331895
O	13.27111836	20.87488441	51.17660064
Ti	15.12516505	18.99371603	48.49071866
Ti	17.06590234	20.84106424	53.30227081
Ti	15.28771638	20.92934078	50.89925893
Ti	17.16925094	18.98997463	55.67230182
O	15.20008851	18.99284474	50.45702379
O	17.13004015	20.91389131	55.20119770
O	15.18343359	20.86365924	52.82462385
O	17.10310850	18.99444582	57.57092425
O	17.10498979	18.99085180	53.60193304
O	15.19716616	20.88171386	48.85620184
O	17.11201367	20.90355204	51.24570869
O	15.16265666	18.98678565	55.92343675
Ti	18.99886310	18.99367999	48.50665957
Ti	20.93334208	20.84099793	53.30150318
Ti	18.99917017	20.94572458	50.88815760
Ti	20.82967153	18.98995931	55.67173820
O	18.99908874	18.99268857	50.46375801
O	20.86904264	20.91385425	55.20050289
O	18.99956401	20.91530127	52.84993414
O	20.89624635	18.99441826	57.57036405
O	20.89425141	18.99083552	53.60131947
O	18.99908792	20.89659539	48.87106105
O	20.88650494	20.90353724	51.24497656
O	18.99951871	18.99344396	55.93930988
Ti	22.87243159	18.99368918	48.48868310
Ti	24.90966859	20.84173826	53.24255659
Ti	22.71063729	20.92920960	50.89763658
Ti	24.59609852	18.98894262	55.66365339
O	22.79797927	18.99281721	50.45518586
O	24.99986452	20.89864279	55.25351371
O	22.81566845	20.86343516	52.82299951
O	24.76422169	18.98447362	57.49954775
O	24.73823141	18.99052924	53.62377401
O	22.80086391	20.88155298	48.85446606
O	24.72734466	20.87464383	51.17425097
O	22.83639125	18.98674917	55.92233168
Ti	26.84472832	18.99412011	48.46548827
Ti	26.48507938	20.90086810	50.88584131
O	26.90995458	18.99301920	50.49268360
O	26.67145333	20.89184930	52.71982528
O	26.66358225	20.86832532	48.84974643
Ti	11.17479341	22.70873702	48.44734342
Ti	13.28252910	24.49649341	53.31698983
Ti	11.62385760	24.71523272	50.91334514

Ti	13.49465378	22.82093609	55.70789450
O	11.11851361	22.79648773	50.46458770
O	13.18922075	24.57764992	55.14078159
O	11.53140517	24.80665958	52.73835045
O	13.41640689	22.92832627	57.53187852
O	13.39815119	22.71764056	53.50376474
O	11.47935707	24.59666639	48.69775061
O	13.39796121	24.60005682	51.10318506
Ti	15.15201362	22.70611575	48.49355481
Ti	17.09572624	24.60567853	53.28244474
Ti	15.28448835	24.90249524	50.84429568
Ti	17.14649950	23.01266067	55.62886288
O	15.24716628	22.81016789	50.42621848
O	17.10176069	24.77837317	55.11679290
O	15.20290258	24.99621040	52.86234522
O	17.09135287	23.13171076	57.63913736
O	17.11934580	22.84296367	53.56275831
O	15.24326931	24.71252838	48.78235573
O	17.12759867	24.74656819	51.24472462
O	15.27414163	22.70568649	55.88896594
Ti	18.99907039	22.73144115	48.50222675
Ti	20.90418887	24.60554315	53.28170494
Ti	18.99953941	24.92364870	50.85247233
Ti	20.85286563	23.01254455	55.62824447
O	18.99924985	22.84094690	50.43797515
O	20.89796253	24.77823924	55.11606857
O	18.99990731	25.02891825	52.88582990
O	20.90844100	23.13158282	57.63858935
O	20.88022166	22.84285668	53.56205564
O	18.99947919	24.73692083	48.79504702
O	20.87161110	24.74647250	51.24397281
O	18.99972329	22.84351592	56.00860274
Ti	22.84597618	22.70584931	48.49145411
Ti	24.71723172	24.49601930	53.31481642
Ti	22.71456942	24.90211902	50.84250324
Ti	24.50472142	22.82057084	55.70626617
O	22.75128857	22.80998385	50.42430014
O	24.81077437	24.57709002	55.13862963
O	22.79692510	24.99592099	52.86071999
O	24.58324950	22.92795677	57.53025406
O	24.60110166	22.71727272	53.50160694
O	22.75533191	24.71216129	48.78043074
O	24.60108587	24.59953883	51.10060267
O	22.72525188	22.70554772	55.88778933
Ti	26.82293901	22.70813991	48.44287125
Ti	26.37514538	24.71438588	50.91008157
O	26.88012989	22.79603938	50.46067248
O	26.46815437	24.80592696	52.73505109
O	26.51862069	24.59580700	48.69358434
Ti	11.37197986	26.37024584	48.50781230
O	11.31121588	26.47032509	50.32984720
Ti	15.21340659	26.46807628	48.48004039
O	15.22924495	26.66249708	50.31569597



Ti	18.99955992	26.49795604	48.48742112
O	18.99966202	26.68556843	50.32057819
Ti	22.78552049	26.46767670	48.47800600
O	22.77013290	26.66210332	50.31366916
Ti	26.62650792	26.36927957	48.50372065
O	26.68837381	26.46921407	50.32572563
Ti	15.17145391	15.34573607	58.09984547
Ti	17.12428825	17.21550536	62.81089503
Ti	15.36004117	17.06591100	60.46889737
O	15.03069711	15.30755058	59.92046075
O	16.96729165	17.23430019	64.61547766
O	15.34203261	16.97484984	62.28955823
O	15.31298897	17.12966290	58.24805054
O	17.14729460	17.12839224	60.58064704
Ti	18.99985976	15.24460971	58.02536890
Ti	20.87505110	17.21559986	62.81059626
Ti	18.99964076	16.86307911	60.34013573
O	18.99978166	15.08536667	59.84932916
O	21.03181884	17.23457527	64.61522548
O	18.99969500	16.64809605	62.34047513
O	18.99961378	17.01643838	58.26169708
O	20.85197855	17.12834197	60.58019497
Ti	22.82824874	15.34588954	58.09888833
Ti	22.63923588	17.06599941	60.46826931
O	22.96898327	15.30777687	59.91954045
O	22.65725891	16.97494020	62.28894723
O	22.68637161	17.12974345	58.24711538
Ti	15.00159057	18.98490057	58.00824583
Ti	17.06963330	20.76961273	62.84050206
Ti	15.36550575	20.90788474	60.44988983
Ti	17.17698048	18.97682647	65.28993091
O	14.88915920	18.98365424	59.99346506
O	16.72484743	20.68062423	64.60380437
O	15.30609293	21.00182796	62.26307734
O	17.16619551	18.94645647	67.05391614
O	17.40175507	18.99425903	62.74225319
O	15.30140620	20.84406834	58.24768576
O	17.15201634	20.84023755	60.59113984
Ti	18.99972108	18.99935948	58.10183371
Ti	20.92967579	20.76950908	62.84014840
Ti	18.99963728	21.15556395	60.40623143
Ti	20.82169879	18.97688956	65.29000767
O	18.99965277	18.97112715	59.90013300
O	21.27413809	20.68043890	64.60352469
O	18.99969212	21.32886796	62.38846713
O	20.83238213	18.94657337	67.05397739
O	20.59730786	18.99425831	62.74158589
O	18.99965285	20.96989939	58.29473969
O	20.84725830	20.84030870	60.59066887
O	18.99933925	19.32118993	65.37612565
Ti	22.99787551	18.98487316	58.00712625
Ti	22.63378345	20.90775531	60.44925800
O	23.11014713	18.98363011	59.99258583

O	22.69318800	21.00166747	62.26246679
O	22.69795567	20.84393761	58.24675271
Ti	15.17108685	22.63184208	58.09636868
O	15.04524016	22.67422479	59.91358310
Ti	18.99989054	22.73299407	58.04228698
O	18.99977552	22.90874853	59.87835782
Ti	22.82867860	22.63163242	58.09540472
O	22.95453341	22.67394018	59.91265959
Ti	18.99924067	19.51385916	67.43413282
O	18.99916228	21.06473746	67.89458807

**(TiO<sub>2</sub>)<sub>455</sub>**

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PBE – Octahedral Shape

Ti	-9.26828516	-9.41621444	-4.94602115
Ti	-9.41851712	-11.15299069	-2.62467664
Ti	-10.83354900	-11.15310924	0.14974248
Ti	-11.18698946	-9.46401955	2.48087436
Ti	-9.49685099	-9.26220716	4.85409107
Ti	-9.35530584	-5.64360915	-4.85700672
Ti	-9.58423908	-7.46710789	-2.41587885
Ti	-11.10348281	-7.46277802	-0.03961472
Ti	-11.31190762	-5.68370898	2.43853984
Ti	-9.70210629	-5.60404696	4.78114946
Ti	-9.23874489	-7.61752905	7.26173443
Ti	-9.38390439	-1.88056242	-4.83796356
Ti	-9.69468764	-3.74474672	-2.38745742
Ti	-11.28369527	-3.76821179	-0.02131277
Ti	-11.33572747	-1.89267666	2.45103666
Ti	-9.74552960	-1.87172448	4.80187919
Ti	-9.36600099	-3.80601039	7.22216078
Ti	-9.38393171	1.88037600	-4.83626346
Ti	-9.71916465	-0.00117457	-2.37880036
Ti	-11.31036789	-0.00216138	-0.01931914
Ti	-11.33577737	1.88625503	2.45266032
Ti	-9.74561711	1.86339262	4.80350765
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O	1.88083404	7.59372753	-0.41761882
O	0.00631195	9.58959927	-9.06850207
O	0.00295806	7.60775589	-2.01413403
O	0.00122993	7.64674976	1.95682682
O	0.00018233	9.82330701	4.41759458
O	1.89482465	7.62829873	5.14472805
O	1.87428120	9.54609482	2.78307119

O	1.86404184	9.57590900	6.67223916
O	1.87802033	7.92429986	9.24828774
O	0.00199185	9.55105919	0.30228110
O	-0.00120678	7.63671578	7.60931806
O	-0.00283396	7.68860281	11.49330468
O	1.88569026	11.51495224	-4.26814267
O	1.89530945	11.69159469	-0.37954090
O	0.00298982	11.68748346	-2.02481027
O	0.00130267	11.49704203	1.85178951
O	3.76930894	-9.57955966	-5.18845773
O	5.71740467	-11.47854563	-4.25335277
O	5.68174677	-9.77074963	-6.81520437
O	5.65842876	-9.52865740	-2.71379369
O	5.64008052	-11.72259088	-0.40190529
O	3.77910326	-9.55563210	-9.06769279
O	3.79085514	-11.64088642	-2.05130365
O	3.79981458	-11.46952129	1.85621898
O	3.74453823	-9.84279290	4.42463422
O	5.58126814	-9.35466704	2.81433460
O	5.60889346	-9.54370567	6.68348394
O	3.76246303	-9.53677233	0.29881625
O	3.72903821	-5.58774659	-14.67735164
O	5.80324390	-7.46006809	-13.91901261
O	5.58789296	-5.80185666	-16.31739528
O	5.59982710	-5.59224130	-12.28316017
O	5.59613300	-7.47048957	-9.88497389
O	3.94089228	-5.57416718	-18.70975623
O	3.79556115	-7.88069303	-11.62594315
O	3.77952032	-7.60759046	-7.53096559
O	3.77289278	-5.69442523	-5.21137993
O	5.63284912	-7.61318738	-4.37680296
O	5.70375996	-5.61828218	-6.77186156
O	5.67781369	-5.66610906	-2.80966042
O	5.63783635	-7.60900512	-0.40457842
O	3.75024591	-5.70413983	-9.18296394
O	3.77315021	-7.58147468	-2.01757821
O	3.71279997	-7.62162374	1.94473804
O	3.78175007	-5.68419206	4.38973985
O	5.60925492	-7.58731956	5.15677961
O	5.66755123	-5.70299170	2.81252043
O	5.62963207	-5.69211119	6.77774130
O	5.66346111	-7.87770524	9.22864848
O	3.79582387	-5.67981307	0.38622053
O	3.73508917	-7.62486513	7.60803113
O	3.75935156	-7.67668505	11.48158741
O	3.79044352	-6.01452966	14.02389539
O	5.59321443	-5.60578389	12.27184723
O	5.80425010	-5.58896415	16.30745960
O	3.75915626	-5.73060591	9.94039188
O	3.68880693	-3.96222175	-21.09758315
O	3.71586737	-3.72003532	-17.06179669
O	3.85994167	-1.87946857	-14.72913931
O	6.01572560	-3.78922580	-14.02926273

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O	5.76036470	-1.86877255	-12.40856118
O	5.73124782	-3.76259050	-9.94284498
O	4.15520026	-1.90305765	-18.80515262
O	3.82470477	-3.74483502	-11.58946967
O	3.80002450	-3.76760710	-7.62310554
O	3.79912717	-1.88953730	-5.23710666
O	5.69520625	-3.78504216	-4.40481261
O	5.74769139	-1.87946431	-6.79237300
O	5.71959112	-1.88604220	-2.82084467
O	5.67431531	-3.71742531	-0.41949015
O	3.81982793	-1.89276380	-9.22846425
O	3.79491453	-3.78714917	-2.00879603
O	3.78845654	-3.79833738	1.98462798
O	3.80467948	-1.89217100	4.41074083
O	5.68742588	-3.77077109	5.20476827
O	5.70865202	-1.89726458	2.82692862
O	5.70125099	-1.89508867	6.80831660
O	5.70364896	-3.75088878	9.18060710
O	3.76980702	-1.88902882	0.41348395
O	3.76684843	-3.79366925	7.61689837
O	3.74560452	-3.82279458	11.58445868
O	3.80999413	-1.87845991	13.98435719
O	5.59107433	-3.73022812	14.66775189
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O	3.79129048	-1.89437234	10.01425207
O	3.72095558	-3.71695966	17.05378571
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O	3.67809922	-1.86780000	19.41568229
O	3.91120489	0.00731230	-21.02380114
O	3.87075226	0.00538000	-17.16389874
O	3.85998273	1.88784426	-14.72739686
O	6.04757386	0.00385390	-14.05148503
O	5.79742820	1.90871184	-16.28105561
O	5.76037823	1.87496258	-12.40682247
O	5.75475146	0.00197882	-9.96398694
O	4.15525556	1.91538486	-18.80332715
O	3.85632313	0.00281205	-11.60816168
O	3.82571482	0.00105844	-7.64147707
O	3.79917287	1.88955337	-5.23547734
O	5.71607091	-0.00033818	-4.40551713
O	5.74772493	1.88082191	-6.79076285
O	5.71956256	1.88400217	-2.81921881
O	5.69622841	-0.00206862	-0.40353566
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O	3.80586636	-0.00306328	1.99954279
O	3.80462389	1.88392465	4.41232566
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O	5.99832581	1.89616280	16.41861484
O	5.75748699	-0.01467955	18.66680396
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O	4.10359663	-0.01422793	21.16056298
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O	6.01576562	3.79689437	-14.02575196
O	5.58820446	5.81157207	-16.31201180
O	5.60001922	5.59841836	-12.27814287
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O	3.80002981	3.76972758	-7.61983257
O	3.77291684	5.69447721	-5.20650262
O	5.69523865	3.78437459	-4.40154608
O	5.70379318	5.61966494	-6.76703999
O	5.67777788	5.66415732	-2.80484184
O	5.67428283	3.71333593	-0.41634209
O	3.75032129	5.70762529	-9.17801262
O	3.79488993	3.78449772	-2.00560721
O	3.78836405	3.79224792	1.98780925
O	3.78169461	5.67605388	4.39452337
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O	5.66743521	5.69622692	2.81726775
O	5.62959374	5.68197954	6.78245745
O	5.70364646	3.73864579	9.18364461
O	3.79578394	5.67509758	0.39098449
O	3.76677534	3.78294753	7.62001587
O	3.74615851	3.80856797	11.58759927
O	3.78913435	5.99662825	14.02973700
O	5.59220090	3.71317612	14.67014895
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O	5.80487698	5.57216168	16.30982668
O	5.57786614	3.92365563	18.69966733
O	3.75869112	5.71766197	9.94541727
O	3.72007598	3.70269825	17.05594457
O	3.94784891	3.67486582	21.08074518
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O	3.79562860	7.88627481	-11.61892137
O	3.77956149	7.60963769	-7.52432720



O	3.76933410	9.57967067	-5.18019101
O	5.63285660	7.61254682	-4.37035397
O	5.68180833	9.77215639	-6.80676822
O	5.65839059	9.52666153	-2.70568314
O	5.63776157	7.60494533	-0.39816998
O	3.77917384	9.55904328	-9.05937126
O	3.77308278	7.57889500	-2.01119513
O	3.71268388	7.61558271	1.95113554
O	3.74444780	9.83470819	4.43292223
O	5.60912895	7.57856790	5.16314720
O	5.58115259	9.34793119	2.82218277
O	5.60849468	9.53362516	6.69154492
O	5.66308334	7.86531197	9.23536043
O	3.76242047	9.53221178	0.30687699
O	3.73483787	7.61376231	7.61456288
O	3.75806532	7.66216962	11.48841365
O	5.71741923	11.47788755	-4.24357459
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O	3.79079163	11.63832415	-2.04138740
O	3.79972581	11.46362813	1.86594776
O	7.49428854	-9.37876937	-5.09179163
O	9.65666831	-11.18889249	-4.40922209
O	9.35898023	-9.49178257	-6.75306726
O	9.34160284	-9.35743020	-2.70332532
O	9.21206305	-11.89027605	0.31309465
O	7.66997376	-9.33510527	-9.12266454
O	7.64424340	-11.57709279	-1.97790932
O	7.19706749	-11.34474093	1.98964617
O	7.50242699	-9.70838983	4.44063060
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O	9.53940947	-9.36544060	6.69748251
O	7.59229975	-9.48645809	0.32088750
O	7.46558631	-7.66783239	-11.52013660
O	7.45689948	-7.46317560	-7.48431459
O	7.60538984	-5.63604187	-5.13488504
O	9.75335766	-7.53116426	-4.43470686
O	9.54895535	-5.63017634	-6.68363331
O	9.52778598	-5.61805399	-2.82344234
O	9.38285388	-7.18207904	-0.37002429
O	7.88218654	-5.66430133	-9.22695551
O	7.56348256	-7.52358255	-1.98634334
O	7.55728516	-7.58237942	1.97084827
O	7.61003913	-5.62353634	4.37187791
O	9.37411811	-7.48980280	5.04976574
O	9.54168275	-5.67021155	2.69760112
O	9.75467561	-5.69124776	6.80043960
O	9.33936874	-7.68980091	9.09583345
O	7.40927478	-5.64165050	0.41987586
O	7.46397394	-7.49012042	7.46844884
O	7.67554956	-7.47008719	11.50277525
O	7.46142968	-5.80919734	13.90619830
O	7.48082639	-5.60107214	9.86722509
O	7.67656531	-3.76479829	-11.48336722

O	7.63743635	-3.74108279	-7.60484869
O	7.63422603	-1.88227967	-5.14503551
O	9.81262642	-3.74900969	-4.42538602
O	9.58767005	-1.86698489	-6.66183718
O	9.55155205	-1.87928805	-2.77295362
O	9.51692720	-3.79210300	-0.29653077
O	7.93205503	-1.88167900	-9.24412162
O	7.63740200	-3.77620510	-1.95906546
O	7.61495710	-3.78041995	2.01379977
O	7.66056014	-1.88811594	4.39432843
O	9.56497388	-3.76303829	5.18536591
O	9.56743852	-1.87888169	2.74037774
O	9.80286337	-1.89703944	6.83421253
O	9.55849351	-3.78489107	9.06255660
O	7.59374912	-1.88557486	0.41956145
O	7.60881865	-3.77008743	7.52761282
O	7.87781756	-3.80026880	11.61768325
O	7.66674209	-1.90418257	13.87773390
O	7.64373688	-1.87922163	10.00002368
O	7.70428580	0.00269427	-11.48947978
O	7.65969919	0.00097723	-7.60900444
O	7.63424610	1.88216920	-5.14338702
O	9.82781408	-0.00035667	-4.40443919
O	9.58769122	1.86815041	-6.66019858
O	9.55153674	1.87719917	-2.77133673
O	9.54696936	-0.00210003	-0.29371396
O	7.93205456	1.88508974	-9.24241831
O	7.65405709	-0.00138930	-1.95352201
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O	9.56737361	1.87220517	2.74197885
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O	9.58599332	-0.00617819	9.07762330
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O	7.63288209	-0.00533307	7.55422361
O	7.90669588	-0.00729491	11.64298158
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O	9.52771832	5.61607051	-2.81859848
O	9.51686285	3.78795917	-0.29331115
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O	7.63735803	3.77343979	-1.95591247
O	7.61476452	3.77426392	2.01690496
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O	9.55819606	3.77272575	9.06571452
O	7.40925863	5.63690434	0.42457398
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O	7.87708375	3.78583736	11.62063979
O	7.46224381	5.79229520	13.90984852
O	7.48076986	5.58830479	9.87187834
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O	7.45708741	7.46518939	-7.47781297
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O	9.35909859	9.49323150	-6.74480156
O	9.34171701	9.35543443	-2.69526741
O	9.38282170	7.17815151	-0.36387895
O	7.67010041	9.33857639	-9.11448665
O	7.56343578	7.52097982	-1.97997504
O	7.55710281	7.57631932	1.97720094
O	7.50229356	9.70027989	4.44882217
O	9.37393229	7.48119899	5.05607080
O	9.36378524	9.52691390	2.74887358
O	9.53919046	9.35547696	6.70528848
O	9.33939348	7.67749797	9.10200979
O	7.59212846	9.48183822	0.32890965
O	7.46372171	7.47966963	7.47483339
O	7.67549151	7.45626079	11.50853696
O	9.65668659	11.18838821	-4.39957038
O	9.21209255	11.88544908	0.32301500
O	7.64418173	11.57445403	-1.96803632
O	7.19703315	11.33874462	1.99918960
O	10.96980380	-11.52353008	-1.67479801
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O	11.26382425	-9.52242047	4.32375786
O	10.75814445	-9.35376120	0.29544178
O	11.36476617	-7.59556498	-1.82393436
O	11.66268293	-7.61446149	1.97918584
O	11.47676483	-5.68923363	4.27567354
O	11.65818811	-5.64304469	0.40177709
O	11.46953996	-3.76360094	-1.83619799
O	11.67342936	-3.78564489	2.06020378
O	11.51432484	-1.88380025	4.29000214
O	11.66772948	-1.89326854	0.40144372
O	11.49656980	-0.00141518	-1.83475001
O	11.70979603	-0.00304983	2.04512497
O	11.51428165	1.87579610	4.29158663
O	11.66768720	1.88855944	0.40305018
O	11.46948390	3.76076350	-1.83301526
O	11.67329872	3.77951293	2.06341450
O	11.47645405	5.68120785	4.28043595
O	11.65816667	5.63831022	0.40648989
O	11.36474880	7.59262162	-1.81753157
O	11.66250581	7.60835442	1.98567612
O	11.26363201	9.51443493	4.33177637
O	10.75843469	9.34914125	0.30321882
O	10.96994922	11.52070049	-1.66507082

O 11.77513596 11.07855784 1.80690349

### ANNEALED SPHERICAL TiO<sub>2</sub> NPs (NanoTiO IP)

(TiO<sub>2</sub>)<sub>43</sub>

129

PBE

O	-2.684080	-4.997992	1.392300
O	-6.142102	-2.403433	0.161339
Ti	-2.556768	-4.573371	-0.315163
O	-4.118808	-4.137343	-1.241351
Ti	-5.112660	-2.602149	-1.288853
O	2.401756	-1.427161	-6.093003
O	1.163731	-4.115768	0.790460
O	0.468318	-5.877725	-3.463580
Ti	0.211349	-5.826647	-1.661796
O	0.858440	-4.061357	-1.823872
Ti	1.312873	-4.240745	-3.704286
O	-1.542925	-5.823792	-1.193409
O	0.437975	-3.101724	-4.854214
Ti	0.706490	-1.339986	-5.344519
O	1.844379	-5.876500	2.747065
Ti	2.081957	-5.662863	0.945271
O	3.812463	-5.144969	0.693612
Ti	4.337844	-3.530943	0.016562
O	1.323075	-6.645438	-0.446176
O	4.726022	-3.801329	-1.746727
Ti	4.159327	-3.696382	-3.486320
O	-3.507295	-0.083001	-4.993647
O	-1.385033	-3.093644	-0.239798
O	-5.320057	-1.540763	-2.818610
Ti	-3.034412	0.106832	-0.433096
O	-4.088041	1.630566	-0.261609
Ti	-4.478966	-0.010430	-3.417915
O	-3.886488	-1.552063	-0.374829
O	-5.314229	1.591262	-3.029591
O	1.707403	-0.287719	-4.070579
O	0.466684	-1.485170	1.269413
O	2.984419	-4.961772	-4.062826
Ti	0.360268	-2.726688	-0.218595
O	0.798029	-1.394176	-1.461935
Ti	0.661651	-0.038130	-2.569350
O	-1.318408	-0.031298	0.018038
O	-0.743123	-0.652972	-3.728808
Ti	-1.702428	0.281012	-4.986617
O	-0.618336	-0.428902	-6.286918
O	4.378176	0.149121	-3.725109
O	3.802568	-0.169011	2.107372
O	5.765053	-2.668566	0.705918
Ti	5.111726	-0.932796	0.839936
O	5.024975	-0.081426	-0.782533
Ti	4.256496	0.928337	-2.109377
O	3.240530	-2.089499	0.544330

O	2.384165	0.941523	-1.788624
Ti	3.486805	-1.259455	-4.592001
O	2.763401	-2.529788	-3.320038
O	6.288227	-0.028972	1.920895
O	-2.627394	3.199430	1.171690
O	-3.064511	0.224082	-2.308628
Ti	-4.438906	2.634026	-1.754927
O	-2.785976	3.239057	-2.322705
Ti	-1.130440	2.909947	-2.981766
O	-5.220509	3.816763	-0.620042
O	0.567446	6.293015	-0.432908
O	0.520777	2.551933	4.508231
O	-0.038252	1.690859	-1.979561
Ti	1.482266	2.096809	-0.544485
O	3.091918	2.965585	-0.077602
Ti	0.927622	5.130573	-1.740231
O	0.045871	3.484647	2.102801
O	-0.236568	4.489660	-3.058986
O	-1.330127	2.044354	-4.576849
O	4.437308	4.434275	3.431822
O	4.864027	2.658273	-2.173675
Ti	4.022245	4.017945	1.717575
O	4.817197	4.857051	0.214221
Ti	4.075948	4.025863	-1.205512
O	2.336180	5.063555	1.581299
O	2.714213	4.918471	-2.093602
O	4.837731	-2.526844	-4.714362
O	5.184314	2.522866	1.588748
O	-2.708066	6.831328	4.133142
O	0.618394	3.816338	-0.467650
Ti	0.674825	5.184154	1.145238
O	-2.014861	4.534546	3.569018
O	-0.179005	6.323246	2.384787
O	-2.917575	-3.562711	4.576077
O	-4.073505	-2.955449	2.174204
O	0.261593	-2.304353	7.858163
O	-2.543830	-1.521887	6.860228
O	-1.661825	-1.981240	2.934186
Ti	-2.419446	-1.838731	4.997232
O	-0.618263	-4.416173	3.153293
Ti	-2.363959	-3.744809	2.848740
O	2.186449	-1.292798	5.932648
O	2.118824	-2.728815	3.121453
Ti	0.965523	-2.625200	6.181530
O	1.253396	-4.238632	5.329960
Ti	1.118011	-4.358431	3.504545
O	-5.193769	1.443995	4.987594
O	-3.284580	-0.182302	1.640818
Ti	-4.605137	0.653729	3.384040
O	-5.719031	-0.590902	2.700167
Ti	-4.883630	-1.647979	1.421906
O	1.472374	0.099144	3.420086
O	2.772574	1.470129	5.549051

Ti	-0.942739	-0.972292	7.433683
O	-1.194702	0.476964	8.617431
O	-0.886913	1.079664	2.635952
Ti	-3.865486	2.586034	5.397848
O	-3.412274	-0.518200	4.362637
Ti	-1.369025	-0.486021	1.836238
O	2.851522	2.557605	2.900184
O	-0.177933	0.557508	6.351582
O	1.257410	1.253270	0.959554
Ti	1.532518	0.309974	5.322275
O	-0.459751	-1.784334	5.418902
Ti	2.164943	-1.312534	2.089818
O	5.160561	1.907372	4.376658
Ti	5.099232	1.150652	2.692087
O	-2.654128	2.293246	6.774714
O	-4.528393	4.921632	2.205870
O	-5.160754	2.104380	2.166605
Ti	-4.532675	3.360199	1.107484
O	0.197904	3.228574	7.347027
O	-4.345284	4.370898	5.187520
Ti	-1.015927	1.842686	7.423236
O	-3.003000	2.151875	3.856129
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O	2.691745	4.121426	5.716212
Ti	1.085662	1.933992	2.783201
Ti	3.733164	3.073329	4.531798
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**(TiO<sub>2</sub>)<sub>115</sub>**

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Ti	4.678663	0.441793	-9.023822
O	4.318676	-0.636361	-10.571448
O	-5.623122	0.692915	0.015644
O	-8.221389	3.396924	-3.660940
Ti	-8.254222	1.567394	-3.706397
O	-6.819510	6.142634	-3.125987
Ti	-6.685793	4.406941	-3.710886
O	-7.302451	1.085256	-2.228100
O	-2.549767	3.240263	-6.328843
O	-1.938996	0.706919	0.898750
O	-4.570232	0.787154	-3.239202
Ti	-2.624673	1.315732	-2.644379
O	-2.991219	3.127432	-3.311222
Ti	-2.281039	4.012987	-4.728174
O	-3.895072	2.326150	-0.985350
O	-5.961789	4.031679	-5.345990
Ti	-5.669322	2.833217	-6.783652
O	-6.959349	1.747509	-7.622882
O	1.784047	4.299377	-6.511678
O	0.884544	0.993383	0.802886
O	-1.893500	0.449932	-3.977053
Ti	1.041550	1.880380	-2.476696
O	0.708272	3.520584	-1.582927
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O	-1.024451	1.630755	-1.678556
O	-0.506155	4.020087	-4.724365
O	-2.948622	5.810266	-7.699545
Ti	-2.444755	6.843918	-6.329059
O	-2.614807	2.153601	-8.736112
Ti	-2.617998	3.931772	-8.029953
O	4.583746	4.657978	-7.897027
O	3.256333	2.356853	0.801259
O	4.754432	2.783944	-4.592707
Ti	4.012305	2.700577	-0.859998
O	5.517010	5.233190	-3.168755
Ti	4.059898	4.243692	-3.844412
O	3.467007	4.143615	-1.785445
O	0.588959	1.491734	-4.232164
O	1.960367	5.235346	-8.730982
Ti	3.113847	5.516667	-7.293297
O	0.497379	2.196318	-6.837409
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O	8.092004	2.996939	-0.642615
O	6.241146	0.177757	-5.300511
Ti	7.355107	2.017182	-2.055465
O	7.518226	2.491178	-3.819632
Ti	6.354118	2.002114	-5.150685
O	5.606382	2.209940	-1.606918
O	6.684081	2.749455	-6.756095
Ti	5.308111	2.935994	-7.993960
O	5.622128	1.941643	-9.519645
O	-5.632560	3.700305	-2.348740
Ti	-5.569821	6.928935	-1.995438

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O	-4.702455	8.330556	-2.772843
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O	2.101269	3.628651	-3.788667
Ti	1.713362	5.113991	-2.225496
O	0.451670	5.949311	-3.281787
Ti	-0.029344	7.396124	-4.241802
O	-1.895115	4.718186	-1.440827
O	-1.599220	8.014986	-3.320667
O	-3.476114	8.082890	-5.445744
O	3.269636	6.303658	1.031587
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Ti	4.878157	6.781331	-2.541454
O	4.749690	7.926905	-4.019595
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O	3.084812	6.364517	-2.856452
O	1.598803	8.132258	-4.470042
O	3.209377	7.306914	-6.743169
O	5.365942	7.017067	-0.767002
O	-3.432247	-4.873941	3.461040
O	-5.628713	-6.255937	2.442179
Ti	-4.367143	-6.357521	3.916548
O	-3.383942	-7.812335	3.156129
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O	-0.639789	-7.172562	6.679471
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Ti	-2.215457	-6.176374	6.699393
Ti	-2.460803	-7.897791	1.615750
O	3.510683	-10.326785	3.374278
O	1.812841	-8.223222	5.091926
O	1.522640	-7.579257	-0.230131
Ti	3.218688	-8.608382	4.008768
Ti	3.296899	-10.019652	1.553209
O	4.722719	-10.108915	0.448963
O	-5.793188	-5.680601	5.148458
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O	-3.026553	-5.544956	8.266720
O	-3.669053	-2.797352	9.443192
Ti	-4.159627	-4.151078	8.362465
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Ti	-6.120748	-4.459183	6.359377
O	-3.424879	-6.777400	5.586165
Ti	-5.839982	-5.198824	1.012321
O	0.970877	-5.322047	5.028341
O	2.016569	-6.166634	7.458766
O	2.122548	-3.503889	9.169372
Ti	2.275090	-4.322320	7.565154

O	0.808879	-3.404034	6.916448
O	-2.379250	-3.388964	1.012679
Ti	-0.275992	-3.685869	5.402408
O	-1.698245	-4.556321	6.019609
Ti	-1.973518	-4.674505	2.389584
O	3.446958	-4.740653	3.967842
O	4.553859	-7.500792	4.499712
Ti	5.152955	-5.882774	3.810900
O	4.214114	-2.160538	3.705803
O	2.654640	-5.223013	-0.274373
Ti	1.807808	-4.496097	3.361808
O	3.009118	-8.245312	2.153309
Ti	2.779403	-6.518955	1.041180
O	7.059026	-4.275157	1.422593
O	6.686911	-6.322318	3.003419
O	6.286815	-5.583910	-0.745583
Ti	6.301522	-6.019246	1.201107
O	6.623892	-7.839439	0.772792
Ti	5.537194	-8.596206	-0.397736
O	-5.430802	-0.180211	6.209146
Ti	-4.298919	1.243181	5.775007
O	-7.205516	2.592400	-0.071199
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O	-4.457258	-3.431819	6.572642
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Ti	-2.189069	-1.605477	9.167645
O	-1.606503	-0.174254	10.083603
Ti	-1.452195	-0.287195	6.208632
O	-2.858992	0.353289	5.127919
O	-4.763321	-1.908558	3.893801
Ti	-5.239100	-1.882020	5.634964
O	-6.777666	-2.828062	5.732519
Ti	-5.322045	-1.820821	2.156118
O	1.778931	-0.618508	2.700691
O	2.353388	-1.124900	7.661007
Ti	1.070463	-1.999872	8.812940
O	1.012602	-0.732362	10.064802
Ti	1.925639	0.092825	6.463111
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O	0.551779	0.160247	5.038620
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O	-0.584266	-4.191622	3.398975
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Ti	4.779347	-3.153911	5.291988
O	5.703790	-1.669589	5.922956
Ti	5.244922	0.066507	5.528875
O	3.734648	-3.716724	6.663021
O	1.305601	-2.737957	4.259906
O	3.979525	-0.040070	1.744082
Ti	3.256062	-1.815083	2.294548

O	2.235679	-3.298768	1.772434
Ti	3.066280	-3.323676	-0.217556
O	6.762381	-1.300453	1.946293
O	5.895424	0.641631	3.906755
O	6.364015	1.526649	1.088013
Ti	5.790689	0.203220	2.183708
O	4.522867	-5.876157	1.812191
Ti	6.414465	-2.733105	0.867064
O	-6.858598	1.979588	2.472205
Ti	-6.073306	2.140474	-1.273460
O	-1.030769	1.886449	6.179606
O	-0.009779	-0.115198	7.675033
Ti	-0.030413	0.698846	9.369412
Ti	-1.978477	2.830359	7.508192
O	-3.703324	2.196495	7.187429
O	-3.925692	2.018684	1.835281
Ti	-5.369321	2.894568	2.822554
O	-4.944345	2.452329	4.524541
Ti	-3.738484	0.844252	0.290011
O	0.474950	4.042600	5.122711
O	1.726193	1.945930	6.653390
Ti	2.225255	2.965363	8.139433
O	1.280397	4.520207	7.962877
Ti	0.120523	5.069441	6.692855
O	1.508052	1.911119	9.406464
O	-1.574897	4.602076	7.194713
O	-0.910284	3.159925	0.787364
Ti	0.279266	2.212286	4.825962
O	-0.876945	1.942463	3.455524
Ti	-1.964588	2.499913	2.119246
O	4.480708	4.092500	2.856599
O	5.718764	1.520062	6.539719
Ti	5.018034	3.214205	6.331420
O	4.027825	3.395676	7.890266
O	3.681881	3.021302	5.184592
O	1.383478	4.840202	2.544763
Ti	2.913160	3.976930	3.797176
O	1.869679	2.226870	3.383882
Ti	2.329308	1.205552	1.895165
O	6.049360	4.430607	5.232153
O	5.445214	4.241910	0.231250
Ti	6.081415	4.756598	3.411853
O	7.352764	3.852789	2.420546
Ti	6.920040	3.210088	0.757272
O	-3.580127	6.713913	2.006589
O	-1.220757	2.218922	8.957075
O	-5.812647	6.864997	-0.171446
O	-5.682210	4.672685	2.381958
Ti	-4.956329	5.875982	1.192665
O	-1.009206	6.208099	3.801416
O	0.519185	6.649727	5.926693
O	-0.727808	5.876357	1.016742
Ti	-1.979998	5.807889	2.410025

O	-2.559228	4.089878	2.747376
Ti	-0.500927	4.510988	-0.333557
O	1.226715	7.395034	2.746691
Ti	0.919738	6.215524	4.139665
O	2.666806	5.561798	4.584549
Ti	1.478589	6.197258	1.389102
O	5.946171	6.300898	2.321424
Ti	5.029952	6.015790	0.762013

**(TiO<sub>2</sub>)<sub>136</sub>**

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O	-3.945951	-2.207687	-9.885814
O	4.560138	-2.249019	-10.729165
O	-3.539321	0.460050	-10.525348
O	-0.694196	1.216272	-10.819592
O	2.150950	-0.147768	-10.928576
O	-6.604493	-8.358109	-1.718825
O	-3.603786	-9.023031	-6.677929
O	-4.672499	-10.787610	-1.310207
O	-4.743158	-9.263256	-3.928159
Ti	-4.977155	-9.138735	-2.134243
O	-3.241295	-8.784945	-1.255845
Ti	-3.876038	-8.133554	-5.103095
O	-5.092932	-6.812731	-5.497084
O	-0.785185	-8.508336	-8.265646
O	-0.527184	-8.000177	-1.882039
O	-0.150680	-9.179298	-4.376833
Ti	-0.490230	-9.710987	-2.620968
O	0.068605	-6.113576	-3.714506
Ti	-0.575889	-7.453014	-4.818626
O	-1.699661	-10.940009	-1.964298
O	-2.127486	-7.019437	-6.063293
Ti	-2.418680	-7.968065	-7.666795
O	2.541328	-7.650998	-8.066628
O	1.652778	-7.732594	0.437911
Ti	1.290436	-8.070963	-1.373665
O	2.507402	-7.990441	-2.750726
Ti	3.747175	-6.669611	-7.090551
O	1.041678	-9.885016	-1.686872
O	0.536020	-7.098077	-6.230589
Ti	0.724689	-7.394782	-8.021014
O	5.294942	-6.381097	-8.042249
O	-6.790377	-4.297320	-4.886360
O	-6.030473	-6.400484	0.317728
O	-7.053117	-5.134827	-2.197378
Ti	-6.203996	-6.584118	-1.456087
O	-7.520081	-2.071136	-2.956866
Ti	-6.592092	-3.647969	-3.189980
O	-1.241925	-3.063765	-4.425838

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O -2.520799 -5.194432 -2.798256  
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O	-3.950848	-4.312718	0.138495
O	-2.368235	-2.319317	-2.357304
Ti	-2.642759	-1.038347	-0.738393
O	-2.631540	0.464527	0.312131
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O	-4.486806	-1.428374	-0.731280
O	-4.336117	-0.357396	-4.347212
O	-6.187536	-1.832909	-9.069599
Ti	-4.479292	-0.349941	-6.193146
O	-4.944760	-2.031253	-6.639743
Ti	-5.048402	-2.930432	-8.259622
O	-0.321896	1.255496	-5.920283
O	2.230021	-1.570469	-0.493053
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Ti	0.815504	-0.435434	-0.142453
O	-0.830611	2.271091	-0.542601
Ti	0.722601	0.450762	-4.467324
O	-2.369918	-2.223700	0.703301
O	-0.970497	-0.344040	-3.885677
O	-1.464987	-1.238670	-8.623953
Ti	-0.893987	-0.170213	-7.261073
O	0.044034	-1.403743	-6.193804
Ti	-2.243026	-2.693435	-9.338585
O	4.468057	0.018338	-7.391055
O	3.254115	-3.920564	0.537467
O	4.020095	0.251367	-2.628283
Ti	2.962495	-1.218638	-2.259873
O	6.823075	1.526774	-2.567592
Ti	5.035496	1.683239	-3.147913
O	1.529384	0.906836	-1.078374
O	2.198870	0.209077	-5.531155
O	0.878327	0.321186	-8.354056
Ti	2.639281	0.164057	-7.280898
O	2.812307	-1.586856	-8.534963
Ti	2.760420	-1.791612	-10.371496
O	6.774787	-0.861553	-5.912966
O	5.608646	-2.150742	1.675515
O	8.380503	-2.958219	-4.725004
Ti	6.601092	-1.309176	-1.107053
O	7.136880	0.207044	-0.214537
Ti	7.795016	-1.254601	-4.486407
O	4.856428	-1.865917	-0.909596
O	6.924275	-1.349795	-2.881407
O	6.682495	-1.014473	-8.922244
Ti	6.231985	0.005723	-7.437549
O	6.932012	-4.077278	-9.548095
Ti	5.883521	-2.535677	-9.528374
O	7.212217	-2.812033	-0.240115
O	-2.904694	2.181672	-4.571103
O	-5.379632	1.139616	1.644398
O	-7.643369	3.454936	-4.971294
Ti	-6.352580	1.077565	-0.337178
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O	-7.353675	-0.345341	0.443083
O	-2.760904	3.569750	-7.060838
O	-2.987592	3.591447	0.483551
O	-2.815922	0.533137	-2.205340
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O	-4.671732	2.036686	-0.490816
O	-5.210959	3.541340	-3.654104
O	-6.348712	0.914613	-9.787298
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O	-4.648341	0.340383	-8.069627
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O	0.173942	3.584719	-7.719503
O	0.857247	3.250279	1.551270
O	4.446782	3.317262	-2.659135
Ti	0.731052	2.516326	-1.572698
O	0.237927	4.253932	-2.324974
Ti	0.687941	4.109453	-4.182708
O	0.839663	2.041754	-3.452806
O	-0.806978	3.825644	-5.101251
O	-2.887030	3.319635	-9.869499
Ti	-1.091625	2.841354	-6.711192
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Ti	-2.256522	1.583975	-9.918237
O	5.249415	4.286178	-6.147491
O	4.436219	4.160807	0.255944
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Ti	3.916985	4.727541	-1.587533
O	4.991505	6.078495	-1.751941
Ti	3.489281	4.875696	-6.126999
O	2.133704	3.551821	-0.814977
O	2.281625	3.912209	-5.134875
O	1.714464	2.656933	-10.008549
Ti	1.909379	3.336291	-8.314713
O	2.767544	2.000685	-7.485427
Ti	0.972863	0.990269	-10.111286
O	8.302074	1.450217	3.540542
O	8.891872	0.213719	-4.279598
Ti	8.064490	1.848870	-0.696417
O	9.270162	2.168586	-2.077561
Ti	8.351055	1.818689	-3.606287
O	7.113291	3.349363	-0.338314
O	7.844143	3.034448	-4.887834
Ti	6.326770	2.839225	-5.932149
O	6.733376	1.781936	-7.369412
O	8.945037	1.580250	0.858423
O	-7.851411	5.486742	0.790319
O	-7.803592	4.500606	-2.188329
Ti	-7.179158	4.350585	-0.493166
O	-4.166743	7.755860	-5.600514
O	-2.917619	6.359091	-0.321221



O	-3.509877	5.366123	-5.134647
Ti	-3.653423	4.799207	-1.118653
O	-4.266513	8.145808	-2.671103
Ti	-4.549621	6.897686	-3.994299
O	-5.425613	4.803936	-0.848383
O	-6.234790	6.182969	-4.084277
O	-5.394375	3.308743	-8.257352
O	-1.368021	7.221993	-6.092542
O	-0.573771	4.984438	0.122376
O	0.644336	5.996306	-4.271896
Ti	0.997283	5.576992	-0.954738
O	0.621851	7.315936	-1.028548
Ti	-2.707108	7.836335	-1.700412
O	-3.569253	5.665320	-2.755074
O	-1.473761	7.708606	-3.091919
Ti	-3.058944	6.595552	-6.444274
O	-3.593255	5.948145	-8.105934
Ti	-3.732680	4.132914	-8.449482
O	4.988100	6.973984	2.699036
O	3.310089	6.520777	-5.386170
Ti	4.359779	7.966056	-1.356604
O	3.801071	8.112156	-3.134877
Ti	2.476899	7.172079	-3.898083
O	2.468002	5.787694	-2.343666
O	1.172986	8.429543	-4.377698
Ti	-0.384760	7.486958	-4.526021
O	2.873777	4.822668	-7.854266
O	5.946447	8.534783	-0.696541
Ti	6.022885	7.610603	0.942234
O	4.197323	7.199840	0.469570
O	0.098255	9.902097	0.446805
O	-2.239654	9.029238	-0.535080
Ti	-1.363750	9.189930	1.359299
O	-3.234717	9.034586	1.917835
O	2.891744	9.087325	-0.798242
O	-3.998133	-6.772220	5.012440
Ti	-3.025373	-5.926554	6.298970
O	-6.339958	-7.204316	3.113169
Ti	-4.536372	-7.454490	3.424627
O	-1.390117	-9.480321	4.237527
Ti	-0.640985	-8.093930	5.196905
O	-1.719582	-7.247945	6.431876
O	-0.956822	-8.148054	1.910583
Ti	-2.084203	-9.468807	2.514020
O	-2.347369	-10.604431	1.052289
Ti	-2.956755	-10.506764	-0.707192
O	4.096393	-8.073050	5.132586
O	0.870019	-8.739304	5.844398
O	1.348189	-5.668733	1.891641
Ti	2.297117	-7.707245	5.103989
O	1.742411	-8.569350	3.249965
Ti	0.788022	-7.590542	2.199010
O	5.683164	-7.175882	2.618990

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O	-5.764453	-1.758153	4.534341
Ti	-7.027603	-1.566068	5.893009
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O	-1.894462	-4.468156	5.918532
O	-4.194247	-5.437196	7.632477
O	-4.148372	-2.476589	8.044740
Ti	-5.043882	-3.801053	7.211934
O	-6.748930	-3.051174	6.937369
O	-5.608032	-4.389517	2.809490
Ti	-4.690230	-3.181324	3.787992
O	-4.538039	-3.958723	5.488932
Ti	-6.520722	-5.800345	1.975964
O	2.337990	-3.315490	3.161015
O	2.235023	-6.642090	6.675366
Ti	2.257944	-4.899304	7.102524
O	1.057225	-3.973983	8.164516
Ti	1.712131	-2.311285	4.847998
O	-0.147954	-3.669910	3.762274
O	-1.410791	-4.666887	1.606832
Ti	-1.593978	-2.975569	4.995005
O	-3.794137	-9.047054	2.930898
Ti	-2.823511	-5.509377	0.892107
O	1.742465	-4.346815	5.408893
O	3.888534	-4.254924	7.624174
O	4.492653	-1.367383	8.456956
Ti	4.524395	-2.619347	7.138453
O	3.108252	-2.110123	6.000823
O	2.946392	-6.202391	3.925846
Ti	1.174788	-4.966321	3.722452
O	0.274692	-6.654728	4.155398
Ti	2.433724	-5.784588	0.311205
O	7.556409	-3.518258	3.473732
O	6.220718	-2.977841	6.500812
O	6.104880	-4.629942	1.243433
Ti	6.229131	-3.482429	4.734944
O	5.429566	-5.130432	4.778115
Ti	5.816079	-6.407798	0.963738
O	-7.181637	0.277369	3.440002
O	-6.497563	-0.006267	6.723357
Ti	-5.739115	1.639041	6.738046
O	-7.964038	-2.338552	2.615324
Ti	-8.619546	-0.803197	3.320111
O	-8.679040	-1.336537	5.125239
Ti	-8.095427	-3.374071	1.131422
O	-1.269225	-1.349751	3.174796
O	-2.456312	-1.647540	5.945806
Ti	-2.703779	-1.371986	7.715273
O	-2.908588	0.391854	8.071586
Ti	-2.930466	1.651212	4.440797
O	-3.929483	1.838089	6.090846
O	-4.861509	-1.857603	2.149694
Ti	-5.480920	-0.237047	2.914001

O	-4.068378	0.342635	3.870105
Ti	-4.801051	-2.723563	0.464326
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O	0.198111	-2.241187	6.032057
Ti	0.474657	-2.258197	7.900919
O	0.261768	2.372224	6.647635
Ti	-0.100531	2.616855	4.920165
O	-1.190753	-2.001864	8.545585
O	1.021670	1.629659	3.824140
O	0.507642	-2.487835	1.241383
Ti	-0.375259	0.181189	3.213984
O	-2.832871	-3.271460	3.535797
Ti	-1.226275	-2.874923	1.965309
O	3.825021	0.496653	4.010040
O	3.337290	0.628876	6.745729
Ti	3.213914	-0.032620	8.410607
O	3.545457	1.499794	9.391684
Ti	4.029101	1.901760	5.614634
O	1.595615	-0.938225	8.512468
O	3.037652	3.033097	4.584696
O	3.159652	1.989032	1.710697
Ti	2.410213	0.768487	2.822567
O	0.783343	0.230438	1.598232
Ti	2.318269	-2.528463	1.482185
O	6.138517	0.449961	2.437995
Ti	7.022027	2.658006	4.034873
O	5.780982	1.967172	5.239458
O	3.233304	-0.926639	1.996777
Ti	4.905595	-0.762790	2.969396
O	5.231793	-2.026746	4.238678
Ti	5.131267	-3.536261	-0.083067
O	8.377570	-1.314809	1.990659
Ti	7.284714	-2.774855	1.787090
O	-6.724268	2.927803	5.926368
O	-5.082073	2.084675	8.369851
O	-9.342557	-2.490090	0.142513
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O	-4.597775	4.677299	4.808082
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O	-3.454824	4.147624	7.491827
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O	-5.682572	4.202203	1.783249
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O	0.622215	4.406810	4.570684
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O	-0.426492	5.076852	7.365760
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O	-1.676816	2.714773	8.846713
O	-2.439644	5.832945	5.242131
O	-1.451086	4.523742	2.502858
Ti	-2.851216	4.695776	3.842506
O	-1.340404	1.704604	2.414207
Ti	-0.885638	3.093431	1.295790
O	4.615096	5.173534	5.202446
O	3.772238	3.302080	7.087942
Ti	3.169097	3.237522	8.792845
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O	1.353989	3.347938	9.067912
O	2.157195	5.519452	6.272230
O	2.136621	5.647195	0.533953
Ti	2.861630	4.831677	4.504356
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O	7.543162	4.096840	5.026825
O	5.981000	5.569587	7.306159
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Ti	6.194765	4.289768	0.891411
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O	-3.784880	8.104102	4.583599
O	-3.246648	7.213521	7.205554
O	-5.838959	7.242064	2.307954
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O	7.326450	0.797932	-1.798927

O	9.630732	3.232249	-5.824015
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O	-5.807916	6.006748	-1.440200
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Ti	-1.085372	6.716480	-7.598920
O	0.397532	3.693089	-8.077198
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O	5.179402	6.202213	-6.713233
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Ti	5.072158	4.122528	-2.850027
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O	-3.607432	-5.023625	7.427682
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O	-3.706486	-2.134213	0.533592
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O	-3.346216	-4.119359	2.723382
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O	-0.500751	-3.858936	2.029249
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O	5.911476	1.310969	2.320365
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Ti	2.668699	0.948337	-8.622596
O	1.453745	-0.059287	-9.307656
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O	-0.854837	5.201137	-9.222212
Ti	-0.726379	4.868331	-7.277977
O	-0.090913	3.225389	-7.745823
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Ti	5.151904	4.152807	-2.471172
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Ti	11.014249	4.488359	0.987868
O	-4.977058	11.013564	2.341666
O	-6.108740	7.390201	3.991517
Ti	-4.556811	6.156543	7.440223
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O	-6.828587	12.778214	1.059700
O	-7.093723	9.391749	2.111176
Ti	-6.446633	10.997186	1.207969
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O	-2.149726	8.978496	9.486922
O	-3.295394	7.269517	4.743395
Ti	-2.711981	9.105917	7.733860
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O	-0.166531	10.050760	3.438118
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PBE

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O	-1.906517	0.061037	9.135162
O	-1.906967	0.033742	5.152109
Ti	-1.954095	0.015638	7.121399
O	-1.895787	1.952908	6.745924
Ti	-1.857714	1.947071	4.769541
O	-3.773555	0.040464	7.540742
O	-3.789645	1.953994	4.354460
O	-3.808934	1.935634	0.381686
Ti	-3.802063	1.901820	2.401807
O	-3.825910	0.037335	1.975545
Ti	-3.826862	0.021371	-0.029058
O	1.954178	1.900074	2.791615
O	1.910496	0.018545	9.127774
O	1.899331	0.013689	5.169211
Ti	1.939337	0.001946	7.127957
O	2.010608	1.920476	6.771956
Ti	1.987088	1.917861	4.776323
O	0.024037	0.026878	7.521522
O	0.040323	1.941298	4.373309
O	0.003240	1.913148	0.383653
Ti	0.019830	1.892264	2.384245
O	0.015160	0.006958	1.959926
Ti	-0.027095	0.000472	-0.035935
O	5.768279	1.901854	2.806525
O	5.651022	0.031446	9.296751
O	5.710346	0.000804	5.249977
Ti	5.717181	-0.013142	7.238027
O	5.788683	1.878140	6.806660
Ti	5.837301	1.895136	4.803155
O	3.859317	-0.056550	7.600467
O	3.861115	1.896771	4.375007
O	3.820437	1.898037	0.379165
Ti	3.834541	1.881571	2.383722
O	3.827172	-0.013625	1.945509
Ti	3.750565	-0.005779	-0.046424
O	9.554855	1.843200	2.765836
O	9.629341	-0.138213	9.597980
O	9.562409	-0.018996	5.293032

Ti	9.588671	0.056292	7.257191
O	9.586960	1.832780	6.869195
Ti	9.675623	1.891131	4.714227
O	7.699952	-0.013282	7.891981
O	7.681934	1.860972	4.381732
O	7.594727	1.888245	0.378902
Ti	7.614366	1.883381	2.324756
O	7.600310	-0.021448	1.940485
Ti	7.504072	-0.031192	-0.073162
O	13.415566	1.687968	2.482571
O	13.406037	0.038648	5.387723
Ti	13.183189	-0.359930	7.388821
O	13.747227	1.325091	7.872880
Ti	13.606332	1.707898	4.439086
O	11.409516	-0.209009	7.676250
O	11.549851	1.817649	4.206813
O	11.307298	1.724050	0.249780
Ti	11.392854	1.900822	2.220346
O	11.379364	-0.121005	1.847172
Ti	11.232906	-0.235482	-0.107154
O	15.382646	1.497042	3.954767
O	15.201089	1.262797	-0.039744
Ti	15.263141	1.507105	2.135097
O	15.677428	-0.382226	1.747223
Ti	14.891795	-0.694344	-0.263438
O	-13.584856	4.145260	5.189531
O	-13.086916	1.719373	6.546770
Ti	-13.173925	2.365029	8.341636
O	-14.091720	3.949250	8.172332
Ti	-13.125595	4.828817	6.856225
O	-15.743751	3.290586	1.827253
Ti	-15.423981	3.297585	-0.008395
O	-9.393754	5.785504	2.851288
O	-9.535546	3.667948	9.098476
O	-9.443413	3.935733	5.177105
Ti	-9.723158	3.849495	7.309789
O	-9.568357	5.777781	6.933846
Ti	-9.286963	5.788775	4.925578
O	-11.962670	2.062418	9.725416
O	-11.634480	3.903584	7.327962
O	-11.982881	5.702387	-0.338146
Ti	-11.196346	5.867274	2.698786
O	-11.576358	4.135065	1.974899
Ti	-11.599618	3.920897	-0.287574
O	-5.614421	5.798582	2.752628
O	-5.733568	3.894058	9.125603
O	-5.696714	3.893452	5.135579
Ti	-5.864966	3.907041	7.168040
O	-5.734819	5.808738	6.750124
Ti	-5.593766	5.850228	4.841423
O	-7.643825	3.716479	7.441133
O	-7.481803	5.885068	4.370863
O	-7.658552	5.820981	0.378706

Ti	-7.457167	5.829100	2.349784
O	-7.557496	3.917205	1.982746
Ti	-7.692304	3.951309	-0.006326
O	-1.789887	5.708397	2.781269
O	-1.891292	3.865619	9.142824
O	-1.862734	3.847224	5.154563
Ti	-1.964813	3.869559	7.182032
O	-1.796500	5.770549	6.732755
Ti	-1.785816	5.701589	4.781726
O	-3.788640	3.928353	7.572795
O	-3.712778	5.758119	4.365832
O	-3.745424	5.727121	0.381366
Ti	-3.715228	5.688961	2.398954
O	-3.750664	3.832547	1.976992
Ti	-3.798170	3.795069	-0.030458
O	2.033648	5.685274	2.823534
O	1.951352	3.866169	9.177247
O	1.992460	3.838686	5.190555
Ti	1.951973	3.857319	7.198165
O	1.991116	5.758026	6.777405
Ti	2.017417	5.699833	4.806670
O	0.056953	3.802746	7.553844
O	0.115376	5.765331	4.389337
O	0.072329	5.703506	0.394954
Ti	0.097507	5.702677	2.379775
O	0.088778	3.807506	1.975169
Ti	0.026496	3.796153	-0.028196
O	5.864956	5.700666	2.808709
O	5.721358	3.636276	9.219354
O	5.762475	3.805117	5.230615
Ti	5.763904	3.813143	7.239569
O	5.903810	5.708952	6.823432
Ti	5.838603	5.696079	4.920962
O	3.872548	3.891841	7.626689
O	3.961532	5.760857	4.424183
O	3.916183	5.704175	0.408291
Ti	3.910858	5.700619	2.413231
O	3.905320	3.786863	1.972027
Ti	3.849498	3.790951	-0.021468
O	9.953684	5.713097	2.981973
O	9.562485	3.653357	9.222653
O	9.623815	3.691539	5.212737
Ti	9.663746	3.726058	7.372097
O	9.675834	5.542045	6.941290
Ti	9.621420	5.595367	4.821560
O	7.677382	3.687113	7.651590
O	7.750743	5.588943	4.394574
O	7.763216	5.710752	0.398874
Ti	7.655939	5.686874	2.396425
O	7.765480	3.795860	1.956563
Ti	7.638425	3.861697	-0.051887
O	13.049697	5.956859	2.885285
O	11.638020	3.487438	7.296058



Ti	13.198284	4.624761	6.417836
O	13.725972	3.258380	5.355076
Ti	12.975451	6.698851	4.562553
O	13.883584	4.232442	8.104414
O	11.742675	5.583503	5.319546
O	11.705787	5.505128	-0.043090
Ti	11.541156	5.817739	1.894706
O	11.481593	3.706093	1.747851
Ti	11.385724	3.527537	-0.282383
O	15.752133	3.171918	1.498897
Ti	15.121493	3.035999	-0.268332
O	-9.496955	9.612254	2.922927
O	-10.507987	8.047389	7.837680
O	-9.424933	7.730191	5.276463
Ti	-11.280147	7.501200	6.233675
O	-9.500461	10.956253	5.677851
Ti	-7.773535	11.548740	5.559821
O	-12.799999	6.609273	6.845359
O	-11.593321	9.005911	5.287648
O	-11.583369	7.290877	1.650468
Ti	-9.866168	9.447638	4.711141
O	-11.259951	6.077048	4.556512
Ti	-11.587757	7.464535	-0.268988
O	-5.579920	9.513490	2.776171
O	-5.634432	7.751945	9.185095
O	-5.581651	7.743098	5.144130
Ti	-5.778942	7.856453	7.117369
O	-5.575090	9.623434	6.739657
Ti	-5.493404	9.719701	4.873442
O	-7.615730	7.923011	7.327913
O	-7.435499	9.868540	4.500925
O	-7.777639	9.651093	0.327370
Ti	-7.702396	9.637628	2.503103
O	-7.580696	7.724422	1.945212
Ti	-7.707765	7.837077	0.002635
O	-1.731066	9.460656	2.760337
O	-1.797367	7.544876	9.060777
O	-1.839317	7.664783	5.122827
Ti	-1.871230	7.761481	7.081585
O	-1.789518	9.618980	6.679080
Ti	-1.734923	9.506539	4.720961
O	-3.736644	7.682177	7.522046
O	-3.652411	9.679627	4.339414
O	-3.655358	9.522804	0.356178
Ti	-3.810323	9.447149	2.405175
O	-3.669531	7.617707	1.972311
Ti	-3.669451	7.558661	-0.031986
O	2.052170	9.391366	2.834615
O	1.962271	7.502951	9.144791
O	2.053354	7.667973	5.215766
Ti	2.026095	7.738137	7.162467
O	2.168853	9.663470	6.801171
Ti	2.025000	9.497486	4.715865

O	0.128654	7.747637	7.478517
O	0.128248	9.556007	4.394939
O	0.084508	9.510720	0.380302
Ti	0.097048	9.528730	2.347741
O	0.156678	7.601061	1.969236
Ti	0.138760	7.595759	-0.005701
O	5.892313	9.409099	2.971405
O	5.797579	7.855332	9.388036
O	5.901518	7.726606	5.314485
Ti	5.854407	7.901363	7.227385
O	5.723026	9.675564	6.934804
Ti	5.805359	9.627256	4.846062
O	3.956423	7.588063	7.684070
O	3.926769	9.677465	4.478713
O	3.940078	9.434953	0.537592
Ti	4.030593	9.481153	2.473323
O	3.987432	7.554976	2.038302
Ti	4.022697	7.586296	0.001564
O	9.754862	9.238918	3.253566
O	9.522363	7.193256	9.260714
O	9.449890	7.429894	5.275498
Ti	9.531695	7.412865	7.355562
O	10.744428	8.616348	7.003711
Ti	8.705521	11.369510	5.440157
O	7.703709	7.884025	7.717868
O	7.725715	9.923184	4.676950
O	7.915858	9.541031	0.558337
Ti	8.106896	9.422297	2.670882
O	7.889474	7.550042	2.015505
Ti	7.865603	7.781313	0.025561
O	14.170610	6.067974	5.777569
O	10.375268	10.730389	5.500653
O	11.530710	7.546369	1.295925
Ti	10.627684	8.958056	5.031758
O	12.300981	8.409638	4.600705
Ti	11.625916	7.307228	-0.543767
O	-7.719749	13.085129	4.612883
O	-5.449427	13.257107	2.420438
O	-4.990368	12.699558	8.980989
O	-5.619894	11.674991	5.160758
Ti	-5.435348	12.484709	7.089979
O	-5.510707	14.046714	6.171682
Ti	-6.005609	13.718005	4.387596
O	-7.174679	11.997707	7.243189
O	-6.729841	15.129995	3.372817
O	-7.622543	13.393856	0.511721
Ti	-6.605513	14.459293	1.655669
O	-7.426084	11.365198	2.041479
Ti	-7.241794	11.593448	0.229169
O	-1.663708	13.516450	2.534245
O	-1.779853	12.000009	9.103695
O	-1.738810	11.551143	4.973633
Ti	-1.927766	11.737641	6.954921

O	-1.912536	13.514543	6.462100
Ti	-1.786289	13.345727	4.639713
O	-3.669679	11.453943	7.364609
O	-3.580241	13.676453	4.091647
O	-3.580760	13.475782	0.310332
Ti	-3.477889	13.173052	2.244292
O	-3.455640	11.402553	1.953620
Ti	-3.525738	11.296173	-0.077641
O	2.046992	13.483539	2.740463
O	0.194863	11.532156	11.246453
O	1.853819	11.495963	5.012478
Ti	1.756986	11.612678	7.015171
O	2.054269	13.367954	6.590996
Ti	1.892077	13.307287	4.722932
O	0.022905	11.540751	7.409819
O	0.107855	13.857325	4.327316
O	0.410593	13.428903	0.202588
Ti	0.214579	13.832494	2.180279
O	0.165450	11.459981	1.948429
Ti	0.161063	11.451945	0.131562
O	5.674419	12.702520	3.036493
O	5.050767	11.567149	8.872269
O	5.753055	11.593227	5.357955
Ti	6.122275	11.772625	7.222356
O	5.699665	13.511098	6.879617
Ti	5.547590	13.519717	5.013819
O	2.016208	11.725785	9.022908
O	3.774278	13.853614	4.427200
O	3.599688	13.294323	0.423256
Ti	3.998416	13.397865	2.441165
O	3.774790	11.346310	2.070060
Ti	3.790056	11.323001	0.156512
O	8.732031	12.698959	4.264203
O	7.915047	11.677987	7.131661
O	6.854464	14.450343	4.263083
O	7.744858	13.390432	1.078842
Ti	7.489012	13.147236	2.898141
O	7.885819	11.274691	2.279597
Ti	7.547874	11.645069	0.385610
O	-5.630805	15.446417	0.460829
Ti	-4.610141	14.584454	-0.795820
O	0.160219	15.457794	1.591168
Ti	0.686565	15.228518	-0.341436
O	4.606855	15.040438	1.899167
Ti	3.879185	15.109438	0.190247
O	-6.997124	-10.338983	8.668797
O	-1.274613	-9.827384	12.752108
O	-3.401113	-8.712963	10.641049
Ti	-2.230714	-8.396176	12.018769
Ti	-6.028030	-11.223377	7.357395
O	1.932034	-9.911060	12.629564
O	0.126540	-9.479577	10.071081
Ti	0.275960	-10.165510	11.883204

Ti	0.006365	-11.279016	9.348735
O	3.254018	-9.095419	10.192680
Ti	3.523830	-9.266408	11.955327
Ti	5.141002	-10.252200	9.652549
O	4.939201	-10.375305	11.527682
O	-5.674331	-6.291470	12.071242
O	-7.660414	-4.959393	10.416142
Ti	-6.837920	-6.573048	10.600998
O	-8.037097	-7.915294	10.305759
Ti	-8.137505	-8.921134	8.678263
O	-1.768726	-5.074214	12.828634
Ti	-2.036184	-4.831120	14.633146
O	-3.838001	-5.137422	14.310092
O	-3.471741	-5.738649	10.381824
Ti	-4.037213	-5.617537	12.530163
O	-3.173582	-7.306547	13.002116
Ti	-3.735440	-7.307181	9.519751
O	1.334238	-5.438710	12.832910
Ti	1.327684	-5.023863	14.690479
O	-0.346788	-5.598761	15.191905
O	0.033398	-5.626516	9.981738
Ti	-0.236180	-5.467995	11.851091
O	-0.677794	-7.410529	11.514219
Ti	-0.058297	-7.478963	9.479396
O	5.435318	-5.421161	12.854983
O	3.132986	-5.600779	14.551224
O	4.042767	-5.763943	9.959074
Ti	3.601373	-5.656348	12.802254
O	3.628655	-7.451389	12.359185
Ti	3.643895	-7.419271	9.345972
O	7.047796	-5.679932	9.976136
Ti	6.927897	-5.623230	11.872042
O	7.413183	-7.357793	11.761333
Ti	7.376647	-7.578312	9.876153
O	-9.226201	-2.577132	12.199617
O	-11.868136	-3.544149	10.570506
Ti	-12.695560	-3.552718	8.906961
O	-4.050745	-1.660588	13.958333
Ti	-5.588765	-1.610337	15.278670
O	-7.219964	-2.289119	14.460550
O	-7.647423	-1.500893	10.162364
Ti	-7.628263	-1.728837	12.845086
O	-5.975687	-2.154521	12.047013
Ti	-7.499565	-3.317576	9.585765
O	-2.063789	-1.747779	12.390199
O	-1.942756	-3.127803	15.155560
Ti	-2.111765	-1.494962	14.266236
O	-5.157521	-2.273056	16.706858
O	-3.717713	-1.890361	10.019798
Ti	-4.227093	-1.858089	12.040217
O	-3.951064	-3.772786	11.694524
Ti	-3.734909	-3.742291	9.758334
O	1.786101	-1.795403	12.420047

O	1.459469	-3.301920	15.110518
Ti	1.768797	-1.624511	14.276897
O	-0.137180	-1.500395	13.898213
O	0.034176	-1.811514	9.900197
Ti	-0.225462	-1.731518	11.980012
O	-0.115415	-3.627467	11.474607
Ti	0.006767	-3.631368	9.475163
O	5.547152	-1.735752	12.280773
Ti	5.593075	-1.728116	14.069168
O	3.726391	-2.118539	14.037659
O	3.716853	-1.979688	10.035704
Ti	3.645052	-2.029987	11.935060
O	3.530946	-3.913562	11.676829
Ti	3.754639	-3.920190	9.594351
O	9.669407	-2.182129	11.952263
O	7.343657	-2.335426	13.962479
O	7.389386	-1.893550	10.233811
Ti	7.867561	-1.970834	12.213528
O	7.725823	-3.949523	11.626880
Ti	7.513602	-3.706762	9.638000
O	11.605343	-0.412919	11.147555
Ti	10.545667	-1.782789	10.407059
O	-9.722702	1.682487	11.773938
O	-11.125389	-0.779934	10.846069
Ti	-10.408308	-2.457416	10.829247
O	-5.983770	1.950121	12.058943
O	-5.978833	0.247635	15.404047
Ti	-6.265140	1.278592	13.975127
O	-7.586737	2.506680	13.944361
O	-7.558424	1.883655	10.096249
Ti	-8.007580	2.347902	12.094754
O	-7.431483	0.092671	12.961456
Ti	-7.523797	0.145977	9.345300
O	-2.105074	1.924963	12.311886
O	-2.146377	0.205478	14.949658
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1785

PBE

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Ti	0.339554	2.443605	-0.859968
O	0.330007	4.319018	-1.275113
Ti	0.314639	4.357297	-3.248220
O	-1.559062	2.394932	-0.461186
O	-1.575836	4.311532	-3.700405
O	-1.559388	4.341444	-7.694282
Ti	-1.552600	4.356136	-5.672972
O	-1.591679	2.440911	-6.089414
Ti	-1.679707	2.461046	-8.073849
O	4.155032	4.425986	-5.276569

O	4.142675	2.454126	1.126066
O	4.151037	2.452231	-2.871877
Ti	4.144901	2.469674	-0.849182
O	4.139426	4.346032	-1.274819
Ti	4.170590	4.364886	-3.251599
O	2.242914	2.414380	-0.462417
O	2.244497	4.364501	-3.685007
O	2.178480	4.386512	-7.680894
Ti	2.238705	4.416302	-5.640996
O	2.249949	2.485885	-6.071064
Ti	2.224895	2.510190	-8.050663
O	7.947151	4.290982	-5.304640
O	7.941762	2.449551	1.121202
O	7.992748	2.459676	-2.866969
Ti	7.953710	2.466682	-0.828965
O	7.956112	4.352686	-1.291045
Ti	7.977189	4.372846	-3.277081
O	6.048969	2.442980	-0.463258
O	6.062462	4.364573	-3.703013
O	6.103374	4.409723	-7.709197
Ti	6.036275	4.430912	-5.707510
O	6.036911	2.499040	-6.102511
Ti	6.130473	2.539640	-8.087186
O	11.797944	4.607470	-5.463824
O	11.798965	2.458130	1.151325
O	11.805372	2.462407	-3.025532
Ti	11.781122	2.476640	-0.714828
O	11.754842	4.288453	-1.330254
Ti	11.936846	4.420087	-3.376368
O	9.873702	2.452334	-0.442542
O	9.898940	4.376008	-3.803224
O	10.194082	4.238091	-7.814065
Ti	9.815145	4.358180	-5.683461
O	9.972160	2.421874	-6.137460
Ti	10.043306	2.264611	-8.175470
O	15.713970	2.404743	1.121537
O	16.209711	4.077703	-1.298030
Ti	15.572536	2.542871	-0.690134
O	15.912434	7.812927	-1.072722
Ti	15.707231	5.961342	-1.204317
O	13.744208	2.595089	-0.446525
O	16.172665	3.723697	-5.171998
O	14.762987	1.800013	-9.274771
Ti	15.117715	5.103725	-4.437385
O	17.099211	1.672012	-7.327417
Ti	15.695256	0.816459	-8.111916
O	-16.428534	4.723014	0.780025
O	-15.334057	6.081729	-1.852218
Ti	-16.367373	4.868804	-1.047796
O	-17.548162	4.296971	-2.373284
O	-11.250065	7.827666	-5.177655
O	-11.016803	6.059096	1.146663
O	-11.093714	6.119344	-2.816282

Ti	-10.894563	6.234766	-0.919461
O	-11.033276	8.046005	-1.207610
Ti	-11.428575	8.139280	-3.197916
O	-12.816013	5.876094	-0.693445
O	-13.201938	7.637248	-3.095437
Ti	-13.537928	6.008347	-2.378536
O	-13.353436	5.779084	-5.918528
Ti	-11.635741	6.281086	-6.161910
O	-7.305188	8.111634	-5.338045
O	-7.215653	6.136674	1.184266
O	-7.270579	6.093340	-2.838317
Ti	-7.196912	6.127811	-0.861902
O	-7.282011	8.038101	-1.325813
Ti	-7.214462	8.038960	-3.328924
O	-9.077130	6.153574	-0.357839
O	-9.205958	8.018047	-3.601682
O	-9.386721	8.450046	-8.369967
Ti	-9.213656	8.170451	-5.384871
O	-9.293806	6.434654	-6.314171
Ti	-9.496369	6.634780	-8.289780
O	-3.442878	8.152569	-5.320347
O	-3.480546	6.209238	1.134730
O	-3.464054	6.188803	-2.862754
Ti	-3.477179	6.263304	-0.866499
O	-3.543078	8.120032	-1.309478
Ti	-3.496676	8.110865	-3.275618
O	-5.362903	6.197677	-0.429673
O	-5.348409	7.958467	-3.784514
O	-5.249687	8.070337	-7.752285
Ti	-5.361830	8.224884	-5.772053
O	-5.355248	6.191371	-6.113857
Ti	-5.422891	6.257342	-8.027853
O	0.317679	8.124696	-5.231541
O	0.309676	6.259264	1.154743
O	0.302337	6.230861	-2.838230
Ti	0.305746	6.274976	-0.829422
O	0.295085	8.133218	-1.244573
Ti	0.303484	8.154826	-3.216544
O	-1.588537	6.211943	-0.441754
O	-1.599265	8.133817	-3.690517
O	-1.486463	8.173257	-7.695793
Ti	-1.597355	8.172850	-5.686256
O	-1.550965	6.252794	-6.134603
Ti	-1.522747	6.265406	-8.095148
O	4.142533	8.149221	-5.225430
O	4.119174	6.286132	1.166026
O	4.146482	6.262347	-2.824446
Ti	4.086702	6.282208	-0.806947
O	4.116372	8.156099	-1.208838
Ti	4.175515	8.154066	-3.200465
O	2.214613	6.223458	-0.423214
O	2.222608	8.140023	-3.643731
O	2.226130	8.164327	-7.658373

Ti	2.175294	8.190053	-5.584781
O	2.223429	6.270935	-6.111444
Ti	2.245720	6.282096	-8.095676
O	7.968702	8.433599	-5.263719
O	7.916352	6.268295	1.136361
O	7.904500	6.249508	-2.860967
Ti	7.850404	6.256047	-0.805520
O	7.996565	8.156962	-1.223734
Ti	8.011825	8.169948	-3.137422
O	6.013224	6.257464	-0.431332
O	6.062950	8.180641	-3.649619
O	6.077744	8.208281	-7.678947
Ti	5.969970	8.175999	-5.643348
O	6.173514	6.303839	-6.107750
Ti	6.283318	6.415175	-8.130181
O	14.305794	5.938174	-5.901202
O	11.786933	6.208880	1.071377
O	11.823154	6.214901	-2.818912
Ti	11.635670	6.102037	-0.809519
O	11.995219	8.058244	-1.028695
Ti	12.126386	8.152283	-3.241255
O	9.835018	6.223056	-0.465201
O	9.832708	8.013877	-3.559456
O	11.774024	6.583027	-7.747828
Ti	10.136211	7.932376	-5.392113
O	9.648854	6.254509	-6.224093
Ti	10.077431	5.998778	-8.216397
O	13.877456	6.159041	-0.765947
Ti	14.188025	8.377794	-0.953085
O	13.737158	4.268202	-3.604824
O	13.848622	8.234221	-2.832777
Ti	12.854589	5.403137	-6.845854
O	15.899984	6.011171	-3.139897
O	-9.167849	10.138249	-0.633373
O	-11.461266	9.904058	-2.830800
Ti	-11.300994	10.167503	-0.988666
O	-10.941855	11.995647	-0.953040
Ti	-9.200444	12.363733	-0.655949
O	-13.022304	10.083877	-0.287498
O	-7.158487	11.850471	-5.624283
O	-7.277306	9.625263	0.966594
O	-7.145112	9.829927	-3.007076
Ti	-7.298548	9.927549	-1.176237
O	-5.681163	13.740784	-0.742129
Ti	-7.447249	12.637133	-3.632927
O	-7.786564	11.957889	-1.882122
O	-9.159578	12.629329	-4.434491
O	-9.152048	11.584778	-7.875761
Ti	-8.915599	11.644795	-5.981375
O	-9.434022	9.959705	-5.684835
Ti	-8.707978	10.151742	-8.917775
O	-3.505407	11.894840	-5.322418
O	-3.621499	10.034237	1.062716

O	-3.641914	10.011813	-2.914629
Ti	-3.596781	10.160793	-0.937487
O	-3.595828	11.977379	-1.371956
Ti	-3.731933	11.911987	-3.380626
O	-5.493672	10.197433	-0.555827
O	-5.495884	12.138021	-3.754127
O	-5.075260	11.857657	-7.842318
Ti	-5.289328	12.177907	-6.014038
O	-5.278250	9.977777	-6.236486
Ti	-5.103619	10.104224	-8.224835
O	0.216611	12.113949	-5.319715
O	0.212437	10.049780	1.133316
O	0.253142	10.022616	-2.832635
Ti	0.257054	10.133526	-0.828907
O	0.157403	11.970690	-1.282105
Ti	0.098500	11.927211	-3.234982
O	-1.676141	10.033119	-0.478222
O	-1.660679	11.790158	-3.751366
O	-1.879651	11.991627	-7.683258
Ti	-1.632984	11.946022	-5.745275
O	-1.518710	10.087875	-6.113073
Ti	-1.441993	10.065751	-8.127961
O	4.075885	11.880044	-5.125747
O	4.103567	10.173395	1.212511
O	4.091925	10.029839	-2.774868
Ti	4.181134	10.094569	-0.700061
O	4.026952	11.976530	-1.214493
Ti	3.906096	11.853378	-3.165760
O	2.177497	10.051711	-0.405209
O	2.088711	11.848609	-3.579610
O	2.366938	12.067008	-7.500214
Ti	2.141827	12.064509	-5.575262
O	2.180341	10.040208	-5.996664
Ti	2.320988	10.019075	-7.934677
O	7.914673	11.754243	-5.100557
O	7.996343	10.039513	1.235959
O	8.160422	10.114593	-2.738785
Ti	8.036981	10.152552	-0.691024
O	7.846180	11.957973	-1.015192
Ti	7.266622	14.906106	-2.165344
O	6.064459	9.988891	-0.364735
O	5.936525	11.925452	-3.416468
O	5.937452	12.117356	-7.430549
Ti	5.895765	12.210043	-5.616213
O	6.120565	10.074319	-5.988019
Ti	6.096125	10.355206	-7.982525
O	11.858077	9.546248	1.677129
O	11.919811	7.879766	-5.054733
Ti	11.772970	9.893024	-0.969410
O	11.633093	9.951277	-2.728116
O	10.008025	10.255828	-0.238199
O	8.155428	13.736334	-3.144030
Ti	7.670218	11.909683	-3.159504



O	10.049650	9.604986	-6.142672
Ti	8.318887	10.170465	-6.097570
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O	-7.054668	14.317439	1.746953
O	-7.206274	14.358813	-3.161213
Ti	-7.119946	14.695086	-1.306357
O	-8.754033	14.144029	-0.685630
O	-2.548460	16.425617	-7.128141
O	-3.848086	14.302716	0.900130
O	-3.289256	13.799627	-3.061452
Ti	-3.763575	13.976274	-1.020659
O	-3.889936	15.734316	-1.602750
Ti	-3.231900	15.622736	-3.333476
O	-6.534341	16.111134	-0.244553
O	-4.127694	15.998323	-4.833641
O	-5.195262	13.924342	-6.067674
Ti	-3.664878	15.069864	-6.413283
O	0.555395	16.109186	-6.848248
O	0.078534	14.056635	1.118066
O	0.050162	13.856517	-2.923254
Ti	0.053698	14.061755	-0.875604
O	0.263147	15.798779	-1.354170
Ti	0.132231	15.699166	-3.203489
O	-1.828008	13.960538	-0.481242
O	-1.543414	16.261026	-3.627125
Ti	-1.062579	15.437635	-7.270058
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O	3.912544	13.963470	-2.926870
Ti	3.782019	13.952441	-0.962366
O	1.414410	16.158527	-4.337832
Ti	4.822243	15.102851	-4.235304
O	1.992708	13.889463	-0.502036
O	3.882720	16.118410	-5.389364
Ti	2.182056	15.575934	-6.043173
O	2.222277	13.870562	-5.502255
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O	6.232420	14.705418	1.426302
O	6.106250	15.923817	-3.199253
Ti	7.092956	13.518964	0.189177
O	5.997148	13.857989	-1.222049
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O	8.183415	14.792687	-0.534215
O	-3.925627	-15.017015	4.457558
Ti	-3.292603	-13.863855	7.873509
O	-4.526704	-14.966587	7.145048
O	-6.948545	-13.572649	2.150868
Ti	-4.995932	-13.918652	5.665257
O	-1.288310	-16.443275	4.372700
O	0.468669	-15.621189	8.096977
Ti	-0.372333	-14.191553	7.293111
O	-1.862866	-14.649812	6.336515

O	-1.002487	-14.765331	2.517537
Ti	-2.169904	-14.803200	4.413474
Ti	0.153204	-16.051348	3.339858
O	4.336480	-15.078105	4.524324
Ti	2.198559	-15.253628	8.497807
O	3.020049	-15.478169	6.886837
O	2.221674	-15.002047	1.509442
Ti	2.801829	-14.556057	5.311449
Ti	5.186292	-15.947873	0.275783
O	5.788469	-14.824389	1.525027
Ti	5.424315	-13.685973	5.089931
O	-11.092151	-10.914573	4.627138
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O	-7.301395	-11.087076	4.438928
O	-6.636127	-13.224216	6.207928
O	-7.207631	-11.085150	8.263185
Ti	-7.115754	-11.473493	6.456719
O	-9.101192	-11.339846	6.122243
O	-8.683088	-11.027226	2.001355
Ti	-9.262956	-11.144123	4.020166
O	-9.513115	-12.877144	3.420570
Ti	-8.549091	-12.851269	1.830396
O	-3.459925	-10.656857	4.455313
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Ti	-3.859548	-11.548431	10.061362
O	-3.542243	-10.840216	8.378029
Ti	-3.366914	-10.722779	6.329796
O	-4.026669	-13.276670	9.433823
O	-5.388230	-10.757482	6.025363
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Ti	-5.457544	-10.796972	4.116975
O	-5.075111	-12.743416	3.909477
Ti	-5.248091	-12.818642	2.049294
O	0.317039	-11.041391	4.332265
O	0.362043	-13.129467	10.815528
O	0.630387	-13.089664	6.293584
Ti	-0.541703	-11.932215	9.823574
O	0.154068	-11.155390	8.230208
Ti	0.449082	-11.155278	6.258081
O	-1.416505	-13.344175	8.578780
O	-1.553462	-11.113670	6.029765
O	-1.534996	-11.140805	2.068831
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O	4.221525	-11.104576	8.114877
Ti	4.150280	-11.033039	6.340173
O	2.031529	-13.430516	8.656785
O	2.290991	-10.964114	5.852137
O	2.264464	-11.021479	1.865845

Ti	2.416516	-10.963988	3.839749
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Ti	2.349809	-13.002517	1.688751
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O	6.670302	-14.069789	6.354146
O	7.544722	-11.634729	8.305792
Ti	7.482234	-12.432046	6.684966
O	2.661227	-15.166466	10.317825
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O	6.094525	-10.958763	1.828976
Ti	6.193732	-10.837725	3.716814
O	6.031390	-12.928545	3.456363
Ti	6.124165	-13.013211	1.593078
O	11.778337	-8.532635	0.909128
O	9.047318	-12.524236	5.822397
O	9.884360	-10.816254	0.972478
Ti	9.669794	-11.413343	4.476439
O	10.311962	-12.487390	3.123250
Ti	9.672016	-12.531476	1.368763
O	-11.006952	-7.085060	4.048823
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Ti	-10.837525	-8.832826	8.419873
O	-10.626816	-8.866517	6.528075
Ti	-11.368022	-7.006562	6.020629
O	-13.102882	-7.095729	5.652555
O	-13.074702	-5.121835	3.003920
Ti	-13.686265	-6.636846	3.873802
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Ti	-11.398389	-7.300672	2.174753
O	-7.157246	-7.223835	4.352269
O	-7.207934	-8.715214	10.764652
O	-7.278107	-8.988815	6.782024
Ti	-7.102987	-9.279202	8.593168
O	-7.448864	-7.099448	8.444533
Ti	-7.277811	-7.149313	6.374307
O	-9.208802	-8.792008	9.164129
O	-9.099550	-6.988950	5.865209
O	-9.189141	-7.258469	1.993951
Ti	-8.964220	-7.215298	4.008332
O	-9.164519	-9.167380	3.571145
Ti	-8.958605	-9.145632	1.598595
O	-3.404357	-7.137266	4.313912
O	-3.445390	-9.378058	10.664688
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Ti	-3.382351	-8.834829	8.738601
O	-3.538386	-7.033611	8.305842
Ti	-3.420693	-6.995934	6.285974
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O	-5.172450	-7.167510	1.882615
Ti	-5.238336	-7.101221	3.935961
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Ti	-5.244789	-8.974520	1.513297

O	0.393991	-7.175818	4.270340
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O	0.422903	-9.189556	6.730896
Ti	0.412715	-9.163723	8.626244
O	0.456873	-7.245132	8.258123
Ti	0.414050	-7.212765	6.301469
O	-1.509826	-8.948679	9.085912
O	-1.484569	-7.186922	5.872388
O	-1.569521	-7.209684	1.864507
Ti	-1.422858	-7.173571	3.908634
O	-1.507526	-9.082082	3.492473
Ti	-1.541899	-9.053395	1.561587
O	4.184212	-7.142316	4.245607
O	4.344570	-9.612216	10.644006
O	4.278515	-9.165764	6.573838
Ti	4.309546	-9.246821	8.589448
O	4.082681	-7.259890	8.215314
Ti	4.195694	-7.196130	6.268392
O	2.214089	-9.337314	9.207042
O	2.296493	-7.267944	5.842940
O	2.255593	-7.162755	1.854813
Ti	2.378292	-7.165798	3.858078
O	2.222732	-9.080812	3.430632
Ti	2.268352	-9.099883	1.480378
O	8.010401	-7.182225	4.240723
O	7.789336	-9.686405	10.559674
O	8.188070	-9.193241	6.785345
Ti	8.022823	-9.886610	8.680164
O	8.119344	-7.181092	8.287602
Ti	7.972566	-7.310648	6.388725
O	6.063807	-9.060092	8.875981
O	6.097456	-7.294791	5.842572
O	6.095064	-7.103464	1.837469
Ti	6.234573	-7.112469	3.883553
O	6.079009	-9.009938	3.396161
Ti	6.125860	-9.010318	1.390092
O	11.823017	-7.100690	3.896452
O	10.720451	-10.360953	5.600228
O	12.397530	-5.846859	9.304711
Ti	10.272395	-9.183702	6.890954
O	9.817101	-9.926706	8.542140
O	9.851452	-7.458984	5.890877
O	9.732365	-7.056950	1.846928
Ti	10.007540	-7.382201	3.850689
O	10.030418	-9.111718	3.193551
Ti	10.048838	-8.851674	1.315837
O	11.716597	-8.198072	7.525373
O	13.541979	-5.812216	-0.647715
Ti	11.562078	-6.406566	7.745707
O	14.032467	-7.247084	1.681597
Ti	13.191974	-7.676148	0.057061
O	-15.324970	-1.602662	5.819987
Ti	-14.487700	-0.471197	6.986548

O	-11.010424	-3.380466	4.217883
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Ti	-11.017235	-5.212496	8.612022
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Ti	-11.418297	-3.335532	6.031220
O	-11.553956	-7.134190	8.217926
O	-13.219682	-3.541363	5.710651
O	-15.402905	-3.508653	3.464966
Ti	-14.375483	-2.608296	4.636032
O	-15.292001	-6.179004	3.383276
Ti	-14.660995	-4.707923	2.206979
O	-7.225548	-3.365644	4.335277
O	-7.135043	-5.802870	10.691182
O	-7.114472	-5.254149	6.812758
Ti	-7.132830	-5.126165	8.719842
O	-7.411323	-3.345881	8.346318
Ti	-7.365594	-3.319866	6.277377
O	-9.322251	-5.329803	9.301358
O	-9.166949	-3.433088	5.911713
O	-9.091436	-3.447532	1.878323
Ti	-9.232443	-3.446254	3.952282
O	-9.035928	-5.321118	3.479959
Ti	-9.062729	-5.252943	1.502070
O	-3.422737	-3.341203	4.267814
O	-3.355922	-5.186687	10.656200
O	-3.364833	-5.193320	6.666134
Ti	-3.340971	-5.117397	8.701396
O	-3.389790	-3.304653	8.244611
Ti	-3.450971	-3.229730	6.248257
O	-5.334017	-5.068272	9.142210
O	-5.311512	-3.350518	5.887425
O	-5.357964	-3.356116	1.888188
Ti	-5.375588	-3.328010	3.950565
O	-5.356295	-5.262273	3.476805
Ti	-5.300240	-5.177527	1.492317
O	0.388070	-3.343915	4.263386
O	0.384983	-5.296687	10.560575
O	0.407814	-5.312407	6.632326
Ti	0.439775	-5.280693	8.585201
O	0.347033	-3.373189	8.230790
Ti	0.384831	-3.317192	6.263841
O	-1.507932	-5.320722	8.991750
O	-1.508789	-3.336316	5.846655
O	-1.526775	-3.340897	1.874344
Ti	-1.521717	-3.337104	3.898017
O	-1.511155	-5.268776	3.453741
Ti	-1.530750	-5.200028	1.511760
O	4.193062	-3.341417	4.289139
O	4.153129	-5.246741	10.583355
O	4.221126	-5.312512	6.632893
Ti	4.202445	-5.359956	8.640981
O	4.220466	-3.408939	8.259924

Ti	4.220532	-3.366461	6.306458
O	2.278971	-5.256866	8.960633
O	2.288262	-3.371690	5.868727
O	2.254031	-3.323802	1.888209
Ti	2.301389	-3.327983	3.900357
O	2.278293	-5.253554	3.461667
Ti	2.264021	-5.252543	1.514974
O	7.999056	-3.283108	4.279230
O	7.977458	-5.269765	10.587102
O	7.938056	-5.320515	6.609542
Ti	8.030173	-5.403225	8.715068
O	8.154691	-3.425528	8.284773
Ti	8.064712	-3.469918	6.399585
O	6.090152	-5.314605	8.991874
O	6.104507	-3.338999	5.889806
O	6.047822	-3.294335	1.903927
Ti	6.104809	-3.295696	3.936502
O	6.121967	-5.217251	3.475840
Ti	6.074119	-5.207430	1.518910
O	11.836672	-3.271549	4.255080
O	10.489360	-3.933977	11.148290
O	12.090374	-5.211993	6.514647
Ti	11.289371	-4.431637	9.592221
O	12.066079	-3.224683	8.407332
Ti	12.049602	-3.325150	6.334156
O	10.083076	-5.361912	8.533728
O	9.943313	-3.420222	5.879999
O	10.008575	-3.268161	1.851575
Ti	9.843588	-3.321335	3.995363
O	9.859142	-5.193589	3.466172
Ti	9.904570	-5.150247	1.616223
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O	12.028379	-4.968351	-2.747987
Ti	13.612926	-3.195141	3.976307
O	14.047075	-4.977729	3.599365
Ti	13.039216	-6.264623	2.834012
O	-15.106182	0.497226	3.465656
O	-15.613722	0.673931	7.692799
O	-15.961187	2.128649	10.301292
Ti	-15.401518	2.252958	8.776471
O	-16.904465	2.346237	2.485657
Ti	-16.103222	0.734257	1.930854
O	-11.174839	0.412586	4.286526
O	-11.322941	-1.630560	10.361567
O	-11.315154	-1.539386	6.561594
Ti	-11.784131	-1.548511	8.541224
O	-11.499689	0.367508	8.216481
Ti	-11.163429	0.508503	6.252889
O	-13.562873	-1.406141	8.308997
O	-13.255998	0.420046	5.811224
O	-12.790585	0.390239	1.946666
Ti	-13.315163	0.595852	3.876624

O	-13.236354	-1.506277	3.597960
Ti	-12.702618	-1.517561	1.750389
O	-7.292912	0.429418	4.305839
O	-7.317341	-1.512496	10.647458
O	-7.230124	-1.481713	6.665214
Ti	-7.208256	-1.434524	8.758600
O	-7.228990	0.408568	8.250587
Ti	-7.305896	0.413397	6.265529
O	-9.219629	-1.400028	8.886889
O	-9.250020	0.371664	5.898925
O	-9.241099	0.427204	1.907517
Ti	-9.347815	0.392353	3.948111
O	-9.118123	-1.497654	3.501433
Ti	-9.041740	-1.457208	1.584185
O	-3.459798	0.473303	4.316926
O	-3.456269	-1.588136	10.691883
O	-3.443819	-1.403195	6.679879
Ti	-3.448806	-1.403908	8.724613
O	-3.506020	0.462729	8.299541
Ti	-3.469113	0.545589	6.322772
O	-5.353752	-1.543298	9.112401
O	-5.375603	0.466762	5.893784
O	-5.330794	0.472167	1.924544
Ti	-5.432928	0.483859	3.944795
O	-5.343032	-1.450608	3.494285
Ti	-5.291895	-1.381974	1.538331
O	0.350048	0.477120	4.311459
O	0.366080	-1.413432	10.609930
O	0.377989	-1.446869	6.655231
Ti	0.442857	-1.470784	8.680722
O	0.368661	0.449316	8.281943
Ti	0.355368	0.482081	6.307447
O	-1.553956	-1.420722	9.048368
O	-1.558928	0.488140	5.902613
O	-1.558211	0.495988	1.920571
Ti	-1.602923	0.491392	3.935682
O	-1.532580	-1.433501	3.481003
Ti	-1.518936	-1.378454	1.524523
O	4.157793	0.497695	4.341194
O	4.190913	-1.482308	10.725682
O	4.182661	-1.477672	6.720070
Ti	4.318998	-1.534098	8.745896
O	4.195191	0.400096	8.344853
Ti	4.170248	0.405789	6.337763
O	2.287872	-1.484682	9.056921
O	2.250972	0.460912	5.905418
O	2.248878	0.508726	1.923572
Ti	2.226022	0.508904	3.928897
O	2.283424	-1.421657	3.492338
Ti	2.277519	-1.420700	1.533094
O	7.937141	0.477478	4.345598
O	8.054375	-1.885349	10.779518
O	8.067735	-1.460399	6.745738

Ti	8.411431	-1.516829	8.831122
O	8.080905	0.438389	8.380722
Ti	7.962915	0.345057	6.439683
O	6.114941	-1.497455	9.187939
O	6.061674	0.419333	5.934419
O	6.042261	0.526505	1.938580
Ti	6.034924	0.523381	3.944445
O	6.064086	-1.399605	3.505194
Ti	6.093620	-1.401621	1.549162
O	11.777854	0.575777	4.254207
O	12.495041	-1.001305	10.597901
O	11.829288	-1.395896	6.591428
Ti	12.376315	-1.315327	8.779311
O	11.839211	0.473330	8.241745
Ti	11.717985	0.456553	6.372104
O	10.092197	-1.480304	9.031682
O	9.863321	0.541233	5.902778
O	9.783913	0.552847	1.960089
Ti	9.747687	0.522118	3.942232
O	9.899734	-1.388774	3.535652
Ti	9.969692	-1.332867	1.600489
O	16.464037	0.313460	7.303970
Ti	14.853288	0.371458	7.549552
O	14.089931	-1.175832	8.359343
O	13.796567	0.527181	5.855542
O	13.780269	0.632813	2.004857
Ti	13.536999	0.673897	4.038188
O	14.060242	-1.281706	3.553724
Ti	13.996569	-1.182449	1.629427
O	-15.126727	4.242386	3.684602
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Ti	-15.658423	3.600646	2.052624
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O	-11.261919	2.148610	10.484712
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Ti	-11.577083	2.242964	8.684067
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Ti	-11.046865	4.449853	6.371967
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O	-13.173920	4.386928	6.037386
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Ti	-13.330303	4.249930	4.147306
O	-13.083505	2.421558	3.467769
Ti	-12.832252	2.304490	1.324131
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O	-7.354576	2.115011	10.622972
O	-7.283651	2.317563	6.660832
Ti	-7.209544	2.277313	8.732967
O	-7.258986	4.179630	8.320966
Ti	-7.265221	4.190044	6.353112
O	-9.284469	2.201383	8.884278
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O	-9.089405	4.261635	2.043570
Ti	-9.336869	4.165043	4.031375
O	-9.199864	2.300527	3.552335
Ti	-9.082126	2.357690	1.568378
O	-3.479242	4.304419	4.394014
O	-3.516335	2.353132	10.727009
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Ti	-3.504218	2.387967	8.771826
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Ti	-3.470441	4.359805	6.428777
O	-5.386158	2.312193	9.104535
O	-5.382535	4.311838	5.971795
O	-5.333541	4.297063	1.994301
Ti	-5.444094	4.318119	3.993008
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Ti	-5.312707	2.433613	1.585259
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O	0.311574	2.357189	10.710435
O	0.325943	2.377658	6.721418
Ti	0.299917	2.312560	8.788477
O	0.235902	4.236818	8.355097
Ti	0.336267	4.249590	6.368204
O	-1.586788	2.323891	9.108785
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Ti	-1.647018	4.316729	3.982091
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Ti	-1.541736	2.434349	1.559612
O	4.111005	4.264688	4.346157
O	4.226760	2.461851	10.796953
O	4.157847	2.295197	6.763203
Ti	4.169200	2.236539	8.831807
O	4.160360	4.140968	8.329865
Ti	4.165827	4.134027	6.301057
O	2.274752	2.338856	9.154148
O	2.203689	4.244450	5.941097
O	2.210682	4.341994	1.965701
Ti	2.173617	4.344313	3.961966
O	2.223141	2.406211	3.522892
Ti	2.254016	2.408832	1.557974
O	7.920343	4.342114	4.360115
O	8.034307	2.610228	10.756824
O	7.898494	2.369873	6.769373
Ti	7.990664	2.360513	8.667636
O	7.853112	4.304911	8.333737
Ti	8.020519	4.310195	6.363473
O	6.098091	2.236580	9.243164
O	6.013297	4.252536	5.929689
O	6.029624	4.359814	1.958354
Ti	6.020690	4.346742	3.968524
O	6.060297	2.421498	3.527872
Ti	6.066161	2.428767	1.560838
O	11.720160	4.358180	3.980715

O	11.814474	1.814381	10.583144
O	11.946430	2.432410	6.749581
Ti	12.514359	2.276901	8.725279
O	12.469322	4.139304	8.491090
Ti	12.030700	4.377281	6.773640
O	9.861519	2.582864	8.937579
O	9.897618	4.255605	5.944322
O	9.778774	4.336714	1.928588
Ti	9.812472	4.272895	4.057747
O	9.824871	2.423918	3.546668
Ti	9.890830	2.494578	1.570001
O	15.877686	5.841286	0.760888
O	14.208191	1.867404	8.614156
O	13.585059	4.677320	5.756693
O	13.814325	4.341432	1.918254
Ti	13.420183	4.589099	3.940825
O	13.897903	2.541038	3.638488
Ti	13.952883	2.505098	1.632065
O	-10.986135	8.594465	3.901456
O	-11.181685	6.077502	10.735242
O	-11.025361	6.150548	6.817365
Ti	-11.413467	6.256565	8.831415
O	-11.131686	8.069380	8.660734
Ti	-10.800742	8.920847	7.099510
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Ti	-12.207177	9.821448	4.433530
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Ti	-7.559779	6.006886	8.873637
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Ti	-7.347839	8.006633	6.463950
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O	-9.255479	8.334313	6.015643
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Ti	-9.240543	7.990867	4.002937
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Ti	-9.071990	6.126667	1.619453
O	-3.499880	8.088138	4.513800
O	-3.598054	6.554487	11.016231
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Ti	-3.706737	6.225480	8.836772
O	-3.524455	8.113810	8.500995
Ti	-3.502999	8.255040	6.562852
O	-5.481736	6.081859	9.338905
O	-5.441540	8.232587	6.106654
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Ti	-5.389919	8.190742	4.066009
O	-5.380830	6.208161	3.606920

Ti	-5.340830	6.247244	1.649844
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O	0.219462	6.340573	10.863025
O	0.327374	6.221692	6.858099
Ti	0.211418	6.085656	8.827795
O	0.314593	8.054827	8.497961
Ti	0.325344	8.103427	6.435335
O	-1.698615	6.102387	9.301471
O	-1.575022	8.177317	6.040197
O	-1.693538	8.112888	1.959710
Ti	-1.648835	8.125861	4.033175
O	-1.584076	6.233181	3.560131
Ti	-1.587117	6.234318	1.578618
O	4.112906	8.187095	4.424887
O	4.034698	5.794971	10.836392
O	4.018584	6.067679	6.747679
Ti	3.990139	5.895160	8.848018
O	3.771778	7.823547	8.395886
Ti	4.117077	7.872013	6.375974
O	2.083008	5.958883	9.290015
O	2.207963	8.201020	5.985797
O	2.172641	8.174083	1.983665
Ti	2.179835	8.217961	3.982015
O	2.230827	6.252033	3.569654
Ti	2.223438	6.240424	1.602018
O	7.867447	7.979315	4.465924
O	6.454781	4.291973	12.047321
O	7.870471	6.172994	6.704988
Ti	7.523608	6.164255	8.560269
O	7.980048	8.089135	8.395902
Ti	7.848409	8.396606	6.523480
O	5.818166	6.240138	8.982923
O	5.939397	8.025352	6.064882
O	5.989316	8.229162	2.074923
Ti	6.028243	8.211416	3.986939
O	5.978723	6.247920	3.565580
Ti	6.049558	6.266650	1.625185
O	11.710282	8.367284	4.139328
O	11.473550	6.210710	7.123715
Ti	11.189952	7.942633	7.314596
O	12.638443	8.947772	6.765377
Ti	12.637665	9.655209	5.097417
O	8.653166	6.345397	10.136208
O	9.795821	8.283173	6.069955
O	9.752048	8.052706	2.078207
Ti	9.691899	7.983412	4.054754
O	9.884700	6.181776	3.612937
Ti	9.932287	6.241574	1.574561
O	13.973657	9.426547	3.827904
O	14.048408	8.024848	1.081460
Ti	13.108162	8.341934	2.673772
O	13.690064	6.508592	3.163303
Ti	14.220209	6.076401	1.265415

O	-10.975295	9.659915	1.117857
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O	-13.349761	9.963352	2.968525
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O	-7.323640	10.086335	7.248015
Ti	-8.534171	11.450086	7.729340
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Ti	-6.899241	13.246727	6.032146
O	-10.181852	10.562074	7.524819
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O	-8.675014	11.894608	1.078103
Ti	-9.582715	11.806903	4.330331
O	-8.946730	10.364430	3.273414
Ti	-9.073593	9.862698	1.442246
O	-3.225096	11.764882	4.639541
O	-3.328403	10.060072	11.017788
O	-3.418118	10.075036	6.938206
Ti	-3.495883	10.224817	8.907791
O	-3.528831	11.998321	8.521123
Ti	-3.459382	12.211205	6.688250
O	-5.283078	10.087719	9.316298
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O	-5.241419	10.021375	3.599251
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O	0.390520	9.990680	11.019178
O	0.410359	10.056759	7.013481
Ti	0.252563	9.847306	8.924717
O	0.630614	11.953576	8.839292
Ti	0.429374	11.909328	6.308171
O	-1.493474	10.126299	9.284278
O	-1.393894	12.241982	6.641928
O	-1.854139	11.951234	1.937269
Ti	-1.619119	11.881838	3.768515
O	-1.582122	9.973498	3.487406
Ti	-1.717712	9.979149	1.483154
O	4.083568	12.205144	3.597017
O	2.517945	8.032943	11.107527
O	4.337904	9.964443	7.209026
Ti	4.015385	9.469299	8.999219
O	5.157462	9.544263	10.392418
Ti	4.092867	11.765291	6.847926
O	2.327790	10.139210	9.364387
O	2.490721	11.864238	5.863972
O	1.947932	11.997566	1.928532
Ti	2.350599	12.007369	3.880591
O	2.207048	10.073549	3.554248
Ti	2.157728	10.061607	1.530523
O	6.687335	13.018425	3.904999

O	8.067513	9.317713	11.080731
O	7.573561	10.122429	6.285934
Ti	9.237282	8.236859	10.124933
O	10.594857	8.576032	8.941057
Ti	7.042315	11.522232	5.058619
O	6.376934	7.149337	11.712715
O	5.690129	12.186388	6.189781
O	6.266293	12.105663	1.434723
Ti	5.400255	13.297764	2.780719
O	6.333122	10.187256	3.692416
Ti	6.184221	10.196720	1.651045
O	11.752470	11.240020	4.980540
O	10.300250	7.561254	11.535393
O	8.766243	12.202698	5.093003
O	10.282546	11.851540	2.300510
Ti	10.160064	11.590343	4.110328
O	9.576308	9.927115	3.685623
Ti	10.127416	10.067542	1.712268
O	-6.314893	14.903185	5.483979
O	-9.264835	13.186547	3.271344
Ti	-7.618929	12.791243	2.389588
O	-3.403463	16.143944	4.574233
O	-3.141882	14.004054	6.670734
Ti	-1.314906	14.212256	6.959421
O	-5.418607	16.227545	2.601571
Ti	-4.995376	15.353327	4.189915
O	-4.609727	13.722692	3.521111
Ti	-5.604506	15.247810	1.091851
O	0.090775	16.153210	3.667035
O	0.642697	13.771127	6.431994
Ti	-0.241231	13.269888	9.876687
Ti	0.929531	15.179598	4.925245
O	-1.050034	14.452383	8.757422
O	-0.935542	15.567204	5.775138
O	-1.994198	15.798657	2.015630
Ti	-1.732872	15.679982	3.885495
O	-1.627625	13.856888	3.565501
Ti	-1.943804	14.111412	1.481383
O	4.449422	17.191420	2.345515
O	3.769215	12.435735	8.522566
Ti	2.399684	12.261105	9.773749
O	1.434956	13.733727	10.390134
O	2.377563	16.243809	5.107048
O	2.547359	15.648403	1.913070
Ti	3.381069	16.224297	3.495864
O	1.724981	13.857557	3.675614
Ti	1.911141	13.871226	1.554547
O	4.233212	15.737921	-0.543100
O	4.545839	14.887768	3.487506
Ti	4.561899	15.666806	1.227885
O	-5.311923	-11.038070	11.042497
O	-2.075273	-11.499223	10.761106
O	2.837088	-11.834399	11.125186

O	-9.587815	-6.879705	11.484012
Ti	-8.270703	-7.285328	10.303810
O	-3.009315	-7.276141	13.983195
O	-4.708492	-7.231249	11.436945
Ti	-4.660426	-7.231020	13.262731
O	-5.456296	-8.909364	13.106172
Ti	-5.406852	-9.188260	11.292542
O	0.441845	-7.408633	13.845016
O	-1.363048	-7.378916	11.333215
Ti	-1.272433	-7.424722	13.228888
O	-1.440973	-9.301318	12.900959
Ti	-1.539905	-9.377003	11.135476
O	3.884671	-7.349922	13.708138
O	2.191452	-7.194843	11.241588
Ti	2.128794	-7.513155	13.018930
O	2.198900	-9.368831	12.653164
Ti	2.539078	-10.027953	11.023907
O	5.766440	-7.187854	11.191996
Ti	5.548487	-7.235982	13.070191
Ti	6.179860	-9.048866	11.013569
O	6.243399	-8.914315	12.885363
O	-7.487316	-3.582638	13.905985
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Ti	-9.171633	-3.215761	13.267207
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Ti	-10.148729	-5.120418	11.365129
O	-3.015555	-3.191571	13.889629
Ti	-3.171213	-3.115395	15.709553
O	-4.946754	-3.714629	15.414323
O	-5.440640	-3.561911	11.640865
Ti	-5.670842	-3.531934	13.727625
O	-5.390848	-5.502493	13.207644
Ti	-5.264019	-5.290509	11.125239
O	0.396422	-3.267689	14.050886
Ti	0.431843	-2.994465	15.930169
O	-1.369353	-3.631753	16.115028
O	-1.412007	-3.412538	11.360373
Ti	-1.341970	-3.416539	13.202192
O	-1.327750	-5.357034	12.928973
Ti	-1.431883	-5.362475	11.014014
O	3.864067	-3.166115	13.843055
Ti	4.051156	-3.069131	15.655937
O	2.211134	-3.621678	16.044889
O	2.203529	-3.367401	11.389113
Ti	2.173861	-3.479788	13.217178
O	2.167091	-5.327186	12.959424
Ti	2.319555	-5.341815	10.988363
O	8.250501	-3.407313	13.357009
O	5.835352	-3.643312	15.344452
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Ti	6.462747	-3.530298	13.595052
O	6.235179	-5.479204	13.071498
Ti	6.203140	-5.208443	10.974726

O	10.412235	-1.431122	12.330954
Ti	9.308831	-2.735568	11.926295
O	-7.518071	0.260116	13.623141
O	-9.374121	0.252204	11.425100
Ti	-9.218859	0.285256	13.306899
O	-9.793821	-1.508997	13.563124
Ti	-9.529857	-1.529339	10.601036
O	-3.486259	0.288947	13.772774
O	-3.349875	-1.469025	16.351894
Ti	-3.542924	0.271436	15.645181
O	-5.393744	0.244667	15.397587
O	-5.358143	0.267577	11.505427
Ti	-5.599044	0.296535	13.614226
O	-5.512074	-1.661378	13.178924
Ti	-5.439519	-1.491416	11.174015
O	0.380352	0.590318	13.825583
O	0.416566	-1.286039	16.354715
Ti	0.369198	0.574427	15.712504
O	-1.540773	0.354157	15.344228
O	-1.633652	0.439134	11.379972
Ti	-1.566761	0.411675	13.439231
O	-1.312419	-1.463521	12.947145
Ti	-1.577873	-1.393293	11.002616
O	4.216559	0.319797	13.765239
O	4.086634	-1.421199	16.277317
Ti	4.267606	0.369060	15.577741
O	2.290665	0.500692	15.402187
O	2.295821	0.479736	11.418386
Ti	2.292065	0.393553	13.432924
O	2.084464	-1.430835	12.990007
Ti	2.241408	-1.340019	11.045671
O	8.365294	0.058472	14.002252
O	6.138152	0.103096	15.466491
O	6.302229	0.396129	11.526525
Ti	6.552803	0.136673	13.748098
O	6.214059	-1.618559	13.130519
Ti	6.071945	-1.540186	11.119743
O	9.726981	0.968296	11.686085
Ti	9.746823	1.117050	13.537373
O	11.565324	0.691263	13.411238
Ti	11.473674	0.066815	11.677947
O	-7.483261	3.884455	13.909221
O	-9.207816	3.776843	11.457429
Ti	-9.134442	3.794996	13.366603
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Ti	-9.440443	2.048222	10.638514
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O	-5.546471	2.182562	13.126527

Ti	-5.468421	2.370041	11.218048
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Ti	0.366915	4.022665	15.782535
O	-1.726745	4.303603	15.571120
O	-1.685122	4.300544	11.545866
Ti	-1.657929	4.325821	13.547035
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O	4.188780	4.344025	13.545198
O	4.551354	2.233070	15.874849
Ti	5.263219	3.207781	14.553675
O	2.203272	3.942909	15.395473
O	2.058462	4.279012	11.559717
Ti	2.254054	4.164416	13.613082
O	2.361583	2.324470	13.070193
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O	6.742236	4.247956	14.932508
O	8.656819	5.570172	13.159029
Ti	7.769334	4.009582	13.452394
O	6.302917	2.157469	13.364559
Ti	6.220966	2.214766	11.169088
O	10.517476	4.349697	11.265997
O	9.206003	2.835541	13.696084
Ti	10.091285	2.645570	10.706474
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O	-5.626340	5.925294	13.230195
Ti	-5.757299	6.200316	11.402988
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O	-1.653058	8.165855	11.643109
Ti	-1.552924	8.376101	13.496934
O	-1.643486	6.147708	13.238913
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O	2.881816	7.928015	15.444844
O	-0.050122	8.105443	14.572316
Ti	1.334561	7.023051	14.990718
O	1.812397	6.136456	13.335690
Ti	2.041570	6.272282	11.291457
O	5.628174	9.336940	13.370794
Ti	4.012267	8.541503	14.062428
O	4.387275	6.953697	13.365391
Ti	5.237011	5.780432	12.189064
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Ti	-6.973579	9.635930	9.059981
O	-1.225348	12.325606	11.109494
O	-1.379051	10.205371	13.182018
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O	2.893765	11.543006	11.338473
O	2.691811	9.523819	13.259637



Ti 2.162452 9.807545 11.551210

### ANNEALED SPHERICAL TiO<sub>2</sub> NPs (MA IP)

(TiO<sub>2</sub>)<sub>43</sub>

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PBE

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O	-3.42935037	-3.90628669	0.42192968
Ti	-4.12458381	-4.23071516	-1.25180349
O	-0.10205600	-5.04006828	-3.75083721
O	-1.14386901	-6.08743210	0.82646033
O	0.24237712	-4.33541425	-1.01646353
Ti	-1.28147450	-4.52784163	-0.09150219
O	-1.67042357	-2.45029221	-1.38997823
Ti	-1.18907032	-3.83936030	-2.97486651
O	-2.35491060	-4.88748663	-1.75576047
O	-2.23944042	-3.31746652	-4.34356846
Ti	-1.45846667	-1.85745088	-5.18143270
O	2.66698278	-5.73436187	0.15050872
Ti	2.32046817	-4.48135261	-1.13842083
O	2.37771658	-2.91563610	-2.64308268
Ti	1.54066448	-4.17324384	-3.87349750
O	2.38759153	-5.37465979	-2.70630561
O	2.10832347	-3.74444670	-5.57006663
Ti	1.59107634	-2.10682475	-6.23447559
O	-2.98904664	-0.96847873	-5.67573874
O	-3.45409580	-2.13336915	2.68585377
O	-4.02843050	-0.35139457	-2.76160358
Ti	-4.39692751	-0.75295193	-0.93622408
O	-5.20880986	0.93052687	-0.77874268
Ti	-3.12013871	0.15599991	-4.20225706
O	-5.38721443	-1.44750458	0.50977031
O	-4.67994743	-2.63285390	-1.67466661
O	2.68686710	1.75996793	-6.77943235
O	-0.55517714	-1.55100074	1.18334371
O	-1.34259663	-0.41434868	-3.89637541
Ti	-1.00061435	-1.01636273	-0.61837705
O	0.65851460	-1.25236931	-1.32622962
Ti	1.52333579	-1.28132962	-2.89059231
O	-2.82898811	-0.33794163	0.14096809
O	1.02473010	0.68061862	-2.94740105
Ti	1.81828804	2.69402842	-5.43335418
O	-0.22963610	-1.99657585	-6.54108144
O	4.80756957	-0.31917521	-5.09195833
O	1.90922759	-0.42956710	0.71101437
O	5.73648774	-2.10743293	-2.42546953
Ti	5.24868762	-2.37106560	-0.58406280
O	4.66825338	-0.64281170	-0.26393973
Ti	5.10552662	-0.62316271	-3.25588535

O	0.18496790	-2.53051578	-3.74779423
O	1.92392447	-0.85121971	-4.91779539
Ti	3.24115851	0.16876749	-5.91999657
O	2.81090414	-1.14246219	-7.18540691
O	3.95580658	-3.58990228	-0.59705514
O	-3.08264440	2.44562886	0.69485869
O	-2.44868786	1.84969084	-4.13623870
Ti	-5.04732781	2.21160223	0.46512189
O	-4.80731764	3.96232869	-0.15380487
Ti	-0.69146474	1.50296490	-3.64826071
O	-6.52282391	2.08096995	1.60765541
O	1.51211911	4.34963758	-4.60030208
O	-0.61879871	1.33105775	1.01961664
O	3.34922788	-0.29307396	-2.61811988
Ti	-0.43427455	2.24691527	-0.69167801
O	-1.25315233	3.90500791	-0.17248106
Ti	0.97641146	4.50418595	-2.81240252
O	-1.20000910	0.87340815	-1.55614757
O	-0.22908916	3.06587121	-2.59286105
O	0.19959742	1.89383181	-5.19940341
O	3.30700817	1.55352335	1.77255409
O	6.02510515	0.71058490	-2.44188850
Ti	5.33363343	0.96160955	-0.72594051
O	3.87605425	1.98689078	-0.99390667
Ti	2.57949178	1.53951729	-2.47754298
O	1.39760316	1.87059727	-0.54313200
O	2.58059011	3.45792398	-2.33930987
O	2.94238110	1.75477891	-4.32652183
O	3.69979630	4.10509583	0.96957332
O	1.37240848	3.24593021	1.64022609
O	-0.09373520	5.93729127	-2.31638932
Ti	-0.54738254	5.67427154	-0.50952187
O	-2.37777991	6.04148908	-0.36262276
O	1.26800479	4.66984704	-0.76236516
O	-0.72002160	-5.31929968	4.11035450
O	-5.74063551	-3.77261330	2.20838511
O	0.37028494	-2.69448269	3.28888443
O	2.03733053	-3.53097104	5.35994339
O	-1.45273536	-3.87295269	1.86950035
Ti	0.83488807	-4.25557461	4.13802586
O	1.86393896	-5.21393475	3.03689609
Ti	-1.67205716	-5.54698890	2.53733651
O	5.29372746	-0.41798226	2.83999329
O	1.84684053	-3.28977725	0.88468766
Ti	5.00111647	-2.32649298	2.65453307
O	4.48589696	-4.16226961	2.27973381
Ti	2.92244788	-4.66561397	1.62721871
O	-2.96745389	0.81737126	5.76051311
O	-4.36792001	0.78299618	2.05449344
Ti	-3.72591916	2.24787580	4.91913252
O	-6.33125502	-0.81731974	3.14923247
Ti	-5.25369351	-1.97939760	2.19209670
O	3.03720026	-2.00836676	2.94458909

O	4.93863063	-2.57007840	4.51666425
Ti	3.18722607	-2.18738453	4.81159428
O	-0.03202533	0.71185039	5.50290194
O	-1.76557738	-0.07465141	3.06037914
Ti	-1.56958994	-0.05177669	4.93501678
O	-1.61171108	-1.85726148	4.76218120
Ti	-1.65767167	-2.07193108	2.88299492
O	4.91887018	2.81716367	3.29171997
O	2.76524386	-0.49360838	5.37956474
O	1.09548682	0.08490356	3.01511595
Ti	1.62675527	0.77079275	4.66944776
O	6.04998925	-2.49288198	1.05612466
Ti	1.33237960	-1.81106001	1.78902871
O	6.14420711	1.56832131	0.79460202
Ti	5.10729081	1.27202718	2.27893063
O	-3.27682429	4.01049498	5.17557358
O	-3.14152973	4.89545502	2.14218709
O	-5.44057513	1.89813542	4.44860679
Ti	-5.93285869	0.96919073	2.93046691
O	-0.54978347	4.57120473	3.62065954
O	0.19217883	6.09999358	1.16010897
Ti	-2.31890139	4.22025656	3.60079556
O	-2.60765288	2.37930122	3.40650257
Ti	-2.45535188	0.93776158	1.54090399
O	2.38940081	5.04977080	3.22743043
Ti	0.80082246	4.88162022	2.39450997
O	2.25828340	2.34090665	4.15507374
Ti	1.46339382	1.10953229	1.49541534
Ti	3.25388434	3.42549643	2.76786938
Ti	-3.10308559	4.50036324	0.34176812
Ti	2.59722333	3.47523730	-0.27435535

**(TiO<sub>2</sub>)<sub>115</sub>**

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O	1.93168890	-3.29161855	-8.06190220
O	-1.75562931	1.29697182	-6.58075663
O	1.06217195	3.91940910	-8.69611613
O	3.83361277	2.86862747	-7.37534986
O	-1.09159802	-7.76471468	-2.75169445
O	-2.35706284	-9.42933507	2.83914890
Ti	-2.81110746	-8.42142683	1.01992144
O	-3.11427546	-7.23115697	-0.49780358
Ti	-2.73648721	-7.01209016	-3.07904327
O	-4.55242628	-7.46708638	-3.03505826
O	1.38936706	-7.70769246	-4.21860848
O	0.16232773	-8.00078334	3.74054355
O	0.77704207	-9.49601496	-1.72486671
Ti	0.14640690	-9.18117029	-0.04493984
O	0.26152755	-7.34714411	-0.43269352

Ti	0.72236663	-7.80122760	-2.44099670
O	-1.59956646	-9.57827210	0.16293479
O	-0.86878999	-7.38954552	-7.21235442
Ti	-2.18665170	-6.24857461	-6.56837529
O	2.71514312	-7.46727136	-1.82932848
Ti	2.43130922	-6.65878560	-5.16154258
O	1.20053279	-9.53645864	1.43573309
O	2.38536824	-7.50050934	-6.79748483
Ti	0.80602794	-6.65780802	-7.40389359
O	-5.77398401	-3.52868554	-5.88280515
O	-7.22079851	-7.04052132	-1.38526811
O	-6.76824075	-5.19995398	-3.64264482
Ti	-5.95520183	-6.40844425	-2.49003990
O	-8.43309032	-4.64219845	-0.45355591
Ti	-6.33742615	-3.48622330	-4.13032814
O	-3.14982301	-3.89815943	-4.90744480
O	-4.03205469	-5.45059436	1.47150989
O	-2.76317798	-5.33400719	-2.34979484
Ti	-3.36972423	-5.43622238	-0.26811756
O	-3.36569665	-3.47359798	-0.84954621
Ti	-3.10320403	-3.46246686	-2.76949037
O	-5.37555585	-5.41252654	-0.99736412
O	-4.86717490	-3.28671641	-3.11412861
Ti	-4.10582741	-3.92970852	-6.46950732
O	-3.84765802	-5.60727391	-7.15775953
O	0.17055941	-2.90106217	-6.35604907
O	0.54662277	-5.39908937	1.66452597
O	0.96208658	-5.53932259	-2.27442444
Ti	0.33955461	-5.42422372	-0.26360157
O	0.22227617	-3.64189076	-0.87253233
Ti	0.59013522	-3.68195972	-2.86156999
O	-1.52547343	-5.17556678	0.30454027
O	-2.47000182	-6.70992829	-4.85445388
O	-0.48775258	-2.63957393	-9.31439137
Ti	-1.51371541	-2.97301535	-5.56662258
O	-1.32205648	-4.67120264	-6.85141358
Ti	0.08977561	-3.80882602	-8.18968338
O	3.92900236	-3.82286081	-5.89696103
O	4.86444004	-5.62489508	-1.01175465
O	3.52463391	-5.62390157	-3.83361475
Ti	3.16153175	-5.82818510	-1.82450137
O	3.21005851	-3.37956678	-2.20533430
Ti	4.05261079	-3.73586933	-3.90793001
O	2.34361404	-5.21496578	-0.10732827
O	1.82692717	-3.41534798	-4.24936231
O	1.26895362	-5.45412784	-5.98880645
Ti	2.04902507	-3.26307873	-6.10744286
O	0.62706593	-5.53259146	-8.78032269
O	7.27380533	-4.11273210	-0.97586133
Ti	6.64071307	-2.71706205	-1.93102948
O	7.15983934	-1.22134013	-0.63708981
Ti	6.95260095	-0.97495212	-5.04501407
O	4.50717508	-1.71350714	-4.56781693

O	6.67129364	-2.49633190	-6.07593272
Ti	4.91676066	-2.20948709	-6.55337500
O	-6.58210154	0.84266301	-4.86146615
O	-7.05563340	-1.26991902	1.86458701
O	-7.21060969	-1.88539341	-3.79335395
Ti	-8.13470732	-3.04611544	0.34117535
O	-7.76392270	-1.64848428	-0.76639353
Ti	-6.49494720	-0.23168741	-3.43351992
O	-9.44401510	-2.49106759	1.52041512
O	-6.62917221	0.79688640	-1.74771071
O	-3.05256847	1.42228022	-4.31672815
O	-3.27029973	-1.32615130	1.66622541
O	-2.74478835	-1.66507380	-2.41654002
Ti	-3.40354206	-1.59903745	-0.32664807
O	-3.40237669	0.23511779	-0.92669540
Ti	-2.98671378	0.20050050	-2.66767050
O	-5.17722755	-1.54766157	0.13766352
O	-4.70375513	-0.26115856	-3.55596509
O	-4.34038962	-0.15184829	-6.59479552
Ti	-4.75930788	1.09176343	-5.35858876
O	-2.95191570	-2.59755621	-7.11465782
Ti	-2.64139673	-0.67415927	-7.08349995
O	0.69818679	-0.58450991	-7.56691198
O	0.46683249	-1.81051893	1.70787070
O	-1.01585481	-3.54078785	-3.74200493
Ti	0.36059724	-1.81155682	-0.22227186
O	0.55074980	-0.00495671	-0.75936591
Ti	0.77238685	-0.07507545	-2.75756097
O	-1.44039485	-1.68389858	0.17447436
O	-1.10635701	0.27900933	-3.07263023
O	-0.02254983	1.24314838	-9.49791782
Ti	-1.01737264	1.12490444	-4.80225910
O	-1.67953057	-1.12846895	-5.48737222
Ti	-0.05079211	-0.61727106	-9.21978772
O	3.40640853	0.91399988	-5.19848449
O	2.39865426	-2.01106178	0.13719493
O	5.17403733	-1.05181111	-2.24883570
Ti	3.62310562	-1.80205588	-1.26886969
O	2.74812223	-0.55998748	-2.55213216
Ti	4.20645006	-0.11800588	-3.65970137
O	0.54727718	-1.85536277	-2.33938772
O	0.77696052	0.23089543	-4.72834182
O	3.18231850	0.37510689	-7.76296618
Ti	1.78155008	0.40723556	-6.39935664
O	2.67790284	-1.56035112	-6.32418767
Ti	2.67855602	-1.45302370	-8.41659500
O	8.08265881	0.38417070	-5.51263240
O	6.31401283	1.40292522	-0.98924329
O	7.51466349	-1.57070355	-3.29071193
Ti	7.04098314	0.13431968	-2.14749826
O	8.22423736	1.23079727	-2.90455434
Ti	7.47331526	1.87459666	-4.57814191
O	4.52208240	-0.40979608	0.04127828

O	6.06336921	0.53794337	-3.90734976
O	4.41339123	-2.10842194	-8.31758397
Ti	4.56176866	1.23330613	-6.61198651
O	5.54688012	-0.33173590	-6.45685631
O	-6.66441606	2.83390472	1.77890086
O	-4.70275269	2.86037765	-0.34532775
Ti	-6.95351885	-0.15067409	0.02224528
O	-7.38952816	3.57358553	-0.93161379
Ti	-6.00143373	2.61573879	-1.58320065
O	-8.14988699	0.90776749	0.76607967
O	-2.66551145	4.10041977	-5.03827407
O	-3.00099235	2.19228020	1.60997909
O	-2.56223205	2.42927892	-2.08576081
Ti	-2.77945233	2.87702109	-0.27721135
O	-2.14712992	4.57219719	0.04432298
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O	0.78730360	1.97342005	1.62622725
O	1.06509822	1.78394186	-2.34317089
Ti	0.72929258	1.91688739	-0.37184324
O	0.61373900	3.73641923	-0.90622014
Ti	0.75685835	3.61822347	-2.70056883
O	-1.13987790	1.93042004	0.13656541
O	-0.40812281	2.70827802	-4.30762935
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Ti	-0.80837191	4.67560988	-5.20027169
O	-0.98170752	3.89240754	-6.88494302
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O	4.53485971	5.67181925	-1.86139360
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O	4.06327864	1.77752200	-2.50729258
Ti	4.41393443	1.46655426	-0.59106559
O	4.74572464	3.39704580	-0.74756578
Ti	4.34639676	3.64916609	-2.59663593
O	2.60130462	1.74469929	-0.04216386
O	2.48424655	4.08786797	-3.14309059
O	3.35422954	5.17959853	-6.65939961
Ti	2.79266150	5.23942598	-4.82608982
O	1.09390464	2.05248545	-6.96604608
Ti	2.13372866	3.77313155	-7.23515281
O	7.58000105	2.60384557	0.86623534
O	8.24923338	3.53761019	-4.60252736
Ti	6.95683774	3.43715463	-0.70503679
O	8.36997547	4.21332868	-1.64554587
Ti	7.63347651	4.66086058	-3.24557190
O	6.27956806	3.48187862	-2.79648928
O	6.30150017	5.07539602	-6.97047095
Ti	5.11150618	4.17177414	-6.32601628
O	5.91716775	2.35236939	-5.85363097

O	-9.10233245	3.30160195	1.87825835
Ti	-7.68543689	4.00050841	0.87304627
O	-3.97072618	6.65198289	-0.00726313
O	-0.49317746	4.94963440	-3.26796614
Ti	-2.63858675	6.16553395	-1.13032410
O	-1.97871060	7.29216606	-2.50660881
Ti	-0.46282038	6.96446375	-3.40990272
O	-3.40497723	4.95613682	-2.32914195
O	2.48853318	6.87463803	-4.36825389
O	0.87005226	6.08326299	1.50859315
O	1.24509722	6.38067817	-2.15982754
Ti	1.23660006	6.81931086	-0.36069833
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Ti	2.17967487	7.97704368	-2.76704857
O	-0.79433355	6.60912211	-0.27965594
O	0.60865079	8.52672292	-3.46849489
O	-0.83926369	6.49881462	-5.16701800
O	4.77179474	6.20491126	2.06119997
O	6.88277122	6.35154936	-3.31702015
Ti	5.02997093	6.05787279	0.07858558
O	5.70331994	7.54881179	-0.65751978
Ti	5.39954344	7.16542314	-2.44585133
O	3.01102380	6.16993038	0.28492262
O	4.07096479	8.32036118	-2.90029051
O	4.55684821	4.53292732	-4.43999442
O	6.50506505	5.01215487	0.11166522
O	-3.66562422	-7.04659673	4.04034820
O	-4.48566368	-8.25442700	1.69885415
Ti	-5.03970328	-6.62620279	2.45837208
O	-1.21046666	-5.60066839	4.12426042
Ti	0.21510881	-6.80554186	5.54379619
O	-1.59787428	-7.59227696	5.63729534
O	-1.79928179	-7.13604129	1.97445796
Ti	-2.90195507	-6.16515378	5.44635175
Ti	-1.80098567	-8.04537174	3.66139470
O	2.89051223	-8.78695138	4.13248750
O	1.49660410	-7.78944583	6.40117956
O	2.68559147	-7.07870347	2.02499328
Ti	2.93306344	-7.37916879	5.32907178
Ti	1.71235897	-8.41960947	2.78842145
O	5.69324752	-3.71880122	-3.24031523
O	-7.86996862	-2.87661965	3.90999992
O	-5.88534230	-5.31850296	3.66137052
O	-3.83362936	-5.76264787	6.94423702
O	-3.33439424	-3.07520671	8.38922026
Ti	-4.00565978	-3.86641965	6.89380525
O	-5.71148413	-3.41032606	6.34366536
O	-6.72754478	-3.95571499	1.27229537
Ti	-6.44227843	-3.73764761	3.09971513
O	-6.65463962	-6.71043982	1.49956290
Ti	-6.99710507	-5.78761264	-0.00336881
O	0.41316889	-3.61389092	4.80514759
O	-0.12543880	-5.51136243	6.74841796

O	0.52422934	-3.61097027	8.75612368
Ti	0.39987674	-3.76050739	7.00371710
O	-1.26715574	-2.92101880	6.57305256
O	-1.58992214	-3.48008491	2.64117049
Ti	-1.44894768	-3.37865343	4.69679766
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Ti	-1.14776777	-5.27480175	2.23062477
O	4.23105267	-3.86971498	4.54785204
O	4.57728429	-6.63228179	5.73768020
Ti	5.23920642	-4.93432532	5.69058454
O	2.37247655	-3.75610433	6.49128816
O	2.36328254	-3.81396084	2.61229264
Ti	2.24237675	-3.61385404	4.50522112
O	1.91892872	-6.03068924	4.63890022
Ti	2.92479850	-5.34100326	1.63463262
O	6.65690129	-3.07077266	1.64778071
O	6.59478783	-4.58576650	4.47783257
O	5.12046017	-2.89573736	-0.50201342
Ti	5.86689087	-3.28223677	3.36522164
O	4.73210121	-4.99958886	1.67032016
Ti	5.76420821	-4.53636580	0.09846033
O	-6.19670529	-0.37876894	5.46425013
Ti	-5.82406559	1.35827427	4.88340587
O	-9.23222572	0.16530776	3.11365391
Ti	-8.61784600	-1.53705415	2.82635676
O	-3.09669284	0.76681709	5.23280260
O	-3.66162354	-1.93599514	6.09687532
Ti	-2.30142439	-1.60007080	7.90478308
O	-3.38290512	-0.11154945	8.12995889
Ti	-3.52006559	1.29313819	6.97923897
O	-5.19254999	1.90516191	6.54090856
O	-4.94389964	0.58026167	3.24406647
Ti	-5.27809759	-1.92336252	5.36399099
O	-5.15003201	-2.36202611	3.46256770
Ti	-5.03900048	-0.90404000	2.04100020
O	0.60513284	0.34135328	4.82417087
O	1.05033535	-1.61883482	7.18229664
Ti	0.95055573	-1.76429605	8.96550569
O	1.15196002	0.28756927	8.91100123
Ti	0.74876825	0.30414906	6.85776474
O	-0.95312618	-1.48536331	9.10388392
O	-1.07002473	-0.08288144	6.58935541
O	-1.21998128	0.26710431	2.64701122
Ti	-1.43114012	0.26714610	4.73677438
O	-1.60052848	-1.57002981	4.16858784
Ti	-1.34327085	-1.60748164	2.15388472
O	4.46161091	-0.01984460	4.49562831
O	5.01274190	-4.21607061	7.37547344
Ti	3.65763310	-2.96447793	7.66559291
O	4.54234028	-1.51731692	7.00257724
Ti	4.50770557	0.21569321	6.58731270
O	2.82332381	-2.39303411	9.15158067
O	2.61678712	0.38159627	6.19637807



O	2.54013678	0.01540434	2.36786685
Ti	2.36198132	0.12294782	4.30526353
O	2.34893521	-1.80784006	4.12009559
Ti	2.68431636	-1.81769410	2.07279248
O	6.58501672	-1.84874827	4.21192291
O	6.34822000	0.71195240	6.09020125
O	6.47083606	-0.03651987	2.14111631
Ti	6.22000843	-0.03086263	4.27007850
O	4.46024968	-2.07705235	2.22625500
Ti	5.98151973	-1.36701930	0.92189089
O	-7.41407989	1.87074575	4.15546960
Ti	-8.35013875	1.73291250	2.52925761
O	-2.52583445	4.89680516	4.36007009
O	-2.40663612	2.63117927	7.47850076
Ti	-1.26365876	3.87297183	8.22887423
Ti	-2.80105680	5.50080012	6.36302160
O	-4.51748542	5.11316200	5.84428892
O	-4.40901571	4.32807078	1.90559429
Ti	-4.37299344	4.76414559	4.03248572
O	-4.89086390	2.94295267	3.90537171
Ti	-4.83321668	2.22221594	2.06504881
O	1.11197688	3.98930519	4.85890793
O	0.67484832	2.18344833	7.27812104
Ti	1.07137968	2.16304599	9.05511835
O	0.47727947	4.87845511	8.34240332
Ti	1.04681440	5.01766516	6.71546858
O	-0.49879517	2.86510585	9.65019229
O	-0.93137138	4.53144535	6.27502115
O	-0.83672364	4.01772485	2.41518500
Ti	-0.76381469	3.98583471	4.33023615
O	-1.13768242	2.24501769	4.18096393
Ti	-1.06455888	2.02518333	2.07111376
O	4.36730010	2.47382884	5.82800635
O	4.34246345	1.16978613	8.12660449
Ti	4.03353793	2.93873350	7.88018051
O	2.75476242	2.98835370	9.21542702
O	2.78969130	4.12769055	6.76472923
O	2.68789447	3.93750296	1.97056806
Ti	2.89499031	3.53440052	4.93973839
O	2.72351747	2.01485555	3.84278569
Ti	2.74509852	2.12191213	1.88905981
O	5.86467846	3.37614397	7.60781334
O	5.81394423	3.76255056	2.52956777
Ti	6.17876587	2.80529745	5.89517888
O	6.80395444	1.80546839	3.90550098
Ti	6.40307005	1.97814894	2.07829870
O	-2.46301607	7.17796271	5.73875332
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O	-6.81367475	5.59281315	1.12708325
O	-4.90563102	6.38723387	3.23743187
Ti	-5.02103251	5.93068662	1.46318654
O	-0.34035697	8.54352190	4.28016407
O	1.44972716	6.75959261	6.26661876

O	-1.98044247	6.83752115	2.30457313
Ti	-1.61659163	7.26316987	4.08931569
O	-0.17422123	6.08996916	4.18319724
Ti	-0.93815465	5.68428013	1.35799247
O	2.38894235	7.15506568	3.37962126
Ti	1.09534105	7.38823638	4.58754983
O	3.75448874	4.92395263	4.13445970
Ti	2.80158475	5.78986994	2.11539021
O	6.42589775	4.42116127	5.04110312
Ti	5.50319497	5.07437148	3.53652030

**(TiO<sub>2</sub>)<sub>136</sub>**

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O	-2.18024704	0.16699582	-7.70083651
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O	-3.28140066	-1.81980213	-9.60132266
O	4.11397939	-2.02984080	-9.28031359
O	-2.63746575	3.42837357	-8.02827436
O	0.10141528	3.41729097	-8.19066093
O	2.64094692	2.42258588	-9.31806832
O	-7.07232268	-6.87327682	-0.80455907
O	-3.26569326	-8.13311445	-3.46848835
O	-4.68006333	-7.36709940	1.24977615
O	-4.62853969	-8.99865319	-1.17126021
Ti	-5.27820169	-7.37328695	-0.61771269
O	-3.21962418	-6.93142731	-0.97597108
Ti	-2.86666369	-8.55145364	-1.68576432
O	-5.28181418	-6.36678542	-2.49021462
O	0.38467511	-7.13726527	-4.60743333
O	0.49969077	-8.97579659	1.86259647
O	1.16356099	-9.43308962	-0.69218677
Ti	-0.19434840	-8.49347465	0.07975176
O	0.47700344	-6.88464942	-0.64519794
Ti	0.30137649	-7.10510554	-2.76512902
O	-2.04385290	-9.11334245	0.18521071
O	-0.95832236	-8.31385203	-2.10075701
Ti	-3.93616364	-6.47327526	-3.71679557
O	3.16500923	-7.75701142	-5.01782074
O	3.27963188	-9.51871704	0.89325394
Ti	2.96157417	-8.89474063	-0.80658257
O	3.76121900	-7.23780818	-0.41980190
Ti	3.66747688	-7.60872784	-3.28207617
O	2.09333807	-6.95121017	1.72419845
O	2.05473140	-7.70092247	-2.49683024
Ti	1.68918892	-6.82302323	-5.84786623
O	4.11751399	-9.10075179	-2.32731883
O	-6.20277288	-3.84003955	-5.99759427
O	-5.31571542	-5.30783290	3.70417115
O	-7.12947279	-4.60930135	-3.29331538
Ti	-6.73440087	-5.21672270	-1.57303489

O	-7.40919117	-3.72949455	-0.75065992
Ti	-6.45689235	-3.19989818	-4.27294656
O	-2.71069546	-3.24259312	-5.47229649
O	-3.08301068	-4.84144252	1.13862209
O	-2.74854628	-5.22051175	-3.01064864
Ti	-3.14153462	-5.00837357	-0.82122835
O	-3.48821910	-3.35403522	-1.54798637
Ti	-2.80968673	-3.34340752	-3.50153844
O	-5.13029305	-5.29360982	-0.20805084
O	-4.67537180	-3.50470872	-4.03285573
O	-3.79451807	-4.06507824	-7.78666670
Ti	-4.41091447	-4.21559064	-6.03937547
O	-4.22266512	-5.92856432	-5.45912067
O	1.15878584	-2.83059250	-5.08377196
O	0.29343524	-4.90722722	1.41390982
O	0.54159832	-5.23307643	-2.61422204
Ti	0.39441619	-5.02796934	-0.54052382
O	0.62939798	-3.21554780	-1.21862416
Ti	0.83723232	-3.34405828	-3.14929110
O	-1.38405851	-4.79666169	-0.64410314
O	-0.93680731	-3.30562275	-3.87408033
O	-1.35191084	-2.40051078	-7.81573490
Ti	-0.80332913	-2.92312606	-5.84898309
O	-0.17837523	-4.41480662	-6.71417929
Ti	-2.50221550	-3.36242120	-8.82345863
O	2.42935949	-5.18498764	-5.67308911
O	4.24492550	-5.37854872	1.61334168
O	4.36219360	-5.85032393	-2.54671075
Ti	4.12166729	-5.50438269	-0.29039926
O	4.13945264	-3.46042364	-1.05852953
Ti	4.54315323	-4.06180015	-2.83546867
O	2.34938922	-4.93636175	-0.03868822
O	2.74256153	-3.54967680	-3.35729022
O	1.63617250	-4.45602722	-9.19182090
Ti	2.89295704	-3.45849481	-5.34915363
O	0.93095421	-6.80948366	-7.52497955
Ti	0.22279232	-5.21897066	-8.30158339
O	7.00624829	-1.51985915	-4.25824627
O	8.50530151	-5.03893657	-0.89660902
O	6.35211819	-3.43057459	-2.49338160
Ti	7.41043174	-3.61605722	-0.97499715
O	8.24046914	-1.96923553	-1.46866708
Ti	6.76129143	-1.08606620	-2.53048207
O	6.10381542	-5.22753257	-0.29289811
O	4.85963172	-4.07670717	-4.72601409
Ti	5.82952681	-2.56827177	-5.28349242
O	6.04643473	-2.74217543	-7.04744233
O	-6.22177316	-1.28950892	-4.97009583
O	-7.26863797	-1.36395423	0.97140759
O	-7.30414787	-1.95097837	-2.86254571
Ti	-7.01200422	-1.91367094	-0.88171750
O	-7.02416204	-0.04075714	-1.40469960
Ti	-6.91827337	-0.09915058	-3.34110944

O	-9.38190437	0.48438855	-0.10224518
O	-6.92151912	1.04685884	-5.02381373
O	-3.43675619	0.10441378	-5.20534180
O	-3.41895928	-1.78236736	1.13978113
O	-2.86816486	-1.51850563	-2.87421738
Ti	-3.30623010	-1.56514849	-0.84763091
O	-3.44626082	0.28913403	-1.27250155
Ti	-3.28557848	0.29090739	-3.24265491
O	-5.24132006	-1.87939416	-0.48968099
O	-5.12344823	0.34651811	-3.35176199
O	-4.33733769	1.31671578	-9.26712754
Ti	-5.35876892	0.17595219	-5.71443014
O	-5.01078043	-0.59788630	-7.35283828
Ti	-3.75539881	-0.29300043	-8.63565144
O	0.78855513	0.66575176	-7.06900691
O	0.31096055	-1.53799064	1.31226438
O	0.67089581	-1.41797224	-2.73051420
Ti	0.36161060	-1.41056106	-0.77467904
O	0.23730526	0.51354828	-1.33181095
Ti	0.41447625	0.41343992	-3.22016734
O	-1.49210309	-1.59736383	-0.33744948
O	-1.25838031	0.37592232	-3.89553455
O	-0.04769217	0.69033363	-9.38570291
Ti	-1.73736197	0.51405364	-5.84154011
O	-0.58085944	-1.02846114	-6.01654294
Ti	-0.24582248	-0.64046715	-8.09040393
O	4.34149972	1.05604178	-5.17760669
O	4.12704550	-1.47521525	1.14124203
O	4.47654946	-1.43272248	-2.81120358
Ti	4.01008111	-1.56052935	-0.91292696
O	3.54767403	0.37763149	-1.38899308
Ti	3.93338525	0.38777240	-3.30909830
O	2.17791041	-1.37860320	-0.24101831
O	2.09408987	0.29569726	-4.22486910
O	3.29055268	-0.15622975	-7.37949644
Ti	2.57436210	0.74079725	-6.08134662
O	3.07631167	-2.99401907	-7.20903243
Ti	2.46862401	-2.83643438	-8.88650031
O	7.22703788	1.84902097	-4.89290109
O	8.00940614	-0.53278169	0.95666951
O	8.09982994	0.36591274	-2.26547870
Ti	9.07358614	-0.29110606	-0.58212329
O	9.74539311	1.38732279	-0.35097497
Ti	7.17844321	1.90959530	-3.08596200
O	5.84025021	-1.11671239	-0.65323007
O	5.80190529	0.68061015	-2.96470484
O	5.96090637	-0.09092213	-7.16114973
Ti	5.87142435	1.40836127	-6.22125189
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O	-8.70419663	3.28427203	-0.67716437
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Ti	-3.70465295	2.23979336	-0.97171805
O	-3.67306476	4.09784280	-1.56306007
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Ti	-4.33510393	2.78247150	-8.06396840
O	0.57437119	4.22904278	-5.44970022
O	0.11767706	2.37622210	1.06680028
O	0.41173137	2.38007766	-3.04458817
Ti	0.09806546	2.44191981	-0.96304824
O	-0.06118059	4.24570679	-1.52138366
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O	-1.46373309	5.63358578	-6.60129518
Ti	-2.28417175	6.22110384	-5.14487829
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O	4.13536018	4.06430721	-5.20320948
O	3.82980580	2.34378680	1.13709189
O	3.59891983	2.28317136	-2.85171406
Ti	3.76460595	2.21436968	-0.91409365
O	4.20135060	4.17282276	-1.16998140
Ti	4.19794657	4.03464917	-3.43863505
O	1.97357124	2.57832889	-0.45797301
O	2.19947912	4.55402206	-3.55230518
O	3.04454650	4.85244468	-7.56367682
Ti	2.43731906	4.72074351	-5.79850282
O	2.48079438	2.51380179	-6.69002409
Ti	1.01928496	1.91249604	-8.53565347
O	7.82079816	2.15232293	1.56606227
O	7.94478192	3.12887493	-1.41512630
Ti	9.12939353	2.96134295	0.49316665
O	8.77922084	4.83126425	0.58560228
Ti	6.36120836	3.95287414	-1.03726091
O	5.66954905	2.12412288	-0.48829224
O	6.00471923	3.48564497	-2.96111064
Ti	3.63403591	3.20052474	-7.99790795
O	5.32014795	2.62713988	-7.47314519
O	10.10995456	2.89596720	2.07725486
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Ti	-7.13934444	7.15142834	-0.98731857
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O	-4.11625399	6.02158446	-3.10545546
Ti	-3.83451355	5.91485498	-1.04189122
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O	-3.75013634	7.32639978	-5.49717743
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O	0.07502795	8.00226609	-1.22122428
Ti	-0.07197542	8.29923458	-3.21584256
O	-1.97634124	6.11853120	-0.70165098
O	1.64323812	8.40630942	-3.74449704
Ti	-4.98239993	7.35782679	-4.20284702
O	-6.03039840	5.89631350	-4.98982521
Ti	-5.57570604	4.31292745	-5.95958689
O	3.89746170	6.76910217	0.74184857
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Ti	4.34308731	6.06456503	-1.13748215
O	4.66682171	9.22562310	0.65253663
Ti	3.14221884	8.73035640	-0.16534351
O	1.92594289	5.87170451	-0.58514839
O	3.45110974	7.74931602	-1.68332243
Ti	2.40727374	6.71945144	-3.50141456
O	2.54838798	6.46423681	-5.29361734
O	7.43702529	4.97093693	3.27052264
Ti	7.37650738	5.48890344	1.54995407
O	6.12676628	5.86857399	-1.09366379
O	-0.32142611	10.13337520	0.91571927
O	-0.41559568	10.05055312	-2.51303385
Ti	0.27130004	9.80740805	-0.85116309
O	-4.70204912	9.95444327	0.10632486
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Ti	-3.61961956	-5.37330672	4.65516078
O	-1.64493209	-5.05735261	4.60080012
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O	-0.03177106	-6.46541886	3.55122778
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O	-3.11756980	-6.36081173	3.00274442
O	-1.32652638	-6.96704793	1.30186853
Ti	-0.23968194	-8.27574720	3.68007872
O	-1.97551107	-8.88828376	3.09522009
Ti	-2.72138135	-8.01188447	1.72031800
O	4.39990602	-6.18005753	5.46287304
O	1.60664990	-6.62819588	5.94787210
O	4.05405553	-7.68750203	3.27763859
Ti	2.85321970	-6.76325171	4.66868970

O	1.70161062	-8.52911986	4.06023878
Ti	2.39746884	-8.59019208	2.26523008
O	6.46068042	-7.25112632	1.50976433
Ti	5.32827881	-6.46342391	2.67702791
O	-9.77340651	-0.40514156	5.15910881
Ti	-9.01495341	1.22038475	4.82673956
O	-9.58929833	-1.21806783	2.40933214
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O	-0.75259547	-7.85868011	5.48661709
O	-3.81146269	-3.00330357	8.28124171
Ti	-4.34571550	-3.40486289	6.49819845
O	-5.98808093	-3.33214773	5.84281212
O	-5.57019936	-3.61736295	1.94261255
Ti	-8.79905065	-1.48213354	3.97831280
O	-7.87910803	-3.14607294	3.92850132
Ti	-4.68354106	-5.42101286	1.77353886
O	0.33913700	-3.25765220	4.71225580
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Ti	3.47956458	-2.54464224	7.66568144
O	1.58528902	-2.60502106	8.38695405
Ti	0.49965593	-3.13996215	6.84233750
O	-1.49140948	-2.69049832	6.46275027
O	-1.50142259	-3.48212443	2.56678419
Ti	-1.56241037	-3.02381505	4.61730505
O	2.40142354	-5.16589418	3.81572771
Ti	-1.39457083	-5.30819949	2.47674573
O	6.19536511	-5.08163486	3.65750155
O	4.54685657	-3.95087872	7.28469351
O	4.08796555	-1.51201729	9.10715183
Ti	5.12507124	-4.46918604	5.54774304
O	2.29316501	-3.11500045	6.14093405
O	2.30457174	-3.19800600	2.27377550
Ti	2.19435708	-3.07857684	4.24311878
O	4.20327542	-3.25675199	4.55947484
Ti	2.10849969	-5.10014237	1.85855208
O	8.84296319	-2.78548591	2.93099479
O	6.53740561	-3.12667580	5.56146947
O	6.94604921	-3.01177509	0.85409102
Ti	7.30358905	-3.68666857	2.59817877
O	8.12047680	-5.19018826	1.78671574
Ti	7.52663229	-6.10093903	0.41166967
O	-7.60887263	-0.09853623	3.85494652
O	-7.89214410	1.76466174	6.17275338
Ti	-6.14687146	2.16278690	6.63077112
O	-9.18354746	1.54702911	2.71939209
Ti	-9.50000940	3.33623528	3.07437494
O	-10.16223431	2.71000037	4.66298727
Ti	-8.61661434	0.11981640	1.49500480
O	-3.61651089	0.43147954	4.20533756
O	-3.67325121	-1.54315714	6.21618868
Ti	-2.61398314	-1.71898019	7.94276266
O	-3.23682360	0.03394744	8.09029861
Ti	-3.61188428	0.33019498	6.28822080

O	-5.53045148	0.52328183	5.85109206
O	-5.18014035	0.14139295	1.90229449
Ti	-5.43114936	0.26295658	3.86822140
O	-5.50946517	-1.69565610	3.51539277
Ti	-5.37323931	-1.73421004	1.54015119
O	0.20347899	0.59793448	4.29870336
O	0.48588843	-0.99782991	6.82946003
Ti	0.46178674	-0.86617435	8.73698931
O	-0.02092557	0.93049433	8.27107385
Ti	0.11661597	0.85230079	6.35394385
O	-1.07950465	-1.71552886	9.06718445
O	-1.72402071	0.54282576	5.84897176
O	-1.65914140	0.32115147	1.93344523
Ti	-1.67432735	0.57031379	3.89076844
O	-1.67461539	-1.38341894	3.72133962
Ti	-1.59364557	-1.52818071	1.74901442
O	4.04751800	0.63657658	4.42542682
O	3.14756842	0.99568310	8.15310238
Ti	3.34830717	0.04605383	9.78287971
O	3.76179167	1.76238157	10.42812788
Ti	3.87561659	0.61380684	6.29841415
O	1.67142010	-0.38922531	10.13245053
O	2.05977677	1.08037081	5.87744638
O	2.08867522	0.54322140	2.01153841
Ti	2.10190674	0.71883720	3.97846363
O	2.23062259	-1.27266522	3.77576835
Ti	2.17097043	-1.37487404	1.70062497
O	6.63170186	-0.28989775	4.86401812
Ti	5.62525852	-1.80245755	4.84710412
O	4.30075134	-1.21193650	6.42153743
O	5.81820533	0.49661087	2.02413809
Ti	6.13082885	1.44811216	4.69442420
O	6.09212072	-2.15129273	2.99412732
Ti	5.93848872	-1.20234350	1.30919616
O	9.65997143	0.17808719	3.09394508
Ti	9.36888681	-1.25193182	2.00946104
O	-7.85639534	3.85240918	3.67145756
O	-5.65917016	2.29997101	8.35892983
O	-8.79237348	6.45357535	-0.76685384
O	-10.18999580	4.32516262	1.64352977
Ti	-9.06255579	4.83258011	0.23937374
O	-3.93389364	3.98380253	4.13168230
O	-3.77904197	2.34482522	6.57243011
Ti	-3.79764275	2.86447223	8.30107582
O	-3.99257885	4.59578732	7.86920627
Ti	-4.00699830	4.73399849	6.01439603
O	-5.86062829	3.82684855	5.73408096
O	-5.55065525	3.78428505	1.78398186
Ti	-6.02650534	3.92291642	3.77616793
O	-5.88343645	1.99188182	3.40538816
Ti	-5.53005857	1.98309109	1.29623239
O	-0.12271033	4.55382296	4.03354107
O	-0.17736174	2.75558106	6.54464092



Ti	-0.36697008	3.00475216	8.38873138
O	-0.35195173	4.85217610	7.94822706
Ti	-0.17864797	5.02446827	6.18046966
O	-2.08113629	2.77446324	9.02963841
O	-2.09894309	4.73336333	5.64095216
O	-1.94101035	4.28586232	1.74954838
Ti	-2.17484452	4.27612086	3.74697499
O	-1.80467755	2.41217461	3.39394205
Ti	-1.77799871	2.48508600	1.42744948
O	3.70083172	4.58670841	4.39872571
O	5.37028333	1.69873390	6.33627509
Ti	3.01319643	2.73215933	9.02838077
O	3.71533602	3.98935661	7.89333567
Ti	3.84582380	4.93849197	6.26563591
O	1.29316919	3.04873346	9.33196575
O	1.72076555	4.71308879	5.82783625
O	2.01605308	4.39594001	1.83708549
Ti	1.68553502	4.48403324	3.93987396
O	1.95702141	2.57905780	3.49844283
Ti	1.95736693	2.47431268	1.55126052
O	7.86132356	2.13148441	4.49864796
O	5.71260196	4.70852922	5.80625495
O	6.13979020	4.17943602	0.95212709
Ti	5.73430289	4.60639216	4.02419603
O	5.55816779	2.82011441	3.35968272
Ti	5.66035121	2.24601544	1.47666864
Ti	8.95546513	1.86669722	3.04933420
O	-4.63488518	8.37142149	2.84231080
O	-4.40027838	6.43804440	5.58506519
O	-6.25454921	7.43664717	0.78352930
O	-5.85332180	5.77683260	3.29123190
Ti	-5.90763540	5.66916487	1.50951596
O	-0.65859894	7.68818015	2.71166181
O	-0.17004985	6.85313854	5.74018406
Ti	-0.70776521	8.11575134	4.56179501
O	-2.46421588	8.50854334	4.80460016
O	-2.57492958	8.10278985	1.01817554
Ti	-3.76970133	7.41239109	4.11868632
O	-2.66548845	6.20686859	3.22165325
Ti	-1.96470759	6.48522508	1.36005119
O	4.22268674	8.44388414	3.34862468
O	3.74091254	6.73326252	6.00148057
O	0.42004978	9.48882570	3.99759390
O	1.80704453	8.23528558	1.24438087
Ti	3.66879726	6.90045717	4.13614181
O	2.06162673	6.40207208	3.34732704
Ti	1.88711048	6.13574911	1.21266337
O	6.85418566	7.28937107	1.47728322
O	5.08233731	6.16748531	3.11099382
Ti	5.14134531	7.81613593	1.81604333
Ti	-4.48050208	8.38491660	0.96483920
Ti	0.42097045	9.08728798	2.19467410

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