Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Band gap engineering of bulk ZrO2 by Ti doping

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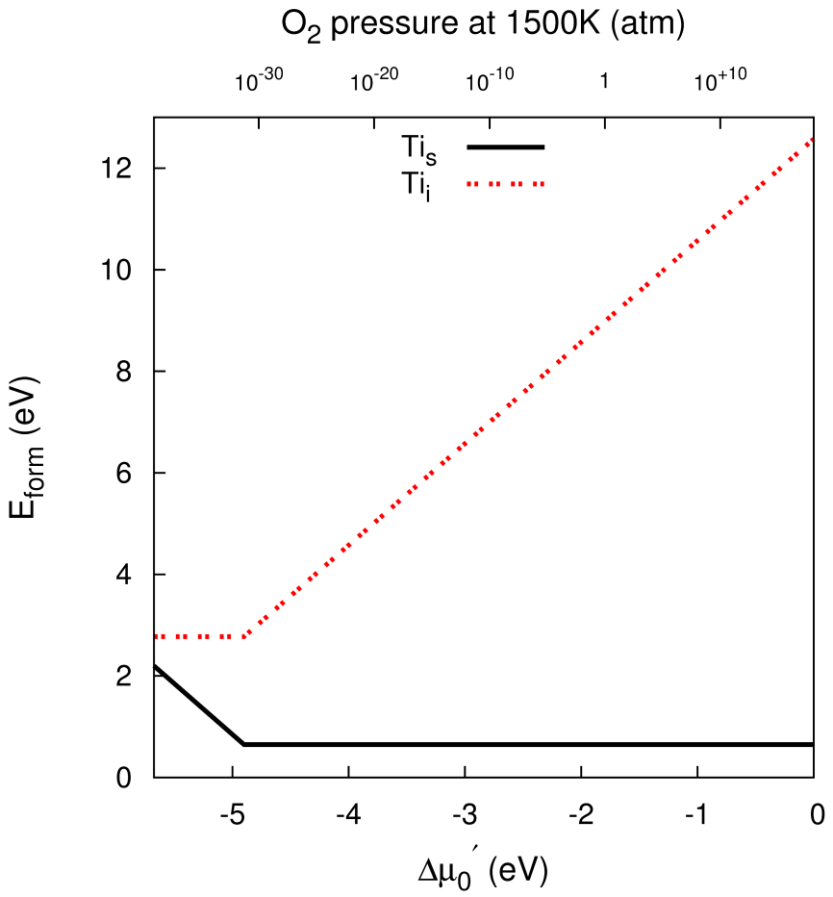

Figure S1. Formation energy E_{form} of substitutional to Zr and interstitial Ti atoms, Ti_s and Ti_i respectively, as a function of delta oxygen chemical potential $\Delta\mu'_O$ at the zero Fermi level ($E_F = 0$). In the upper x-axis $\Delta\mu'_O$ is expressed in terms of O_2 pressure assuming a temperature of 1500 K (*t*-ZrO_2 phase thermodynamic stable region). Note that this stability diagram is referred to the diluted case with one Ti atom in the supercell model (<0.03 molar fraction).

Table S1. Cartesian coordinates of all the atoms in the supercell for the two most representative geometrical configurations of $2Ti_s$ reported in Fig. 3(a-b) and discussed in the text. All the values are in Å.

		$2Ti_s$ Fig. 3a			**$2Ti_s$ Fig. 3b**		
ID Number	**Atom**	**x**	**y**	**z**	**x**	**y**	**z**
1	Zr	-0,01853	3,64715	-0,02300	-0,00042	3,65384	-0,00398
2	Zr	0,03064	3,61846	5,27369	-0,00058	-3,65424	-0,00411
3	Zr	0,01344	-3,64551	0,01030	5,46211	5,46246	-2,62966
4	Zr	-0,01548	-3,63108	5,26142	5,46258	5,46216	2,58125
5	Zr	-0,01627	0,01486	-0,00820	0,00066	3,63025	-5,28907
6	Zr	-1,82675	-1,80970	-2,65165	0,00053	-3,62997	-5,28887
7	Zr	3,64857	3,63117	0,00521	-3,63595	0,00027	-5,27626
8	Zr	3,63199	3,66492	5,30726	3,63698	0,00011	-5,27676
9	Zr	3,62737	-3,62728	0,02897	-0,00061	-0,00015	0,07348
10	Zr	3,65405	-3,64523	5,28839	0,00065	0,00027	-5,25038
11	Zr	3,67227	0,01645	0,00930	3,64136	3,60076	-0,01654
12	Zr	3,56487	-0,01588	-5,27873	-3,64218	-3,60114	-0,01626

13	Zr	-3,64165	3,64373	0,00955	-3,64206	3,60025	-0,01616
14	Zr	-3,63638	3,61907	5,26334	3,64098	-3,60079	-0,01637
15	Zr	-3,63344	-3,63477	-0,02999	3,64854	3,64722	5,27211
16	Zr	-3,64744	-3,65257	5,32811	-3,64755	-3,64666	5,27244
17	Zr	-3,64440	-0,00228	0,02317	-3,64775	3,64711	5,27291
18	Zr	-3,60919	0,01309	-5,31206	3,64841	-3,64660	5,27236
19	Zr	-1,81124	-1,84249	2,63380	1,79696	1,81744	2,64712
20	Zr	1,83770	1,80638	-2,63913	-1,79599	-1,81794	2,64693
21	Zr	1,83434	5,45154	2,67895	-1,79606	1,81745	2,64698
22	Zr	1,80785	5,46644	-2,65512	1,79682	-1,81766	2,64685
23	Zr	1,78969	-1,79701	2,66624	-1,83628	-1,82507	-2,61414
24	Zr	1,83978	-1,82555	-2,62347	1,83515	1,82530	-2,61416
25	Zr	5,43010	1,80737	2,66576	1,83534	-1,82496	-2,61428
26	Zr	5,46543	1,82353	-2,67025	-1,83631	1,82521	-2,61404
27	Zr	5,46660	5,47326	2,61144	1,83836	5,46209	2,64939
28	Zr	5,45482	5,45655	-2,61656	-1,83743	5,46217	2,64924
29	Zr	5,45663	-1,79806	2,67631	5,46196	-1,85424	-2,66736
30	Zr	5,46312	-1,82207	-2,65605	5,46192	1,85459	-2,66811
31	Zr	-1,74401	1,83715	2,63097	1,81495	5,46232	-2,67083
32	Zr	-1,85126	1,80453	-2,65656	-1,81568	5,46224	-2,67097
33	Zr	-1,83431	5,46612	2,65147	5,46265	-1,77379	2,65123
34	Zr	-1,80599	5,44845	-2,67513	5,46269	1,77326	2,65057
35	O	-1,83366	-0,00629	-1,03932	5,46257	-3,64603	4,22071
36	O	-1,59614	0,06974	4,30904	5,46276	3,64636	4,22055
37	O	1,86010	3,52950	1,65625	1,89857	3,64340	1,58771
38	O	1,77858	3,61684	-3,68149	-1,89813	-3,64390	1,58735
39	O	1,83056	-3,63328	1,61510	-1,89856	3,64353	1,58745
40	O	1,76741	-3,61900	-3,70019	1,89856	-3,64373	1,58761
41	O	1,77997	0,14605	1,73420	-3,67323	-1,89079	-1,63141
42	O	1,93600	-0,01428	-3,60821	3,67239	1,89097	-1,63198
43	O	5,47430	3,65009	1,60651	3,67243	-1,89109	-1,63170
44	O	5,45706	3,65949	-3,69898	-3,67330	1,89143	-1,63203
45	O	5,42172	-3,61749	1,60539	1,81258	3,63265	-3,69257
46	O	5,47645	-3,66498	-3,68736	-1,81228	-3,63254	-3,69264
47	O	5,47808	-0,01599	1,60434	-1,81278	3,63260	-3,69273
48	O	5,46594	-0,00097	-3,70005	1,81227	-3,63271	-3,69250
49	O	-1,84326	3,66825	1,58611	-3,63659	-1,81576	3,66019
50	O	-1,77092	3,60410	-3,71930	3,63790	1,81548	3,66011
51	O	-1,79710	-3,65132	1,57695	3,63714	-1,81545	3,66024
52	O	-1,78820	-3,62745	-3,70775	-3,63707	1,81534	3,65999
53	O	-1,81948	-0,01295	1,62674	1,58286	-0,00005	1,70069
54	O	-1,92208	0,00308	-3,67426	-1,58279	-0,00022	1,70094
55	O	-0,11638	1,83581	0,96096	-0,00050	-1,68057	-1,56256
56	O	0,04009	1,67478	-4,38105	-0,00039	1,68096	-1,56229
57	O	0,05508	5,43994	1,05454	1,83894	0,00046	-3,63041
58	O	-0,00972	5,45419	-4,26090	-1,83923	0,00022	-3,63025
59	O	0,04211	-1,79584	1,03442	0,00041	-1,84558	3,72847
60	O	-0,03934	-1,70933	-4,30319	0,00024	1,84569	3,72855
61	O	3,74248	1,81804	1,02670	5,46221	3,55978	1,56143
62	O	3,64074	1,83393	-4,27367	5,46207	-3,56020	1,56175
63	O	3,61018	5,44834	1,06154	-3,61543	5,46251	-1,60752
64	O	3,61899	5,47233	-4,22294	3,61485	5,46225	-1,60730

65	O	3,59103	-1,78264	1,07245	5,46257	3,65871	-3,71894
66	O	3,66521	-1,84690	-4,23373	5,46238	-3,65799	-3,71861
67	O	-3,64537	1,82196	1,05330	-3,65441	5,46267	3,67003
68	O	-3,65668	1,83671	-4,25148	3,65516	5,46235	3,67041
69	O	-3,65658	5,48660	1,04144	5,46263	-0,00034	1,63937
70	O	-3,60187	5,43827	-4,25179	-0,00038	5,46216	-1,60514
71	O	-3,63654	-1,83809	1,05240	5,46240	-0,00024	-3,64707
72	O	-3,65400	-1,82992	-4,25267	0,00037	5,46206	3,67504
73	O	0,20457	2,01680	3,52200	-0,00030	1,90093	1,06627
74	O	-0,00696	1,80636	-1,67109	-0,00011	-1,90119	1,06595
75	O	-0,03099	5,49723	3,68943	-2,00221	0,00013	-0,90006
76	O	0,00024	5,46137	-1,60073	2,00121	-0,00020	-0,90062
77	O	-0,03293	-2,05005	3,63107	0,00126	1,81787	-4,21553
78	O	0,00281	-1,80783	-1,62050	-0,00006	-1,81760	-4,21561
79	O	3,41738	1,74672	3,62982	-1,81713	0,00083	4,29818
80	O	3,65444	1,82800	-1,60801	1,81802	-0,00043	4,29762
81	O	3,71220	5,49159	3,70354	-0,00015	5,46216	1,05692
82	O	3,62682	5,46003	-1,59190	5,46193	-0,00020	-0,91897
83	O	3,62343	-1,77117	3,71308	0,00037	5,46226	-4,25432
84	O	3,64890	-1,82958	-1,57868	5,46284	0,00005	4,27434
85	O	-3,59560	1,74658	3,67835	3,58484	1,65766	0,95483
86	O	-3,64979	1,82816	-1,59746	-3,58510	-1,65834	0,95526
87	O	-3,67306	5,39755	3,69722	-3,58514	1,65787	0,95490
88	O	-3,63012	5,47491	-1,61200	3,58476	-1,65786	0,95497
89	O	-3,61092	-1,68341	3,70256	-1,79806	-3,61326	-1,05705
90	O	-3,64540	-1,83924	-1,59995	1,79733	3,61328	-1,05692
91	O	1,81857	3,63066	-1,02620	1,79721	-3,61319	-1,05704
92	O	1,85398	3,86797	4,30851	-1,79796	3,61333	-1,05692
93	O	1,82063	-3,64111	-1,04486	3,64466	1,82709	-4,26762
94	O	1,85123	-3,67885	4,25101	-3,64410	-1,82688	-4,26692
95	O	1,82801	0,01510	-0,97646	-3,64505	1,82706	-4,26672
96	O	1,61483	-0,19761	4,41758	3,64512	-1,82684	-4,26709
97	O	5,46689	3,66068	-1,04654	-1,82212	-3,65406	4,24152
98	O	5,43083	3,50212	4,23806	1,82298	3,65407	4,24120
99	O	5,45143	-3,65304	-1,03424	1,82287	-3,65350	4,24151
100	O	5,49293	-3,57850	4,24214	-1,82247	3,65358	4,24196
101	O	5,47043	-0,00664	-1,04957	3,71218	5,46219	1,01611
102	O	5,41722	0,07254	4,26067	-3,71287	5,46216	1,01590
103	O	-1,82773	3,65084	-1,06741	5,46190	-3,68261	-1,05990
104	O	-1,80329	3,59159	4,22645	5,46194	3,68256	-1,06019
105	O	-1,80536	-3,63822	-1,05459	3,62512	5,46243	-4,26070
106	O	-1,89253	-3,67332	4,23662	-3,62494	5,46260	-4,26038
107	**Ti**	1,82182	1,86011	2,58629	3,70257	-0,00011	-0,01204
108	**Ti**	-0,00145	-0,03929	5,35387	-3,70411	-0,00061	-0,01156

Table S2. Cartesian coordinates of all the atoms in the supercell for the two most representative geometrical configurations of $4Ti_s$ reported in Fig. 3(c-d) and discussed in the text. All the values are in Å.

		$4Ti_s$ Fig. 3c			**$4Ti_s$ Fig. 3d**		
ID Number	**Atom**	**x**	**y**	**z**	**x**	**y**	**z**
1	Zr	0,00000	3,62498	-0,06538	0,00291	-3,64449	-0,02245
2	Zr	0,00000	-3,62498	-0,06538	-3,64733	0,00707	0,00020
3	Zr	-3,62498	0,00000	0,06538	3,61928	0,01440	-0,01366
4	Zr	3,62498	0,00000	0,06538	-0,03294	3,64270	5,28156
5	Zr	0,00000	3,62460	5,22788	0,01076	-3,64983	-5,27870
6	Zr	0,00000	-3,62460	5,22788	-3,63205	0,01149	5,27842
7	Zr	-3,62460	0,00000	-5,22788	3,64235	0,00486	-5,27453
8	Zr	3,62460	0,00000	-5,22788	0,01140	0,01186	-0,01974
9	Zr	3,63611	3,63611	0,00000	0,01374	0,00139	-5,27830
10	Zr	-3,63611	-3,63611	0,00000	-3,64812	-3,62847	0,00807
11	Zr	-3,63611	3,63611	0,00000	-3,68052	3,64414	0,01187
12	Zr	3,63611	-3,63611	0,00000	3,62578	-3,64706	-0,01665
13	Zr	3,63634	3,63634	5,29318	3,68996	3,64226	5,28355
14	Zr	-3,63634	-3,63634	5,29318	-3,63239	-3,65167	-5,30669
15	Zr	-3,63634	3,63634	5,29318	-3,63225	3,63679	-5,23624
16	Zr	3,63634	-3,63634	5,29318	3,64793	-3,65212	-5,27695
17	Zr	1,82610	1,82605	2,64640	1,83115	1,85114	2,67604
18	Zr	-1,82610	-1,82605	2,64640	-1,78384	-1,81474	2,65821
19	Zr	-1,82605	-1,82610	-2,64640	-1,84434	-1,82147	-2,67946
20	Zr	1,82605	1,82610	-2,64640	-1,84000	1,83591	2,61807
21	Zr	-1,82610	1,82605	2,64640	1,82879	-1,81765	2,61836
22	Zr	1,82610	-1,82605	2,64640	-1,75949	1,82417	-2,62119
23	Zr	-1,82605	1,82610	-2,64640	1,81845	-1,83126	-2,56804
24	Zr	1,82605	-1,82610	-2,64640	1,83150	5,44325	2,67904
25	Zr	1,83765	5,46229	2,58161	-1,84125	-5,46796	2,61809
26	Zr	-1,83765	5,46229	2,58161	-5,45059	-1,82075	-2,68532
27	Zr	5,46229	-1,83765	-2,58161	5,36855	1,83152	-2,60702
28	Zr	5,46229	1,83765	-2,58161	-1,76544	5,45333	-2,62805
29	Zr	1,83720	5,46229	-2,71231	5,43918	-1,81454	2,66068
30	Zr	-1,83720	5,46229	-2,71231	-5,42694	1,82998	2,62736
31	Zr	5,46229	-1,83720	2,71231	-5,42562	5,46054	2,62266
32	Zr	5,46229	1,83720	2,71231	5,37635	5,44901	-2,61674
33	O	1,75131	3,59284	1,54081	1,85854	3,64859	1,69794
34	O	-1,75131	-3,59284	1,54081	-1,76888	-3,63641	1,58710
35	O	-3,59284	-1,75131	-1,54081	-3,65033	-1,81910	-1,58812
36	O	3,59284	1,75131	-1,54081	3,38674	1,64710	-1,73650
37	O	-1,75131	3,59284	1,54081	-1,99113	3,64498	1,61387
38	O	1,75131	-3,59284	1,54081	1,82716	-3,70051	1,60701
39	O	-3,59284	1,75131	-1,54081	-3,64864	2,04762	-1,59889
40	O	3,59284	-1,75131	-1,54081	3,75869	-1,83378	-1,58260
41	O	1,75031	3,59225	-3,75234	1,80919	3,65260	-3,50294
42	O	-1,75031	-3,59225	-3,75234	-1,80961	-3,63617	-3,69666
43	O	-3,59225	-1,75031	3,75234	-3,63466	-1,81727	3,66901
44	O	3,59225	1,75031	3,75234	3,66394	1,83417	3,65154
45	O	-1,75031	3,59225	-3,75234	-1,81830	3,63435	-3,66899

46	O	1,75031	-3,59225	-3,75234	1,82097	-3,76667	-3,61743
47	O	-3,59225	1,75031	3,75234	-3,63293	1,78238	3,70334
48	O	3,59225	-1,75031	3,75234	3,62566	-1,81652	3,70668
49	O	1,99380	0,00000	1,69121	1,82521	0,06648	1,60682
50	O	-1,99380	0,00000	1,69121	-1,76147	0,00597	1,58792
51	O	0,00000	-1,99380	-1,69121	-0,12251	-1,83306	-1,58341
52	O	0,00000	1,99380	-1,69121	0,22837	1,61787	-1,75059
53	O	1,99507	0,00000	-3,60171	1,82334	0,10217	-3,62298
54	O	-1,99507	0,00000	-3,60171	-1,79607	-0,00479	-3,69667
55	O	0,00000	-1,99507	3,60171	0,02935	-1,81877	3,70512
56	O	0,00000	1,99507	3,60171	-0,00782	1,83921	3,64280
57	O	5,46229	3,81088	1,71246	-5,24776	3,64400	1,63597
58	O	5,46229	-3,81088	1,71246	5,41471	-3,63531	1,59100
59	O	-3,81088	5,46229	-1,71246	-3,64897	5,19993	-1,60876
60	O	3,81088	5,46229	-1,71246	3,40409	5,62346	-1,73557
61	O	5,46229	3,81307	-3,58092	5,46399	3,63384	-3,66017
62	O	5,46229	-3,81307	-3,58092	-5,47490	-3,64051	-3,69196
63	O	-3,81307	5,46229	3,58092	-3,63437	-5,41851	3,70005
64	O	3,81307	5,46229	3,58092	3,66612	5,45490	3,64909
65	O	5,46229	0,00000	1,66143	-5,51566	0,00526	1,59228
66	O	0,00000	5,46229	-1,66143	0,20860	-5,27596	-1,73946
67	O	5,46229	0,00000	-3,63147	5,43450	0,00150	-3,69121
68	O	0,00000	5,46229	3,63147	-0,00864	-5,47296	3,64499
69	O	0,00000	1,65083	0,93400	-0,01892	1,95639	0,92995
70	O	0,00000	-1,65083	0,93400	0,02592	-1,81858	1,06186
71	O	-1,65083	0,00000	-0,93400	-1,85010	0,12064	-1,05945
72	O	1,65083	0,00000	-0,93400	1,81824	-0,34659	-0,93446
73	O	0,00000	1,65013	-4,35901	-0,01530	1,84212	-4,29122
74	O	0,00000	-1,65013	-4,35901	0,08467	-1,82550	-4,21775
75	O	-1,65013	0,00000	4,35901	-1,80155	-0,01876	4,24912
76	O	1,65013	0,00000	4,35901	1,82703	0,02280	4,27067
77	O	0,00000	5,46229	0,98518	-0,02948	5,33780	0,93767
78	O	5,46229	0,00000	-0,98518	5,47578	0,13164	-1,05381
79	O	0,00000	5,46229	-4,30823	-0,04776	5,44082	-4,29116
80	O	5,46229	0,00000	4,30823	-5,46637	-0,01597	4,25240
81	O	3,71126	1,86949	1,10571	3,66605	1,95735	0,93243
82	O	-3,71126	-1,86949	1,10571	-3,64266	-1,81171	1,04140
83	O	-1,86949	-3,71126	-1,10571	-1,86078	-3,77091	-1,05986
84	O	1,86949	3,71126	-1,10571	1,78462	3,66047	-0,79954
85	O	-3,71126	1,86949	1,10571	-3,64006	1,76560	1,04585
86	O	3,71126	-1,86949	1,10571	3,61643	-1,81814	1,06363
87	O	-1,86949	3,71126	-1,10571	-1,50255	3,63086	-1,00662
88	O	1,86949	-3,71126	-1,10571	1,81743	-3,33192	-0,94416
89	O	3,71167	1,86991	-4,18734	3,66600	1,84570	-4,28331
90	O	-3,71167	-1,86991	-4,18734	-3,64191	-1,81677	-4,25900
91	O	-1,86991	-3,71167	4,18734	-1,80299	-3,61993	4,24792
92	O	1,86991	3,71167	4,18734	1,82782	3,64687	4,33277
93	O	-3,71167	1,86991	-4,18734	-3,62859	1,80380	-4,22481
94	O	3,71167	-1,86991	-4,18734	3,56486	-1,82572	-4,21800
95	O	-1,86991	3,71167	4,18734	-1,84095	3,64276	4,24921
96	O	1,86991	-3,71167	4,18734	1,82855	-3,66365	4,27414
97	O	3,46938	5,46229	0,95576	3,67746	-5,59081	0,93272

98	O	-3,46938	5,46229	0,95576	-3,64105	-5,40152	1,03924
99	O	5,46229	-3,46938	-0,95576	5,48591	-3,78444	-1,05475
100	O	5,46229	3,46938	-0,95576	5,13537	3,62853	-0,98180
101	O	3,46594	5,46229	-4,33839	3,70341	-5,48615	-4,29054
102	O	-3,46594	5,46229	-4,33839	-3,63073	5,47262	-4,22873
103	O	5,46229	-3,46594	4,33839	5,45930	-3,61947	4,25031
104	O	5,46229	3,46594	4,33839	-5,42992	3,64043	4,25681
105	**Ti**	0,00000	0,00000	0,00000	0,08230	3,65205	0,04831
106	**Ti**	0,00000	0,00000	5,29318	3,47207	3,64808	0,04790
107	**Ti**	5,46229	5,46229	2,64485	1,80421	1,81735	-2,75619
108	**Ti**	5,46229	5,46229	-2,64485	1,80133	5,45711	-2,72078

Table S3. Cartesian coordinates of all the atoms in the supercell for the most representative geometrical configurations of $5Ti_s$ and $6Ti_s$ discussed in the text. All the values are in Å.

		$5Ti_s$			**$6Ti_s$**			
ID Number	**Atom**	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
1	Zr	0,00000	3,65164	5,24016	Zr	0,00000	3,62215	5,25924
2	Zr	0,00000	-3,65164	5,24016	Zr	0,00000	-3,62215	5,25924
3	Zr	-3,59720	0,00000	-5,30783	Zr	-3,62215	0,00000	-5,25924
4	Zr	3,59720	0,00000	-5,30783	Zr	3,62215	0,00000	-5,25924
5	Zr	0,00000	0,00000	-0,03345	Zr	0,00000	0,00000	0,00000
6	Zr	0,00000	0,00000	5,33660	Zr	0,00000	0,00000	5,29318
7	Zr	3,58717	3,60616	0,00078	Zr	3,59210	3,59210	0,00000
8	Zr	-3,58717	-3,60616	0,00078	Zr	-3,59210	-3,59210	0,00000
9	Zr	-3,58717	3,60616	0,00078	Zr	-3,59210	3,59210	0,00000
10	Zr	3,58717	-3,60616	0,00078	Zr	3,59210	-3,59210	0,00000
11	Zr	3,68115	3,63822	5,32025	Zr	3,65310	3,65310	5,29318
12	Zr	-3,68115	-3,63822	5,32025	Zr	-3,65310	-3,65310	5,29318
13	Zr	-3,68115	3,63822	5,32025	Zr	-3,65310	3,65310	5,29318
14	Zr	3,68115	-3,63822	5,32025	Zr	3,65310	-3,65310	5,29318
15	Zr	1,79255	1,82231	2,59014	Zr	1,80314	1,83121	2,60593
16	Zr	-1,79255	-1,82231	2,59014	Zr	-1,80314	-1,83121	2,60593
17	Zr	-1,83011	-1,81122	-2,62358	Zr	-1,83121	-1,80314	-2,60593
18	Zr	1,83011	1,81122	-2,62358	Zr	1,83121	1,80314	-2,60593
19	Zr	-1,79255	1,82231	2,59014	Zr	-1,80314	1,83121	2,60593
20	Zr	1,79255	-1,82231	2,59014	Zr	1,80314	-1,83121	2,60593
21	Zr	-1,83011	1,81122	-2,62358	Zr	-1,83121	1,80314	-2,60593
22	Zr	1,83011	-1,81122	-2,62358	Zr	1,83121	-1,80314	-2,60593
23	Zr	1,96958	5,46229	2,70435	Zr	1,94371	5,46229	2,67834
24	Zr	-1,96958	5,46229	2,70435	Zr	-1,94371	5,46229	2,67834
25	Zr	5,46229	-1,85597	-2,65914	Zr	5,46229	-1,94371	-2,67834
26	Zr	5,46229	1,85597	-2,65914	Zr	5,46229	1,94371	-2,67834
27	Zr	1,77310	5,46229	-2,69172	Zr	1,78882	5,46229	-2,73692
28	Zr	-1,77310	5,46229	-2,69172	Zr	-1,78882	5,46229	-2,73692
29	Zr	5,46229	-1,78168	2,71539	Zr	5,46229	-1,78882	2,73692
30	Zr	5,46229	1,78168	2,71539	Zr	5,46229	1,78882	2,73692

31	Zr	5,46229	5,46229	-2,51474	O	2,04138	3,67181	1,63195
32	O	2,03706	3,67092	1,64050	O	-2,04138	-3,67181	1,63195
33	O	-2,03706	-3,67092	1,64050	O	-3,67181	-2,04138	-1,63195
34	O	-3,66693	-2,03653	-1,64040	O	3,67181	2,04138	-1,63195
35	O	3,66693	2,03653	-1,64040	O	-2,04138	3,67181	1,63195
36	O	-2,03706	3,67092	1,64050	O	2,04138	-3,67181	1,63195
37	O	2,03706	-3,67092	1,64050	O	-3,67181	2,04138	-1,63195
38	O	-3,66693	2,03653	-1,64040	O	3,67181	-2,04138	-1,63195
39	O	3,66693	-2,03653	-1,64040	O	1,75400	3,58781	-3,66708
40	O	1,80020	3,62983	-3,66439	O	-1,75400	-3,58781	-3,66708
41	O	-1,80020	-3,62983	-3,66439	O	-3,58781	-1,75400	3,66708
42	O	-3,57588	-1,74167	3,64443	O	3,58781	1,75400	3,66708
43	O	3,57588	1,74167	3,64443	O	-1,75400	3,58781	-3,66708
44	O	-1,80020	3,62983	-3,66439	O	1,75400	-3,58781	-3,66708
45	O	1,80020	-3,62983	-3,66439	O	-3,58781	1,75400	3,66708
46	O	-3,57588	1,74167	3,64443	O	3,58781	-1,75400	3,66708
47	O	3,57588	-1,74167	3,64443	O	1,45775	0,00000	1,65341
48	O	1,46194	0,00000	1,63030	O	-1,45775	0,00000	1,65341
49	O	-1,46194	0,00000	1,63030	O	0,00000	-1,45775	-1,65341
50	O	0,00000	-1,45021	-1,67092	O	0,00000	1,45775	-1,65341
51	O	0,00000	1,45021	-1,67092	O	1,91233	0,00000	-3,65870
52	O	1,84434	0,00000	-3,67350	O	-1,91233	0,00000	-3,65870
53	O	-1,84434	0,00000	-3,67350	O	0,00000	-1,91233	3,65870
54	O	0,00000	-1,96774	3,65016	O	0,00000	1,91233	3,65870
55	O	0,00000	1,96774	3,65016	O	5,46229	3,61177	1,66824
56	O	5,46229	3,61302	1,66414	O	5,46229	-3,61177	1,66824
57	O	5,46229	-3,61302	1,66414	O	-3,61177	5,46229	-1,66824
58	O	-3,52320	5,46229	-1,56877	O	3,61177	5,46229	-1,66824
59	O	3,52320	5,46229	-1,56877	O	5,46229	3,92050	-3,56522
60	O	5,46229	3,67662	-3,64552	O	5,46229	-3,92050	-3,56522
61	O	5,46229	-3,67662	-3,64552	O	-3,92050	5,46229	3,56522
62	O	-3,93550	5,46229	3,61485	O	3,92050	5,46229	3,56522
63	O	3,93550	5,46229	3,61485	O	5,46229	0,00000	1,68562
64	O	5,46229	0,00000	1,64597	O	0,00000	5,46229	-1,68562
65	O	0,00000	5,46229	-1,65337	O	5,46229	0,00000	-3,55663
66	O	5,46229	0,00000	-3,62053	O	0,00000	5,46229	3,55663
67	O	0,00000	5,46229	3,57051	O	0,00000	2,11426	0,91738
68	O	0,00000	2,09790	0,92416	O	0,00000	-2,11426	0,91738
69	O	0,00000	-2,09790	0,92416	O	-2,11426	0,00000	-0,91738
70	O	-2,11418	0,00000	-0,93692	O	2,11426	0,00000	-0,91738
71	O	2,11418	0,00000	-0,93692	O	0,00000	1,78996	-4,27058
72	O	0,00000	1,83373	-4,27667	O	0,00000	-1,78996	-4,27058
73	O	0,00000	-1,83373	-4,27667	O	-1,78996	0,00000	4,27058
74	O	-1,75406	0,00000	4,24624	O	1,78996	0,00000	4,27058
75	O	1,75406	0,00000	4,24624	O	0,00000	5,46229	0,89464
76	O	0,00000	5,46229	0,90649	O	5,46229	0,00000	-0,89464
77	O	5,46229	0,00000	-0,94139	O	0,00000	5,46229	-4,32594
78	O	0,00000	5,46229	-4,30306	O	5,46229	0,00000	4,32594
79	O	5,46229	0,00000	4,29282	O	3,58955	1,65010	0,97813

80	O	3,58609	1,64887	0,96232	O	-3,58955	-1,65010	0,97813
81	O	-3,58609	-1,64887	0,96232	O	-1,65010	-3,58955	-0,97813
82	O	-1,63187	-3,56006	-0,96696	O	1,65010	3,58955	-0,97813
83	O	1,63187	3,56006	-0,96696	O	-3,58955	1,65010	0,97813
84	O	-3,58609	1,64887	0,96232	O	3,58955	-1,65010	0,97813
85	O	3,58609	-1,64887	0,96232	O	-1,65010	3,58955	-0,97813
86	O	-1,63187	3,56006	-0,96696	O	1,65010	-3,58955	-0,97813
87	O	1,63187	-3,56006	-0,96696	O	3,70198	1,85653	-4,23426
88	O	3,63003	1,81427	-4,25195	O	-3,70198	-1,85653	-4,23426
89	O	-3,63003	-1,81427	-4,25195	O	-1,85653	-3,70198	4,23426
90	O	-1,88093	-3,75472	4,26925	O	1,85653	3,70198	4,23426
91	O	1,88093	3,75472	4,26925	O	-3,70198	1,85653	-4,23426
92	O	-3,63003	1,81427	-4,25195	O	3,70198	-1,85653	-4,23426
93	O	3,63003	-1,81427	-4,25195	O	-1,85653	3,70198	4,23426
94	O	-1,88093	3,75472	4,26925	O	1,85653	-3,70198	4,23426
95	O	1,88093	-3,75472	4,26925	O	3,78586	5,46229	0,96170
96	O	3,78758	5,46229	1,01562	O	-3,78586	5,46229	0,96170
97	O	-3,78758	5,46229	1,01562	O	5,46229	-3,78586	-0,96170
98	O	5,46229	-3,77693	-0,96579	O	5,46229	3,78586	-0,96170
99	O	5,46229	3,77693	-0,96579	O	3,34739	5,46229	-4,39934
100	O	3,63343	5,46229	-4,25096	O	-3,34739	5,46229	-4,39934
101	O	-3,63343	5,46229	-4,25096	O	5,46229	-3,34739	4,39934
102	O	5,46229	-3,30891	4,37120	O	5,46229	3,34739	4,39934
103	O	5,46229	3,30891	4,37120	**Ti**	0,00000	3,75273	-0,04451
104	**Ti**	0,00000	3,74534	-0,01558	**Ti**	0,00000	-3,75273	-0,04451
105	**Ti**	0,00000	-3,74534	-0,01558	**Ti**	-3,75273	0,00000	0,04451
106	**Ti**	-3,74194	0,00000	0,03125	**Ti**	3,75273	0,00000	0,04451
107	**Ti**	3,74194	0,00000	0,03125	**Ti**	5,46229	5,46229	2,35674
108	**Ti**	5,46229	5,46229	2,36949	**Ti**	5,46229	5,46229	-2,35674