

Figure 9(b):

Coordinates (Angstroms)			
Atom	X	Y	Z
O	-1.692036	-1.142932	-1.286570
O	1.988003	-0.994863	-0.696408
O	-1.875328	2.576654	-1.076856
O	1.804711	2.724723	-0.486694
Ti	-1.673263	-3.032356	-0.929579
Ti	-1.856555	0.687230	-0.719865
Ti	2.006775	-2.884287	-0.339417
Ti	1.823483	0.835300	-0.129703
Ti	-2.039848	4.406817	-0.510150
Ti	1.640191	4.554886	0.080012
O	-1.508743	-4.862519	-1.496285
O	2.171295	-4.714450	-0.906122
O	-3.586156	-3.136022	-0.762812
O	0.093882	-2.987952	-0.172650
O	-3.769448	0.583565	-0.553098
O	-0.089410	0.731634	0.037064
O	-5.372074	-1.291002	-1.876732
O	3.773921	-2.839883	0.417512
O	3.590629	0.879704	0.627227
O	5.668042	-0.846794	-0.106246
O	-2.058620	6.296241	-0.867141
O	1.621419	6.444310	-0.276979
O	-3.952741	4.303152	-0.343383
O	-0.272702	4.451221	0.246779
O	-5.555366	2.428585	-1.667018
O	3.407337	4.599290	0.836941
O	5.484749	2.872793	0.103469
Ti	-1.489971	-6.751943	-1.139294
Ti	2.190068	-6.603873	-0.549131
Ti	-5.353302	-3.180426	-1.519741
Ti	-5.536594	0.539161	-1.310027
Ti	5.686814	-2.736217	0.250745
Ti	5.503522	0.983369	0.460459
Ti	-2.223140	8.126403	-0.300436
Ti	1.456899	8.274473	0.289726
Ti	-5.719886	4.258747	-1.100313
Ti	5.320230	4.702956	0.670174
O	-1.325451	-8.582105	-1.705999
O	2.354588	-8.434036	-1.115837
O	-3.402864	-6.855608	-0.972526
O	0.277175	-6.707539	-0.382364

O	-5.188782	-5.010588	-2.086447
O	3.957213	-6.559469	0.207798
O	5.851334	-4.566380	-0.315960
O	-7.266195	-3.284091	-1.352974
O	-7.449487	0.435496	-1.143260
O	-9.052113	-1.439071	-2.466895
O	7.453960	-2.691813	1.007674
O	7.270667	1.027773	1.217389
O	9.348080	-0.698724	0.483916
O	-2.241912	10.015827	-0.657427
O	1.438126	10.163896	-0.067265
O	-4.136033	8.022738	-0.133669
O	-0.455994	8.170807	0.456493
O	-5.738659	6.148171	-1.457304
O	3.224044	8.318877	1.046655
O	5.301457	6.592379	0.313183
O	-7.632779	4.155082	-0.933546
O	-9.235405	2.280515	-2.257180
O	7.087375	4.747360	1.427103
O	9.164788	3.020862	0.693631
Ti	-5.170009	-6.900012	-1.729456
Ti	5.870106	-6.455804	0.041031
Ti	-9.033340	-3.328495	-2.109904
Ti	-9.216633	0.391091	-1.900189
Ti	9.366853	-2.588148	0.840907
Ti	9.183560	1.131438	1.050622
Ti	-5.903178	7.978334	-0.890598
Ti	5.136937	8.422542	0.879888
Ti	-9.399925	4.110678	-1.690475
Ti	9.000268	4.851025	1.260336
O	-5.005490	-8.730175	-2.296161
O	6.034626	-8.285967	-0.525675
O	-7.082902	-7.003677	-1.562689
O	-8.868821	-5.158658	-2.676609
O	7.637252	-6.411400	0.797960
O	9.531372	-4.418311	0.274202
O	-5.921951	9.867758	-1.247589
O	5.118165	10.311966	0.522897
O	-7.816071	7.874669	-0.723831
O	-9.418697	6.000102	-2.047466
O	6.904083	8.466946	1.636817
O	8.981496	6.740449	0.903345
Ti	-8.850048	-7.048082	-2.319618
Ti	9.550145	-6.307735	0.631193
Ti	-9.583217	7.830264	-1.480761
Ti	8.816976	8.570612	1.470050

O	-8.685528	-8.878244	-2.886323
O	9.714665	-8.137897	0.064488
O	-9.601989	9.719688	-1.837751
O	8.798204	10.460035	1.113059
O	-1.595794	-6.382164	0.823374
O	1.649850	-6.272487	1.347800
V	1.163653	-5.974240	3.055038
V	-1.933222	-6.208676	2.582932
O	-0.276693	-6.167196	3.702838
O	2.461735	-6.257950	3.909960
O	-3.353362	-6.249760	3.274247
O	1.308802	0.561533	1.783450
O	1.500897	-3.156266	1.576337
O	-1.835710	-3.299012	1.045897
O	-2.018999	0.420483	1.255599
V	-0.074097	0.322393	3.151662
V	0.124333	-3.394812	2.951026
O	-0.028551	-1.552708	3.602852
O	0.451276	-4.940603	2.957386
O	3.159050	-11.049581	6.715252