Modelling the structure of Zr-rich $Pb(Zr_{1-x}Ti_x)O_3$, x=0.4 with a multiphase approach. Supplementary information.

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Final set structures

System: 0.25^I_1, Contribution: 6 %			
	5.871	-5.815	-0.007
	5.871	5.815	-0.007
	-0.078	0.000	4.187
Zr	0.234	0.738	0.521
Zr	0.738	0.234	0.521
Zr	0.735	0.735	0.524
Ti	0.239	0.239	0.504
Pb	0.016	0.016	0.978
Pb	0.012	0.497	0.970
Pb	0.497	0.012	0.970
Pb	0.504	0.504	0.978
O	0.987	0.222	0.567
O	0.222	0.987	0.567
O	0.223	0.223	0.061
O	0.981	0.712	0.568
O	0.712	0.981	0.568
O	0.220	0.713	0.036
O	0.713	0.220	0.036
O	0.221	0.467	0.560
O	0.467	0.221	0.560
O	0.477	0.715	0.567
O	0.715	0.477	0.567
O	0.716	0.716	0.040

Table I. Final set structures (lattice vectors (Å) and fractional coordinates) and their contributions to the $g_m(r)$

System:	0.375^{f}_{1},	Contribution:	25 %
	8.075	-0.000	0.000
	-0.000	8.346	-0.074
	0.000	-0.075	8.177
Zr	0.250	0.262	0.728
Zr	0.250	0.772	0.742
Zr	0.750	0.261	0.726
Zr	0.750	0.764	0.236
Zr	0.750	0.771	0.737
Ti	0.250	0.287	0.235
Ti	0.250	0.773	0.230
Ti	0.750	0.279	0.237
Pb	0.001	0.065	0.995
Pb	0.004	0.042	0.436
Pb	0.997	0.527	0.953
Pb	0.012	0.555	0.470
Pb	0.499	0.065	0.995
Pb	0.496	0.041	0.436
Pb	0.503	0.527	0.953
Pb	0.488	0.555	0.470
O	0.250	0.229	0.013
O	0.250	0.249	0.478
O	0.250	0.754	0.007
O	0.250	0.723	0.489
O	0.750	0.222	0.013
O	0.750	0.257	0.479
O	0.750	0.752	0.992
O	0.750	0.706	0.490
O	0.002	0.237	0.242
O	0.000	0.256	0.787
O	0.011	0.746	0.265
O	0.001	0.716	0.739
O	0.498	0.237	0.242
O	0.500	0.256	0.787
O	0.489	0.746	0.265
O	0.499	0.716	0.739
O	0.250	0.988	0.264
O	0.250	0.010	0.747
O	0.250	0.496	0.240
O	0.250	0.502	0.776
O	0.750	0.005	0.270
O	0.750	0.009	0.736
O	0.750	0.490	0.228
O	0.750	0.500	0.784

System:	$0.375\frac{l}{2}$,	Contribution:	10 %
	8.221	0.068	-0.045
	0.068	8.221	-0.045
	-0.045	-0.045	8.100
Zr	0.238	0.238	0.767
Zr	0.237	0.736	0.768
Zr	0.736	0.237	0.768
Zr	0.732	0.732	0.262
Zr	0.737	0.737	0.761
Ti	0.226	0.226	0.267
Ti	0.230	0.724	0.266
Ti	0.724	0.230	0.266
Pb	0.964	0.964	0.046
Pb	0.964	0.964	0.534
Pb	0.964	0.452	0.051
Pb	0.959	0.453	0.523
Pb	0.452	0.964	0.051
Pb	0.453	0.959	0.523
Pb	0.457	0.457	0.053
Pb	0.457	0.457	0.525
O	0.259	0.259	0.020
O	0.258	0.258	0.491
O	0.256	0.762	0.018
O	0.254	0.757	0.490
O	0.762	0.256	0.018
O	0.757	0.254	0.490
O	0.765	0.765	0.010
O	0.764	0.764	0.503
O	0.007	0.254	0.251
O	0.994	0.256	0.734
O	0.007	0.757	0.246
O	0.996	0.762	0.741
O	0.503	0.255	0.249
O	0.493	0.259	0.736
O	0.486	0.759	0.249
O	0.493	0.760	0.735
O	0.254	0.007	0.251
O	0.256	0.994	0.734
O	0.255	0.503	0.249
O	0.259	0.493	0.736
O	0.757	0.007	0.246
O	0.762	0.996	0.741
O	0.759	0.486	0.249
O	0.760	0.493	0.735

System: 0.375_3^I, Contribution: 7 %			
	8.409	-0.127	-0.000
	-0.127	8.409	-0.000
	-0.000	-0.000	8.153
Zr	0.261	0.239	0.750
Zr	0.262	0.737	0.750
Zr	0.763	0.238	0.750
Zr	0.767	0.733	0.250
Zr	0.763	0.737	0.750
Ti	0.271	0.229	0.250
Ti	0.270	0.727	0.250
Ti	0.773	0.230	0.250
Pb	0.044	0.964	0.010
Pb	0.044	0.964	0.490
Pb	0.039	0.461	0.010
Pb	0.039	0.461	0.490
Pb	0.534	0.966	0.999
Pb	0.534	0.966	0.501
Pb	0.536	0.456	0.010
Pb	0.536	0.456	0.490
O	0.241	0.259	0.012
O	0.241	0.259	0.488
O	0.245	0.760	0.011
O	0.245	0.760	0.489
O	0.740	0.255	0.011
O	0.740	0.255	0.489
O	0.736	0.764	0.002
O	0.736	0.764	0.498
O	0.995	0.258	0.250
O	0.005	0.261	0.750
O	0.010	0.761	0.250
O	0.006	0.763	0.750
O	0.492	0.256	0.250
O	0.504	0.259	0.750
O	0.494	0.757	0.250
O	0.503	0.765	0.750
O	0.244	0.008	0.250
O	0.241	0.996	0.750
O	0.242	0.505	0.250
O	0.239	0.495	0.750
O	0.743	0.006	0.250
O	0.735	0.997	0.750
O	0.739	0.490	0.250
O	0.737	0.494	0.750

System: 0.375_1^{II}, Contribution: 10 %			
	8.665	-0.000	-0.019
	-0.000	8.175	0.000
	-0.025	0.000	8.169
Zr	0.270	0.250	0.744
Zr	0.270	0.750	0.244
Zr	0.771	0.250	0.742
Zr	0.770	0.750	0.240
Zr	0.768	0.750	0.746
Ti	0.273	0.250	0.240
Ti	0.276	0.750	0.736
Ti	0.780	0.250	0.244
Pb	0.054	0.987	0.983
Pb	0.052	0.008	0.488
Pb	0.054	0.513	0.983
Pb	0.052	0.492	0.488
Pb	0.544	0.013	0.997
Pb	0.546	0.003	0.482
Pb	0.544	0.487	0.997
Pb	0.546	0.497	0.482
O	0.241	0.250	0.002
O	0.234	0.250	0.486
O	0.254	0.750	0.985
O	0.220	0.750	0.500
O	0.733	0.250	0.004
O	0.736	0.250	0.485
O	0.706	0.750	0.995
O	0.745	0.750	0.493
O	0.990	0.250	0.250
O	0.006	0.250	0.742
O	0.005	0.750	0.219
O	0.000	0.750	0.774
O	0.485	0.250	0.246
O	0.504	0.250	0.747
O	0.503	0.750	0.267
O	0.487	0.750	0.720
O	0.237	0.008	0.249
O	0.237	0.992	0.740
O	0.237	0.492	0.249
O	0.237	0.508	0.740
O	0.734	0.009	0.243
O	0.726	0.001	0.751
O	0.734	0.491	0.243
O	0.726	0.499	0.751

System: 0.5_2^V, Contribution: 5 %			
	8.199	0.000	0.000
	0.000	7.926	0.000
	-0.149	0.000	8.117
Zr	0.244	0.000	0.765
Zr	0.750	0.000	0.254
Zr	0.742	0.000	0.752
Zr	0.235	0.500	0.252
Ti	0.235	0.000	0.257
Ti	0.241	0.500	0.759
Ti	0.739	0.500	0.269
Ti	0.724	0.500	0.755
Pb	0.956	0.270	0.010
Pb	0.956	0.730	0.010
Pb	0.981	0.260	0.537
Pb	0.981	0.740	0.537
Pb	0.478	0.248	0.040
Pb	0.478	0.752	0.040
Pb	0.457	0.251	0.514
Pb	0.457	0.749	0.514
O	0.278	0.242	0.249
O	0.278	0.758	0.249
O	0.018	0.000	0.275
O	0.239	0.000	0.012
O	0.259	0.260	0.726
O	0.259	0.740	0.726
O	0.003	0.000	0.702
O	0.293	0.000	0.489
O	0.757	0.262	0.221
O	0.757	0.738	0.221
O	0.506	0.000	0.210
O	0.806	0.000	0.997
O	0.778	0.263	0.742
O	0.778	0.737	0.742
O	0.501	0.000	0.768
O	0.739	0.000	0.498
O	0.991	0.500	0.240
O	0.259	0.500	0.988
O	0.019	0.500	0.730
O	0.275	0.500	0.501
O	0.514	0.500	0.230
O	0.770	0.500	0.981
O	0.509	0.500	0.745
O	0.757	0.500	0.492

System: 0.5_1^{III}, Contribution: 15 %			
	8.213	0.007	-0.048
	0.038	8.212	-0.048
	0.003	0.003	8.213
Zr	0.255	0.256	0.748
Zr	0.251	0.251	0.249
Zr	0.752	0.255	0.244
Zr	0.256	0.752	0.245
Ti	0.757	0.263	0.745
Ti	0.755	0.757	0.237
Ti	0.263	0.755	0.743
Ti	0.762	0.762	0.738
Pb	0.013	0.009	0.975
Pb	0.525	0.012	0.972
Pb	0.013	0.013	0.487
Pb	0.525	0.013	0.491
Pb	0.012	0.528	0.975
Pb	0.525	0.525	0.975
Pb	0.009	0.525	0.487
Pb	0.528	0.525	0.488
O	0.996	0.197	0.233
O	0.267	0.996	0.303
O	0.263	0.204	0.001
O	0.499	0.263	0.296
O	0.713	0.988	0.248
O	0.715	0.250	0.994
O	0.988	0.252	0.787
O	0.231	0.987	0.730
O	0.197	0.267	0.504
O	0.506	0.230	0.735
O	0.753	0.991	0.766
O	0.770	0.231	0.513
O	0.987	0.770	0.269
O	0.203	0.499	0.237
O	0.230	0.766	0.994
O	0.506	0.715	0.250
O	0.765	0.506	0.270
O	0.749	0.736	0.004
O	0.991	0.734	0.747
O	0.250	0.506	0.785
O	0.252	0.713	0.512
O	0.496	0.749	0.764
O	0.736	0.496	0.751
O	0.734	0.753	0.509

System: 0.5_1^{IV}, Contribution: 11 %			
	8.089	0.031	-0.027
	0.031	8.089	-0.027
	-0.028	-0.028	7.990
Zr	0.233	0.238	0.260
Zr	0.238	0.233	0.760
Zr	0.232	0.738	0.262
Zr	0.738	0.232	0.762
Ti	0.225	0.732	0.767
Ti	0.732	0.225	0.267
Ti	0.733	0.725	0.273
Ti	0.725	0.733	0.773
Pb	0.952	0.962	0.031
Pb	0.962	0.952	0.531
Pb	0.954	0.471	0.032
Pb	0.960	0.477	0.529
Pb	0.477	0.960	0.029
Pb	0.471	0.954	0.532
Pb	0.479	0.470	0.032
Pb	0.470	0.479	0.532
O	0.304	0.224	0.005
O	0.224	0.304	0.505
O	0.239	0.788	0.995
O	0.268	0.724	0.515
O	0.724	0.268	0.015
O	0.788	0.239	0.495
O	0.761	0.741	0.002
O	0.741	0.761	0.502
O	0.985	0.237	0.216
O	0.993	0.285	0.776
O	0.981	0.773	0.258
O	0.001	0.731	0.738
O	0.510	0.279	0.282
O	0.494	0.237	0.702
O	0.505	0.733	0.234
O	0.505	0.768	0.765
O	0.285	0.993	0.276
O	0.237	0.985	0.716
O	0.237	0.494	0.202
O	0.279	0.510	0.782
O	0.731	0.001	0.238
O	0.773	0.981	0.758
O	0.768	0.505	0.265
O	0.733	0.505	0.734

System: 0.5_1^V, Contribution: 9 %			
	8.125	0.000	0.000
	0.014	8.238	0.000
	0.021	0.148	8.273
Zr	0.750	0.752	0.755
Zr	0.754	0.253	0.757
Zr	0.252	0.755	0.759
Zr	0.253	0.257	0.254
Ti	0.758	0.766	0.259
Ti	0.754	0.261	0.259
Ti	0.253	0.259	0.758
Ti	0.263	0.757	0.257
Pb	0.016	0.018	0.026
Pb	0.009	0.528	0.036
Pb	0.021	0.024	0.518
Pb	0.019	0.520	0.513
Pb	0.518	0.022	0.027
Pb	0.520	0.520	0.033
Pb	0.508	0.027	0.518
Pb	0.515	0.520	0.512
O	0.706	0.998	0.751
O	0.999	0.761	0.707
O	0.756	0.725	0.005
O	0.771	0.498	0.710
O	0.005	0.208	0.754
O	0.727	0.252	0.004
O	0.756	0.991	0.226
O	0.991	0.731	0.259
O	0.717	0.757	0.486
O	0.736	0.490	0.255
O	0.991	0.247	0.223
O	0.760	0.223	0.487
O	0.270	0.001	0.724
O	0.498	0.696	0.754
O	0.221	0.754	0.005
O	0.213	0.487	0.751
O	0.489	0.267	0.720
O	0.259	0.226	0.989
O	0.233	0.989	0.250
O	0.495	0.750	0.224
O	0.264	0.727	0.487
O	0.251	0.506	0.229
O	0.508	0.228	0.252
O	0.227	0.253	0.501

System: 0.25_1^{III}, Contribution: 2 %			
	8.222	0.020	-0.023
	0.016	8.243	-0.042
	-0.021	-0.033	8.166
Zr	0.254	0.261	0.237
Zr	0.267	0.759	0.247
Zr	0.756	0.248	0.242
Zr	0.767	0.259	0.747
Zr	0.754	0.761	0.737
Zr	0.256	0.748	0.742
Ti	0.755	0.769	0.242
Ti	0.255	0.269	0.743
Pb	0.042	0.016	0.968
Pb	0.038	0.027	0.483
Pb	0.002	0.552	0.001
Pb	0.002	0.529	0.455
Pb	0.502	0.028	0.955
Pb	0.501	0.052	0.501
Pb	0.537	0.527	0.982
Pb	0.542	0.517	0.468
O	0.251	0.244	0.990
O	0.252	0.224	0.510
O	0.232	0.739	0.001
O	0.225	0.762	0.497
O	0.724	0.264	0.997
O	0.733	0.237	0.501
O	0.752	0.722	0.010
O	0.750	0.746	0.489
O	0.002	0.253	0.276
O	0.013	0.238	0.751
O	0.989	0.731	0.246
O	0.999	0.744	0.771
O	0.499	0.245	0.272
O	0.489	0.230	0.746
O	0.513	0.737	0.250
O	0.502	0.753	0.776
O	0.229	0.004	0.248
O	0.249	0.999	0.767
O	0.239	0.505	0.269
O	0.256	0.490	0.743
O	0.755	0.990	0.241
O	0.741	0.005	0.771
O	0.749	0.498	0.268
O	0.728	0.504	0.746