Appendix 1

Selected bond lengths (Å) and bond angles (°) of synthetic $(Mg_{1-x}Zn_x)TiO_3$ ($0 \leq x \leq 0.8$) at ambient conditions

	x	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
***A*O$_6$ octahedron**										
3 x *A*-O1	Å	1.998(3)	2.036(3)	2.027(3)	2.026(3)	2.024(3)	2.022(3)	2.028(4)	2.035(4)	2.053(4)
3 x *A*-O1	Å	2.177(3)	2.189(3)	2.201(3)	2.211(3)	2.225(3)	2.231(3)	2.232(4)	2.242(5)	2.258(6)
3 x O-*A*-O	°	77.02	76.11	75.61	75.39	75.09	74.89	74.38	74.34	73.87
3 x O-*A*-O	°	87.98	89.88	89.71	89.75	89.77	89.72	89.80	90.18	91.10
3 x O-*A*-O	°	88.46	88.28	88.59	88.25	87.90	88.07	88.31	88.03	88.21
3 x O-*A*-O	°	103.34	102.59	102.79	103.16	103.58	103.60	103.67	103.62	103.10
3 x O-*A*-O	°	161.04	161.04	160.60	160.10	159.54	159.40	159.02	159.01	159.10
TiO$_6$ octahedron										
3 x Ti-O1	Å	1.888(3)	1.861(3)	1.865(3)	1.862(3)	1.861(3)	1.864(4)	1.867(4)	1.855(4)	1.836(4)
3 x Ti-O1	Å	2.122(3)	2.100(3)	2.098(3)	2.099(3)	2.097(3)	2.094(4)	2.084(4)	2.085(5)	2.075(6)
3 x O-Ti-O	°	162.91	162.04	161.96	162.14	162.55	162.64	162.37	162.38	162.04
3 x O-Ti-O	°	84.24	82.55	82.55	88.47	82.45	82.37	82.10	81.70	81.68
3 x O-Ti-O	°	79.42	79.98	80.00	80.17	80.57	80.74	80.70	81.04	80.64
3 x O-Ti-O	°	92.74	92.94	92.50	92.67	92.83	92.60	92.72	92.79	92.63
3 x O-Ti-O	°	101.64	102.56	102.85	102.67	102.36	102.45	102.62	102.68	103.29
***A*-Ti**	Å	2.946	2.945	2.961	2.970	2.976	2.979	2.982	2.985	2.986
A*-*A ***a***	Å	2.994	2.992	2.698	2.983	3.014	3.018	3.020	3.023	3.023
A*-*A ***b***	Å	3.968	3.981	3.956	3.936	3.910	3.901	3.893	3.889	3.892
Ti-Ti ***a***	Å	2.978	2.981	2.983	3.006	2.981	2.983	2.983	2.984	2.985
Ti-Ti ***b***	Å	4.044	4.036	4.033	4.041	4.057	4.062	4.066	4.065	4.060
O-O ***c***	Å	2.711	2.699	2.698	2.704	2.712	2.713	2.698	2.709	2.714
O-O ***d***	Å	3.135	3.178	3.168	3.175	3.180	3.179	3.188	3.199	3.216
O-O ***e***	Å	2.916	2.986	2.985	2.993	3.002	3.004	3.010	3.033	3.081
O-O ***f***	Å	2.903	2.944	2.955	2.953	2.952	2.960	2.971	2.975	3.004
O-O ***g***	Å	2.927	2.904	2.918	2.908	2.899	2.907	2.914	2.897	2.879
O-O ***h***	Å	2.695	2.619	2.621	2.618	2.614	2.613	2.600	2.583	2.537
O-O ***i***	Å	2.907	2.876	2.868	2.871	2.871	2.866	2.863	2.857	2.832
Ti-O-*A* ***j***	°	120.37	119.88	119.75	119.82	119.93	119.89	119.43	119.64	119.66
A*-O-*A ***k***	°	91.54	90.12	90.28	90.25	90.23	90.28	90.20	89.81	88.90
Ti-O-Ti ***l***	°	95.76	97.45	97.45	97.25	97.57	97.63	97.89	98.29	99.36
Ti-O-*A* ***m***	°	128.01	127.61	127.83	127.40	126.94	127.07	127.14	126.70	126.40
Ti-O-*A* ***n***	°	86.49	86.71	87.02	87.04	86.98	87.00	87.35	87.15	87.02
Ti-O-*A* ***o***	°	134.52	135.10	134.62	134.84	135.10	134.90	135.00	135.21	135.28

The metal-metal distances: ***a*** across shared edge between adjacent metal sites; ***b*** across vacant octahedral position, along $[001]_h$.

The oxygen-oxygen distances: ***c*** *A*-Ti shared face; ***d*** *A* site, face opposite the shared face; ***e*** *A* site, shared edge; ***f*** *A* site, unshared edge; ***g*** Ti site, face opposite the shared face; ***h*** Ti site, shared edge; ***i*** Ti site, unshared edge.

Framework angles: ***j***, ***m***, and ***o*** at the shared vertex; ***k*** and ***l*** at the shared edge; ***n*** shared face.

TABLE 1

Refinement parameters and crystallographic characteristics of synthetic $(Mg_{1-x}Zn_x)TiO_3$ $(0 \leq x \leq 0.8)$ at ambient conditions

		0	1	2	3	4	5	6	7	8
$^{vi}R_A^{2+}$	Å	0.72	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.74
t*		0.748	0.748	0.749	0.750	0.750	0.751	0.752	0.753	0.755
Phase composition										
$ATiO_3$	%	≥ 95	≥ 95	≥ 95	≥ 95	≥ 95	97.07	98.60	99.22	99.88
Other	%	Arm	Arm, Ru	Arm, Ru	Arm, Ru	Arm, Ru	Ru 2.93	Ru (1.40)	Ru (0.78)	Ru (0.22)
Agreement factors										
R_{wp}	%	13.37	12.81	12.68	12.03	11.43	11.27	11.18	12.04	11.26
R_{Bragg}	%	4.570	2.131	2.139	1.951	2.342	2.427	1.571	2.161	2.264
GOF		1.60	1.57	1.54	1.55	1.51	1.48	1.55	1.61	1.58
DW		0.95	1.04	1.00	1.02	1.06	1.06	1.05	0.92	0.94
Unit cell parameters										
a	Å	5.05669(4)	5.05758(4)	5.05968(3)	5.06232(4)	5.06422(4)	5.06690(3)	5.06893(4)	5.07109(3)	5.07191(4)
c	Å	13.9034(2)	13.9067(1)	13.9114(1)	13.9158(1)	13.9182(1)	13.9216(1)	13.9232(1)	13.9235(1)	13.9243(2)
c*/*a		2.750	2.750	2.749	2.749	2.748	2.748	2.747	2.746	2.745
V	Å^3	307.883(6)	308.064(5)	308.422(4)	308.844(6)	309.127(6)	309.532(5)	309.814(6)	310.085(4)	310.204(6)
Coordination polyhedra characteristics										
<*A*-O1>	Å	2.088(3)	2.113(3)	2.114(3)	2.119(3)	2.124(3)	2.126(3)	2.130(4)	2.138(5)	2.156(6)
V_{AO6}	Å^3	11.644(4)	12.062(4)	12.062(4)	12.120(4)	12.183(4)	12.206(5)	12.245(5)	12.392(6)	12.694(7)
***A*-shift**	Å	0.158	0.134	0.151	0.161	0.176	0.182	0.178	0.180	0.176
Δ_{AO6}		1.838	1.311	1.694	1.906	2.238	2.415	2.293	2.342	2.261
δ_{AO6}		75.62	75.95	79.87	83.52	88.11	89.37	92.95	93.14	93.47
<Ti-O1>	Å	2.005(3)	1.980(3)	1.982(3)	1.981(3)	1.979(3)	1.979(4)	1.975(4)	1.970(5)	1.955(6)
V_{TiO6}	Å^3	10.394(3)	9.975(4)	9.993(4)	9.986(4)	9.971(4)	9.973(4)	9.906(4)	9.826(5)	9.582(6)
Ti-shift	Å	0.206	0.213	0.209	0.212	0.212	0.206	0.195	0.207	0.219
Δ_{TiO6}		3.405	3.641	3.457	3.580	3.555	3.377	3.017	3.408	3.734
δ_{TiO6}		61.74	69.06	70.04	68.78	65.72	65.71	67.62	68.09	72.82

- no data available. * Tolerance factor for ABO_3 compounds, $t = (R_O + R_A)/[\sqrt{2}\,(R_O + R_B)]$ (Goldschmidt, 1926). Arm armalcolite, Ru rutile.