Table 1

Evolution of unit cell parameters and superstructure formation in tetragonal tungsten bronze (TTB) related phases along the BaO-Ta_2O_5 binary. From 43 to 39 mol% BaO, no superstructure formation is observed. From 38 to 31 mol% BaO, the *a*- and *b*-parameters are related to those of the TTB structure by a factor of √2. From 30 to 26 mol% BaO, tripling of the TTB *b*-parameter is observed. Despite the large variation in Ba-content, the change in specific volume is less than 1%. Indexed X-ray powder diffraction data are given in Tables X, Y, and Z for the compounds listed here.

mol BaO:Ta_2O_5	Space Group	a (Å)	b (Å)	c (Å)	Vol (Å^3)
43.0:57.0	*P4bm*	12.513(1)		3.9296(2)	615.29(3)
32.5:67.5	*P4bm*	17.695(1)		3.9188(2)	613.52(4)*
27.5:72.5	*Pbam*	12.517(1)	37.482(2)	3.9124(2)	611.87(4)*

*normalized on the basis of a 12 Å x 4 Å TTB-type unit cell for comparison with the other table entries

Table 2

X-Ray powder diffraction data for 43:57 $BaO:Ta_2O_5$, indexed with a tetragonal-tungsten-bronze-type (TTB) unit cell and reflection conditions of *P4bm*: *a*=12.513(1), *c*=3.9296(2) Å.

h	k	l	$2\theta_{obs}$	I_{obs}	$2\theta_{calc}$	$\Delta 2\theta$	d_{obs}
1	1	0	9.990	2	9.988	0.002	8.847
2	0	0	14.118	1	14.144	-0.026	6.268
2	1	0	15.836	1	15.823	0.013	5.592
2	2	0	20.061	3	20.054	0.007	4.4225
3	1	0	22.445	33	22.450	-0.005	3.9578
0	0	1	22.605	31	22.609	-0.004	3.9302
3	2	0	25.647	32	25.647	0.000	3.4705
2	0	1	26.770	10	26.768	0.002	3.3274
2	1	1	27.728	48	27.717	0.011	3.2146
4	0	0	28.511	3	28.509	0.002	3.1280
4	1	0	29.410	100	29.406	0.004	3.0344
3	3	0	30.291	34	30.279	0.012	2.9482
2	2	1	30.411	17	30.399	0.012	2.9368
4	2	0	31.974	53	31.959	0.015	2.7967
3	1	1	32.074	83	32.074	0.000	2.7882
3	2	1	34.456	44	34.449	0.007	2.6007
4	0	1	36.697	15	36.689	0.008	2.4469
4	1	1	37.419	5	37.410	0.009	2.4013
5	2	0	38.721	1	38.719	0.002	2.3235
4	2	1	39.502	8	39.504	-0.002	2.2793
4	4	0	40.762	1	40.757	0.005	2.2117
5	3	0	42.063	11	42.070	-0.007	2.1463
4	3	1	42.784	1	42.804	-0.020	2.1118
6	0	0	43.345	2	43.350	-0.005	2.0857
5	1	1	43.445	1	43.439	0.006	2.0812
6	1	0	43.983	1	43.979	0.004	2.0570
5	2	1	45.305	4	45.302	0.003	2.0000
6	2	0	45.827	16	45.825	0.002	1.9784
0	0	2	46.168	33	46.164	0.004	1.9646
5	4	0	46.427	3	46.427	0.000	1.9542
5	3	1	48.287	1	48.281	0.006	1.8832
6	3	0	48.770	27	48.779	-0.009	1.8656
6	0	1	49.412	6	49.434	-0.022	1.8429
6	1	1	49.982	1	50.003	-0.021	1.8232
2	2	2	50.812	1	50.804	0.008	1.7954
7	1	0	51.611	79	51.606	0.005	1.7694
6	2	1	51.661	52	51.684	-0.023	1.7678
3	1	2	51.893	5	51.916	-0.023	1.7605
5	4	1	52.233	28	52.235	-0.002	1.7498
7	2	0	53.254	5	53.249	0.005	1.7186
3	2	2	53.573	11	53.553	0.020	1.7092
6	3	1	54.395	23	54.401	-0.006	1.6853
4	0	2	55.138	1	55.156	-0.018	1.6643
4	1	2	55.677	44	55.683	-0.006	1.6494
7	3	0	55.938	1	55.914	0.024	1.6424
3	3	2	56.215	14	56.208	0.007	1.6349

7	1	1	57.019	48	57.029	-0.010	1.6138
4	2	2	57.237	15	57.246	-0.009	1.6081
6	5	0	57.479	3	57.473	0.006	1.6019
7	2	1	58.558	7	58.568	-0.010	1.5750
8	0	0	58.999	6	59.005	-0.006	1.5642
8	1	0	59.517	6	59.510	0.007	1.5519
8	2	0	61.000	10	61.010	-0.010	1.5176
6	5	1	62.562	6	62.558	0.004	1.4834
6	6	0	62.981	2	62.978	0.003	1.4746
8	3	0	63.462	9	63.464	-0.002	1.4646
7	5	0	63.962	4	63.948	0.014	1.4543
5	3	2	64.240	6	64.219	0.021	1.4487
8	1	1	64.521	1	64.498	0.023	1.4431
6	0	2	65.171	1	65.180	-0.009	1.4302
8	2	1	65.944	2	65.933	0.011	1.4153
8	4	0	66.826	1	66.815	0.011	1.3988
6	2	2	67.085	9	67.079	0.006	1.3940
5	4	2	67.530	1	67.550	-0.020	1.3859
8	3	1	68.286	9	68.290	-0.004	1.3724
7	5	1	68.765	5	68.757	0.008	1.3640
6	3	2	69.409	16	69.417	-0.008	1.3529

Table 3

X-Ray powder diffraction data for TTB-related 32.5:67.5 $BaO:Ta_2O_5$, indexed with a tetragonal unit cell and reflection conditions of *P4bm*: *a*=17.695(1), *c*=3.9188(2) Å. The *a*-parameter is related to that of the tetragonal tungsten bronze structure by √2.

h	k	l	$2\theta_{obs}$	I_{obs}	$2\theta_{calc}$	$\Delta 2\theta$	d_{obs}
2	0	0	10.018	2	9.989	0.029	8.822
2	2	0	14.161	1	14.145	0.016	6.249
4	0	0	20.040	3	20.055	-0.015	4.4271
4	2	0	22.460	32	22.452	0.008	3.9552
0	0	1	22.680	55	22.672	0.008	3.9174
1	1	1	23.800	2	23.773	0.027	3.7355
2	0	1	24.838	2	24.828	0.010	3.5817
2	1	1	25.369	2	25.341	0.028	3.5079
5	1	0	25.641	30	25.649	-0.008	3.4713
2	2	1	26.839	6	26.822	0.017	3.3190
3	1	1	27.780	26	27.769	0.011	3.2087
4	4	0	28.519	4	28.511	0.008	3.1272
5	3	0	29.419	100	29.408	0.011	3.0335
6	0	0	30.299	30	30.281	0.018	2.9474
4	0	1	30.459	15	30.448	0.011	2.9323
6	1	0	30.717	1	30.709	0.008	2.9082
4	1	1	30.900	1	30.874	0.026	2.8914
3	3	1	31.298	2	31.294	0.004	2.8556
6	2	0	31.980	32	31.961	0.019	2.7962
4	2	1	32.121	62	32.120	0.001	2.7842
5	1	1	34.500	40	34.493	0.007	2.5975
5	2	1	35.601	1	35.627	-0.026	2.5197
4	4	1	36.739	12	36.731	0.008	2.4442
5	3	1	37.459	20	37.451	0.008	2.3988
6	0	1	38.132	2	38.159	-0.027	2.3580
6	1	1	38.520	1	38.510	0.010	2.3352
6	2	1	39.520	11	39.544	-0.024	2.2783
8	0	0	40.751	1	40.760	-0.009	2.2123
8	2	0	42.060	9	42.073	-0.013	2.1464
7	1	1	42.841	1	42.842	-0.001	2.1091
6	6	0	43.360	2	43.354	0.006	2.0851
6	4	1	43.480	1	43.476	0.004	2.0796
7	3	1	45.318	2	45.338	-0.020	1.9994
8	4	0	45.820	12	45.828	-0.008	1.9787
0	0	2	46.300	48	46.297	0.003	1.9593
9	2	0	47.321	1	47.323	-0.002	1.9193
2	0	2	47.501	1	47.487	0.014	1.9125
9	3	0	48.760	19	48.783	-0.023	1.8660
6	6	1	49.462	1	49.469	-0.007	1.8412
4	0	2	50.957	1	50.929	0.028	1.7906
8	6	0	51.620	62	51.610	0.010	1.7691
8	4	1	51.729	51	51.717	0.012	1.7657
4	2	2	52.022	13	52.039	-0.017	1.7564
9	1	1	52.260	14	52.269	-0.009	1.7490

9	2	1	53.103	1	53.088	0.015	1.7232
9	5	0	53.279	1	53.253	0.026	1.7179
4	3	2	53.400	1	53.404	-0.004	1.7143
5	1	2	53.662	13	53.674	-0.012	1.7065
9	3	1	54.432	26	54.434	-0.002	1.6842
4	4	2	55.278	1	55.275	0.003	1.6604
5	3	2	55.800	53	55.802	-0.002	1.6461
6	0	2	56.320	16	56.325	-0.005	1.6321
8	6	1	57.060	45	57.061	-0.001	1.6127
6	2	2	57.359	16	57.362	-0.003	1.6050
9	5	1	58.618	1	58.600	0.018	1.5735
8	8	0	59.000	9	59.009	-0.009	1.5642
11	3	0	59.520	6	59.515	0.005	1.5518
10	6	0	61.000	9	61.015	-0.015	1.5176
6	5	2	62.620	4	62.630	-0.010	1.4822
8	0	2	63.362	3	63.361	0.001	1.4666
11	5	0	63.482	4	63.469	0.013	1.4641
8	8	1	64.039	5	64.047	-0.008	1.4527
8	2	2	64.321	5	64.329	-0.008	1.4471
12	3	0	65.163	1	65.156	0.007	1.4304
10	6	1	65.979	5	65.964	0.015	1.4147
8	4	2	67.199	7	67.187	0.012	1.3919
9	1	2	67.641	1	67.657	-0.016	1.3839
11	5	1	68.300	6	68.321	-0.021	1.3721
12	2	1	68.769	3	68.787	-0.018	1.3639
9	3	2	69.501	14	69.523	-0.022	1.3513

Table 4

X-Ray powder diffraction data for TTB-related 27.5:72.5 $BaO:Ta_2O_5$, indexed with an orthorhombic unit cell and reflection conditions of *Pbam*: *a*=12.517(1), *b*=37.482(2), *c*=3.9124(2) Å. The *b*-parameter is related to that of the tetragonal tungsten bronze structure by √2.

h	k	l	$2\theta_{obs}$	I_{obs}	$2\theta_{calc}$	$\Delta 2\theta$	d_{obs}
1	3	0	10.021	2	9.995	0.026	8.820
0	6	0	14.185	1	14.166	0.019	6.238
2	6	0	20.081	4	20.066	0.015	4.4181
1	9	0	22.480	36	22.481	-0.001	3.9518
0	0	1	22.720	72	22.709	0.011	3.9105
0	10	0	23.723	1	23.718	0.005	3.7474
1	1	1	23.946	4	23.928	0.018	3.7130
1	2	1	24.279	3	24.283	-0.004	3.6629
0	4	1	24.660	3	24.638	0.022	3.6071
1	3	1	24.859	1	24.865	-0.006	3.5787
2	9	0	25.679	37	25.672	0.007	3.4662
0	6	1	26.878	6	26.866	0.012	3.3143
1	6	1	27.821	17	27.811	0.010	3.2040
2	4	1	28.521	5	28.518	0.003	3.1270
2	5	1	29.420	100	29.418	0.002	3.0334
3	9	0	30.300	43	30.297	0.003	2.9473
2	6	1	30.486	18	30.484	0.002	2.9297
4	5	0	30.941	4	30.940	0.001	2.8877
3	1	1	31.408	2	31.409	-0.001	2.8458
4	6	0	31.974	35	31.961	0.013	2.7967
3	3	1	32.150	59	32.144	0.006	2.7818
2	8	1	33.059	3	33.058	0.001	2.7074
3	5	1	33.563	1	33.572	-0.009	2.6678
1	10	1	33.874	1	33.857	0.017	2.6441
2	9	1	34.539	44	34.537	0.002	2.5947
4	0	1	36.760	11	36.746	0.014	2.4428
4	3	1	37.474	28	37.468	0.006	2.3979
5	5	0	37.838	2	37.857	-0.019	2.3757
3	9	1	38.202	5	38.197	0.005	2.3539
4	6	1	39.552	14	39.566	-0.014	2.2766
4	12	0	40.781	1	40.783	-0.002	2.2108
5	9	0	42.080	12	42.078	0.002	2.1455
5	2	1	43.123	1	43.134	-0.011	2.0960
6	0	0	43.339	2	43.336	0.003	2.0860
4	14	0	44.519	1	44.499	0.020	2.0334
5	6	1	45.374	1	45.354	0.020	1.9971
6	6	0	45.820	12	45.818	0.002	1.9787
0	0	2	46.381	50	46.378	0.003	1.9560
0	2	2	46.634	2	46.645	-0.011	1.9460
2	19	0	48.323	2	48.335	-0.012	1.8819
6	9	0	48.780	27	48.782	-0.002	1.8653
2	17	1	49.598	1	49.604	-0.006	1.8364
7	3	0	51.601	59	51.590	0.011	1.7697
6	6	1	51.719	35	51.727	-0.008	1.7660

1	9	2	52.139	12	52.127	0.012	1.7527
5	12	1	52.283	15	52.302	-0.019	1.7483
1	10	2	53.283	2	53.283	0.000	1.7178
3	6	2	53.750	15	53.749	0.001	1.7039
6	9	1	54.459	30	54.451	0.008	1.6834
2	22	0	55.879	50	55.883	-0.004	1.6440
3	9	2	56.400	16	56.405	-0.005	1.6300
7	3	1	57.061	43	57.060	0.001	1.6127
4	6	2	57.421	16	57.431	-0.010	1.6034
7	6	1	58.617	1	58.604	0.013	1.5735
8	0	0	58.981	6	58.984	-0.003	1.5647
4	8	2	59.006	7	59.025	-0.019	1.5641
7	12	0	59.517	8	59.519	-0.002	1.5519
8	6	0	61.006	9	60.996	0.010	1.5175
3	21	1	61.217	1	61.196	0.021	1.5128
6	15	1	62.614	7	62.628	-0.014	1.4823
6	18	0	63.000	2	63.020	-0.020	1.4742
4	12	2	63.430	5	63.443	-0.013	1.4652
8	9	0	63.458	4	63.457	0.001	1.4646
7	15	0	63.961	6	63.970	-0.009	1.4543
8	1	1	64.078	3	64.093	-0.015	1.4520
5	9	2	64.399	6	64.397	0.002	1.4455
6	0	2	65.328	1	65.339	-0.011	1.4272
8	6	1	65.971	6	65.962	0.009	1.4148
8	12	0	66.835	1	66.818	0.017	1.3986
6	6	2	67.250	9	67.242	0.008	1.3910
9	3	0	67.716	2	67.733	-0.017	1.3825
8	9	1	68.339	6	68.325	0.014	1.3714
7	15	1	68.804	6	68.819	-0.015	1.3633
6	9	2	69.571	16	69.584	-0.013	1.3501

Table 5

Unit cell parameters (space group *Cmcm*) for the orthorhombic homologous series $BaTi_nTa_4O_{11+2n}$, n=3,5,7,9, with "rutile-slab" type structures. Successive members are generated by adding $2TiO_2$ to the width of the slabs, thus increasing the c-axis by ~4.4 Å, while the other cell parameters remain relatively unaffected.

Formula	n	a (Å)	b (Å)	c (Å)
$BaTi_3Ta_4O_{17}$	3	6.6220(8)	8.9438(9)	21.115(3)
$BaTi_5Ta_4O_{21}$	5	6.6073(3)	8.9205(5)	25.541(1)
$BaTi_7Ta_4O_{25}$	7	6.5911(4)	8.9051(5)	29.960(2)
$BaTi_9Ta_4O_{29}$	9	6.5832(4)	8.8942(6)	34.343(2)

Table 6

Crystallographic data for *13L* $Ba_{18}Ti_{53}Ta_2O_{129}$ and *7L* $Ba_{10}Ti_{27}Ta_2O_{69}$ from single-crystal X-ray diffraction studies

Formula	$Ba_{18}Ti_{53}Ta_2O_{129}$	$Ba_{10}Ti_{27}Ta_2O_{69}$
Space Group	*C2/m*	*C2/m*
a	9.859(2) Å	9.855(3) Å
b	17.067(5) Å	17.081(7) Å
c	30.618(8) Å	16.719(7) Å
β	96.11(2)º	101.18(3)º
V	5123(2) $Å^3$	2761(2) $Å^3$
Z	2	2
dimensions	0.24 x 0.08 x 0.17 mm^3	0.14 x 0.08 x 0.06 mm^3
transmission factors	0.069 to 0.173	0.34 to 0.54
Reflections measured	45843	8812
unique	9529	4169
observed	6824	3017
R_F	0.095	0.072
R_{wF} (all reflections)	0.094	0.078
secondary extinction	0.168(15) μm	0.32(4) μm

Table 7

Refined structural parameters for *13L* $Ba_{18}Ti_{53}Ta_2O_{129}$. The symbol M represents mixed Ti/Ta octahedral sites; the occupancies were refined as mixed-atom sites containing xTi + (1−x)Ta. The refined occupancies correspond to Ti (= x). (*C2/m*, No.12; ***a***=9.859(2) Å, ***b***=17.067(5) Å, ***c***=30.618(8) Å, β=96.11(2)°; Z=2)

atom	pos	x	y	z	B_{iso}	occ. Ti
Ba 1	8j	0.65431(8)	0.14632(5)	0.45841(3)	0.82 (3)	
Ba 2	4g	½	0.14403(8)	0	0.92 (4)	
Ba 3	8j	0.10535(8)	0.14643(5)	0.31046(3)	0.77 (3)	
Ba 4	8j	0.74300(8)	0.14641(5)	0.22721(3)	0.80 (3)	
Ba 5	8j	0.19673(8)	0.14811(6)	0.07954(3)	1.03 (3)	
M 1	4i	0.85168(23)	0	0.03045(7)	0.88 (7)	0.784(8)
M 2	4i	0.0654 (3)	0	0.19843(9)	0.64 (9)	0.899(8)
M 3	4i	0.7826 (3)	0	0.34011(9)	0.40 (10)	0.956(8)
M 4	4i	0.5402 (3)	0	0.11043(9)	0.36 (10)	0.942(8)
M 5	8j	0.55046(18)	0.17695(11)	0.11378(6)	0.49 (5)	0.921(6)
M 6	4h	0	0.18372(20)	½	0.44 (11)	0.992(8)
M 7	8j	0.07447(19)	0.17567(12)	0.19273(6)	0.54 (6)	0.932(6)
M 8	8j	0.42224(22)	0.18304(15)	0.26892(8)	0.64 (7)	0.978(6)
M 9	8j	0.85544(19)	0.17779(13)	0.03649(7)	0.70 (6)	0.923(6)
M10	2c	0	0	½	0.51 (17)	1.0
M11	8j	0.29832(20)	0.17577(13)	0.42406(7)	0.66 (7)	0.950(6)
M12	4i	0.4223 (3)	0	0.26881(11)	0.67 (12)	0.983(8)
M13	4i	0.3130 (3)	0	0.42932(10)	0.61 (10)	0.938(8)
M14	8j	0.77215(20)	0.17577(13)	0.34504(7)	0.57 (7)	0.946(6)
M15	8j	0.02722(22)	0.09244(14)	0.41618(7)	0.47 (7)	0.992(6)
M16	8j	0.50673(22)	0.09224(14)	0.35281(8)	0.49 (8)	0.995(5)
M17	8j	0.82089(22)	0.09141(14)	0.12050(7)	0.41 (7)	1.0
M18	8j	0.34209(24)	0.09220(15)	0.18592(8)	0.42 (8)	1.0
O 1	8j	0.3985 (10)	0.1548 (6)	0.1488 (3)	0.529(23)	
O 2	8j	0.8291 (10)	0.0837 (6)	0.3084 (3)	0.529(23)	
O 3	8j	0.3801 (10)	0.0851 (6)	0.4619 (3)	0.529(23)	
O 4	4i	0.5773 (14)	0	0.3140 (4)	0.529(23)	
O 5	8j	0.9133 (10)	0.0880 (6)	0.4648 (3)	0.529(23)	
O 6	8j	0.1984 (10)	0.0861 (6)	0.3922 (3)	0.529(23)	
O 7	4i	0.7264 (14)	0	0.0822 (4)	0.529(23)	
O 8	8j	0.4895 (10)	0.0870 (6)	0.2344 (3)	0.529(23)	
O 9	8j	0.9008 (10)	0.1591 (6)	0.1593 (3)	0.529(23)	
O10	4i	0.1242 (14)	0	0.4563 (4)	0.529(23)	
O11	8j	0.0175 (10)	0.0839 (6)	0.2307 (3)	0.529(23)	

O12	2a	0	0	0	0.529(23)
O13	8j	0.3591 (10)	0.0886 (6)	0.3046 (3)	0.529(23)
O14	4e	¼	¼	0	0.529(23)
O15	8j	0.2377 (10)	0.0885 (6)	-0.0041 (3)	0.529(23)
O16	4i	0.2711 (14)	0	0.2257 (4)	0.529(23)
O17	4i	0.4464 (14)	0	0.3854 (4)	0.529(23)
O18	8j	0.6962 (10)	0.0865 (6)	0.3771 (3)	0.529(23)
O19	8j	0.2647 (10)	0.1729 (6)	0.2266 (3)	0.529(23)
O20	8j	0.4681 (10)	0.0833 (6)	0.0782 (3)	0.529(23)
O21	4i	0.9463 (14)	0	0.3841 (4)	0.529(23)
O22	8j	0.1305 (10)	0.1695 (6)	0.4567 (3)	0.529(23)
O23	8j	0.6515 (10)	0.0857 (6)	0.1465 (3)	0.529(23)
O24	8j	0.1528 (10)	0.0878 (6)	0.1612 (3)	0.529(23)
O25	8j	0.5829 (10)	0.1718 (6)	0.3126 (3)	0.529(23)
O26	4i	0.9049 (14)	0	0.1525 (4)	0.529(23)
O27	8j	0.3294 (10)	0.2538 (6)	0.3018 (3)	0.529(23)
O28	4g	0	0.1778 (8)	0	0.529(23)
O29	8j	0.2212 (10)	0.2501 (6)	0.3851 (3)	0.529(23)
O30	8j	0.9355 (10)	0.0879 (6)	0.0736 (3)	0.529(23)
O31	8j	0.4502 (10)	0.1607 (6)	0.3914 (3)	0.529(23)
O32	8j	0.3848 (10)	0.2452 (6)	0.4686 (3)	0.529(23)
O33	8j	0.9434 (10)	0.1617 (6)	0.3765 (3)	0.529(23)
O34	4i	0.4042 (14)	0	0.1560 (4)	0.529(23)
O35	8j	0.7179 (10)	0.1752 (6)	0.0816 (3)	0.529(23)
O36	8j	0.1288 (10)	0.2496 (6)	0.1548 (3)	0.529(23)
O37	8j	0.0134 (10)	0.2455 (6)	0.2369 (3)	0.529(23)
O38	8j	0.4567 (10)	0.2437 (6)	0.0734 (3)	0.529(23)

Table 8

Refined structural parameters for *7L* $Ba_{10}Ti_{27}Ta_2O_{69}$. The symbol M represents mixed Ti/Ta octahedral sites; the occupancies were refined as mixed-atom sites containing xTi + (1−x)Ta. The refined occupancies correspond to Ti (= x). (*C2/m*, No.12; ***a***=9.855(3) Å, ***b***=17.081(7) Å, ***c***=16.719(7) Å, β=101.18(3)°; Z=2)

atom	site	x	y	z	B_{iso}	occ. Ti
Ba 1	8j	0.21936(13)	0.14844(8)	0.14807(7)	0.92(4)	
Ba 2	4g	½	0.14394(10)	0	0.76(6)	
Ba 3	8j	0.80719(12)	0.14653(7)	0.42241(7)	0.70(4)	
M 1	4i	0.8577 (3)	0	0.05634(18)	0.40(13)	0.84(1)
M 2	4h	½	0.1828 (3)	½	0.51(18)	0.97(1)
M 3	4i	0.1208 (4)	0	0.36801(22)	0.61(16)	0.90(1)
M 4	4i	0.5714 (4)	0	0.20498(22)	0.35(15)	0.92(1)
M 5	8j	0.5825 (3)	0.17702(16)	0.21148(15)	0.51(10)	0.906(7)
M 6	8j	0.1283 (3)	0.17564(16)	0.35800(15)	0.51(10)	0.914(7)
M 7	2d	½	0	½	0.8 (3)	0.97(1)
M 8	8j	0.8664 (3)	0.17719(16)	0.06789(16)	0.61(10)	0.922(7)
M 9	8j	0.8549 (3)	0.09135(19)	0.22380(17)	0.43(12)	0.973(7)
M10	8j	0.3947 (3)	0.09214(20)	0.34508(18)	0.41(12)	0.994(7)
O 1	8j	0.4386 (13)	0.1581 (7)	0.2749 (7)	0.14(17)	
O 2	8j	0.5550 (13)	0.0867 (8)	0.4347 (7)	0.34(18)	
O 3	8j	0.3299 (13)	0.1723 (7)	0.4197 (7)	0.13(17)	
O 4	4i	0.3341 (20)	0	0.4181 (11)	0.4 (3)	
O 5	8j	0.0810 (14)	0.0833 (8)	0.4267 (8)	0.55(19)	
O 6	4i	0.7481 (20)	0	0.1537 (12)	0.5 (3)	
O 7	8j	0.2376 (15)	0.0897 (8)	-0.0052 (8)	0.69(20)	
O 8	4e	¼	¼	0	0.7 (3)	
O 9	8j	0.9573 (14)	0.0879 (8)	0.1368 (8)	0.58(19)	
O10	8j	0.4899 (15)	0.0830 (9)	0.1452 (8)	0.82(21)	
O11	8j	0.0824 (13)	0.2446 (7)	0.4395 (7)	0.15(17)	
O12	8j	0.1733 (14)	0.2501 (8)	0.2859 (8)	0.38(18)	
O13	2a	0	0	0	0.4 (4)	
O14	8j	0.6931 (14)	0.0867 (8)	0.2716 (8)	0.47(19)	
O15	8j	0.2008 (14)	0.0861 (8)	0.2993 (8)	0.57(19)	
O16	4i	0.9497 (21)	0	0.2849 (12)	0.6 (3)	
O17	4i	0.4493 (22)	0	0.2868 (12)	0.8 (3)	
O18	8j	0.9467 (14)	0.1610 (8)	0.2957 (8)	0.41(19)	
O19	8j	0.7411 (15)	0.1726 (9)	0.1500 (9)	0.84(21)	
O20	4g	0	0.1768 (14)	0	1.1 (3)	
O21	8j	0.4768 (15)	0.2439 (9)	0.1334 (9)	0.85(21)	

Table 9

Unit cell parameters (space group *P4bm*) for the tetragonal tungsten bronze type solid solution $Ba_{6-x}Ti_{2-2x}Ta_{8+2x}O_{30}$, $0 \leq x \leq 0.723$, which forms on the join between $Ba_6Ti_2Ta_8O_{30}$ and $BaTa_2O_6$.

x	a (Å)	c (Å)	Vol (Å^3)
0	12.560(1)	3.9559(3)	624.01(6)
0.253	12.562(1)	3.9539(2)	623.98(4)
0.500	12.560(1)	3.9513(3)	623.38(6)
0.723	12.562(1)	3.9487(2)	623.15(3)