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Tungsten Bronze Barium Neodymium Titanate ($\text{Ba}_{6-3n}\text{Nd}_{8+2n}\text{Ti}_{18}\text{O}_{54}$): An Intrinsic Nanostructured Material and Its Defect Distribution

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Table S1. Cation – Oxygen bond distances for composition n = 0.3

Ba – O bond distances for n = 0.3		
Number	Atoms	Bond length (Å) and uncertainty (Å)
1	Ba6 - O9	(2.7386 (0.0090))
2	Ba7 - O9	2.7421 (0.0084)
3	Ba6 - O8	2.8325 (0.0101)
4	Ba7 - O18	2.8638 (0.0088)
5	Ba6 - O1	2.9029 (0.0055)
6	Ba6 - O16	2.9198 (0.0111)
7	Ba7 - O4	2.9265 (0.0065)
8	Ba7 - O8	2.9304 (0.0100)
9	Ba6 - O10	2.9774 (0.0090)
10	Ba7 - O15	3.0090 (0.0111)
11	Ba7 - O1	3.0588 (0.0059)
12	Ba7 - O17	3.1123 (0.0089)
13	Ba6 - O4	3.2851 (0.0066)
14	Ba6 - O11	3.3744 (0.0088)
15	Ba6 - O15	3.5752 (0.0111)
16	Ba6 - O5	3.6333 (0.0065)
17	Ba6 - O14	3.6711 (0.0087)
18	Ba7 - O5	3.7317 (0.0061)
19	Ba7 - O12	3.7718 (0.0090)
20	Ba7 - O16	3.8822 (0.0111)
Nd – O bond distances		
1	Nd5 - O6	2.3902 (0.0070)
3	Nd1 - O2	2.3936 (0.0058)
5	Nd1 - O12	2.4164 (0.0092)
6	Nd1 - O11	2.4185 (0.0087)
7	Nd3 - O15	2.4219 (0.0112)
8	Nd4 - O5	2.4236 (0.0076)
9	Nd5 - O14	2.4344 (0.0088)
10	Nd2 - O7	2.4465 (0.0082)
11	Nd4 - O13	2.4913 (0.0092)
12	Nd3 - O3	2.4939 (0.0052)
13	Nd4 - O12	2.5201 (0.0098)
14	Nd3 - O10	2.5231 (0.0108)

15	Nd3 - O4	2.5257 (0.0070)
16	Nd4 - O16	2.5268 (0.0112)
17	Nd2 - O11	2.5345 (0.0090)
18	Nd2 - O17	2.561 (0.0080)
19	Nd1 - O6	2.5641 (0.0074)
20	Nd2 - O7	2.5906 (0.0085)
21	Nd5 - O3	2.5936 (0.0052)
22	Nd3 - O5	2.5988 (0.0079)
23	Nd2 - O18	2.6022 (0.0090)
24	Nd5 - O13	2.6368 (0.0096)
25	Nd4 - O14	2.6389 (0.0080)
26	Nd2 - O1	2.6986 (0.0056)
27	Nd4 - O4	2.7146 (0.0073)
28	Nd5 - O2	2.7682 (0.0062)
29	Nd1 - O17	2.7865 (0.0086)
30	Nd1 - O13	2.8213 (0.0098)
31	Nd3 - O2	2.8767 (0.0055)
32	Nd5 - O7	2.8869 (0.0074)
33	Nd4 - O3	2.9604 (0.0052)
34	Nd2 - O14	2.968 (0.0078)
35	Nd1 - O7	2.9741 (0.0077)
36	Nd5 - O10	2.9755 (0.0094)
37	Nd5 - O18	2.9812 (0.0087)
38	Nd1 - O3	3.0602 (0.0052)
39	Nd2 - O1	3.1801 (0.0058)
40	Nd3 - O17	3.1897 (0.0078)
41	Nd4 - O2	3.2298 (0.0059)
42	Nd3 - O13	3.428 (0.0092)

Ti – O bond distances

1	Ti2 - O9	1.79 (0.0046)
2	Ti5 - O8	1.8295 (0.0049)
3	Ti4 - O4	1.835 (0.0048)
4	Ti1 - O3	1.8793 (0.0045)
6	Ti2 - O6	1.898 (0.0049)
7	Ti2 - O5	1.9056 (0.0051)
8	Ti3 - O8	1.9089 (0.0047)
9	Ti4 - O1	1.9139 (0.0042)
10	Ti2 - O10	1.9291 (0.0041)
11	Ti3 - O1	1.9297 (0.0041)

12	Ti3 - O6	1.9396 (0.0052)
13	Ti3 - O18	1.9438 (0.0040)
14	Ti5 - O16	1.952 (0.0050)
15	Ti3 - O11	1.9567 (0.0041)
16	Ti4 - O17	1.96 (0.0048)
17	Ti5 - O5	1.965 (0.0050)
18	Ti5 - O15	1.9669 (0.0050)
19	Ti5 - O9	1.9691 (0.0041)
20	Ti1 - O2	1.9747 (0.0049)
22	Ti4 - O14	1.9747 (0.0049)
23	Ti1 - O13	1.9854 (0.0022)
25	Ti2 - O12	2.0023 (0.0043)
26	Ti3 - O7	2.0468 (0.0045)
27	Ti4 - O7	2.0589 (0.0046)
28	Ti4 - O2	2.06 (0.0052)
29	Ti2 - O3	2.1393 (0.0048)
30	Ti5 - O4	2.4057 (0.0048)
31	Ti5 - O6	3.5011 (0.0046)
32	Ti2 - O8	3.7318 (0.0051)
33	Ti3 - O9	3.8876 (0.0044)
34	Ti1 - O6	3.9128 (0.0046)
36	Ti1 - O12	3.9857 (0.0079)
38	Ti3 - O7	3.99 (0.0048)
39	Ti2 - O8	3.9979 (0.0048)