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Supporting information for article:

Novel borate Lu5Ba6B9O27 with a new structure type: synthesis, disordered crystal structure and negative linear thermal expansion

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Table S1 Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for of $Lu_5Ba_6B_9O_{27}$.

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq} (Å^2)	Occupancy
Lu1	0.5	0	0	0.00822 (11)	1
Lu2	0.26103 (2)	−0.00756 (3)	0.066162 (14)	0.00822 (8)	1
Lu3	0.36450 (2)	0.24784 (3)	0.212196 (14)	0.00974 (8)	1
Ba1	0.48188 (3)	0.37268 (4)	0.07664 (2)	0.01094 (11)	1
Ba2	0.74687 (3)	0.11058 (4)	0.14021 (2)	0.01546 (13)	1
Ba3	0.56852 (3)	−0.25023 (5)	0.15923 (3)	0.02098 (14)	1
O1	0.5840 (4)	0.1921 (4)	0.0196 (2)	0.0131 (15)	1
O2	0.2920 (4)	0.3363 (5)	0.1078 (2)	0.0168 (16)	1
O3	0.5376 (4)	−0.0040 (5)	0.1119 (2)	0.0164 (16)	1
O4	0.8365 (4)	0.2913 (5)	0.0714 (2)	0.0167 (9)	1
O5	0.6869 (4)	0.4256 (5)	0.1427 (2)	0.0201 (17)	1
O6	0.5036 (8)	0.3968 (9)	0.2771 (5)	0.016 (2)*	0.5
O7	0.4537 (7)	0.6346 (9)	0.2168 (5)	0.017 (3)	0.5
O8	0.5466 (4)	0.1841 (5)	0.1846 (2)	0.0167 (9)	1
O9	0.3432 (3)	0.0938 (4)	−0.0073 (2)	0.0119 (14)	1
O10	0.7513 (4)	−0.1127 (5)	0.2366 (2)	0.0155 (16)	1
O11	0.7363 (4)	−0.3916 (5)	0.2203 (3)	0.0162 (16)	1
O12	0.4546 (7)	0.5346 (10)	0.1764 (5)	0.016 (3)	0.5
O13	0.1607 (4)	0.1799 (5)	0.0485 (3)	0.0165 (16)	1
O14	0.3924 (4)	0.0599 (5)	0.1533 (3)	0.0198 (17)	1
O15	0.1249 (4)	−0.0937 (5)	−0.0155 (2)	0.0167 (9)	1
B1	0.5	0.5202 (11)	0.25	0.012 (2)*	1
B2	0.2062 (6)	0.3058 (7)	0.0547 (4)	0.009 (2)	1
B3	0.4938 (6)	0.0752 (8)	0.1502 (4)	0.014 (2)	1
B4	0.8724 (5)	0.2318 (7)	0.0222 (4)	0.0092 (13)*	1
B5	0.7750 (6)	−0.0274 (8)	0.2921 (4)	0.012 (2)	1

Table S2 Anisotropic atomic displacement parameters (Å^2) of $Lu_5Ba_6B_9O_{27}$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Lu1	0.00680 (16)	0.00809 (17)	0.00940 (18)	0.00033 (14)	0.00176 (14)	0.00171 (15)
Lu2	0.00879 (12)	0.00692 (12)	0.00902 (13)	−0.00089 (10)	0.00269 (10)	0.00025 (10)
Lu3	0.00939 (12)	0.00834 (13)	0.01087 (13)	0.00005 (10)	0.00196 (10)	0.00119 (10)
Ba1	0.01000 (17)	0.01309 (19)	0.00999 (18)	0.00075 (15)	0.00330 (15)	0.00045 (15)
Ba2	0.00929 (18)	0.0210 (2)	0.0145 (2)	−0.00102 (16)	0.00082 (16)	0.00691 (17)
Ba3	0.01235 (19)	0.0164 (2)	0.0304 (3)	−0.00111 (17)	0.00027 (18)	0.00768 (19)
O1	0.018 (2)	0.007 (2)	0.016 (3)	−0.0030 (18)	0.007 (2)	0.0008 (19)
O2	0.018 (2)	0.022 (3)	0.009 (2)	0.001 (2)	0.002 (2)	0.001 (2)
O3	0.012 (2)	0.025 (3)	0.012 (2)	0.003 (2)	0.005 (2)	0.009 (2)
O4	0.0210 (15)	0.0136 (14)	0.0128 (15)	−0.0043 (12)	0.0004 (12)	0.0017 (11)
O5	0.017 (3)	0.033 (3)	0.010 (2)	−0.013 (2)	0.005 (2)	−0.002 (2)
O7	0.016 (5)	0.017 (5)	0.019 (5)	−0.002 (4)	0.007 (4)	0.009 (4)
O8	0.0210 (15)	0.0136 (14)	0.0128 (15)	−0.0043 (12)	0.0004 (12)	0.0017 (11)
O9	0.013 (2)	0.013 (2)	0.011 (2)	0.0040 (18)	0.0059 (19)	0.0044 (19)
O10	0.019 (2)	0.012 (2)	0.015 (2)	0.003 (2)	0.004 (2)	−0.005 (2)
O11	0.016 (2)	0.013 (2)	0.019 (3)	−0.001 (2)	0.005 (2)	0.005 (2)
O12	0.012 (5)	0.025 (5)	0.009 (5)	0.004 (4)	0.001 (4)	0.000 (4)
O13	0.014 (2)	0.010 (2)	0.023 (3)	−0.0025 (19)	0.000 (2)	−0.002 (2)
O14	0.009 (2)	0.027 (3)	0.021 (3)	0.001 (2)	0.000 (2)	−0.007 (2)
O15	0.0210 (15)	0.0136 (14)	0.0128 (15)	−0.0043 (12)	0.0004 (12)	0.0017 (11)
B2	0.015 (3)	0.005 (3)	0.009 (3)	0.003 (3)	0.007 (3)	0.000 (3)
B3	0.018 (4)	0.010 (3)	0.013 (4)	−0.002 (3)	0.001 (3)	0.002 (3)
B5	0.009 (3)	0.016 (4)	0.011 (4)	0.003 (3)	0.002 (3)	−0.006 (3)

Table S3 Selected bond lengths (Å) and bond valence sums (v.u.) of $Lu_5Ba_6B_9O_{27}$.

Atom	Distance (Å)	Bond valence sum (v.u.)	Atom	Distance (Å)	Bond valence sum (v.u.)
Lu1—O1	2.192 (4)	0.516	Lu2—O5^{iv}	2.174 (6)	0.541
Lu1—O1^{i}	2.192 (4)	0.516	Lu2—O14	2.196 (4)	0.510
Lu1—O3	2.201 (5)	0.503	Lu2—O4^{iv}	2.230 (5)	0.465
Lu1—O3^{i}	2.201 (5)	0.503	Lu2—O15	2.235 (4)	0.459
Lu1—O9	2.222 (5)	0.476	Lu2—O13	2.257 (5)	0.433
Lu1—O9^{i}	2.222 (5)	0.476	Lu2—O9	2.321 (5)	0.364
<Lu1—O>$_6$	2.21	2.99	<Lu2—O>$_6$	2.24	2.77
Lu3—O8^{vi}	2.193 (4)	0.514	Ba1—O5	2.686 (5)	0.358
Lu3—O10^{vii}	2.195 (5)	0.512	Ba1—O1	2.705 (5)	0.341
Lu3—O11^{vii}	2.225 (5)	0.472	Ba1—O12	2.711 (10)	0.168
Lu3—O6^{vi}	2.242 (10)	0.225	Ba1—O15^{iii}	2.719 (5)	0.329
Lu3—O2	2.255 (5)	0.435	Ba1—O13^{iii}	2.751 (4)	0.303
Lu3—O14	2.319 (5)	0.366	Ba1—O2	2.763 (5)	0.275
Lu3—O6	2.429 (9)	0.272	Ba1—O8	2.842 (5)	0.240
<Lu3—O>$_7$	2.27	2.80	Ba1—O6^{vi}	2.957 (10)	0.089
Ba2—O12^{ii}	2.712 (9)	0.158	Ba1—O15^{viii}	3.038 (6)	0.145
Ba2—O7^{ii}	2.718 (8)	0.155	<Ba1—O>$_9$	2.80	2.25
Ba2—O4	2.755 (5)	0.281	Ba3—O7^{x}	2.451 (11)	0.319
Ba2—O11^{ix}	2.801 (5)	0.248	Ba3—O11	2.607 (4)	0.419
Ba2—O3	2.869 (5)	0.206	Ba3—O3	2.634 (5)	0.389
Ba2—O1	2.875 (4)	0.203	Ba3—O12^{x}	2.698 (10)	0.164
Ba2—O2^{ii}	2.921 (5)	0.179	Ba3—O10	2.816 (4)	0.238
Ba2—O10	2.970 (5)	0.157	Ba3—O7^{xi}	2.879 (10)	0.100
Ba2—O8	3.102 (5)	0.110	Ba3—O13^{ii}	2.946 (6)	0.168
Ba2—O5	3.249 (5)	0.074	Ba3—O4^{iv}	3.078 (4)	0.117
Ba2—O9^{i}	3.335 (4)	0.059	<Ba3—O>$_8$	2.76	1.92
Ba2—O15	3.444 (7)	0.044	B1—O6	1.348 (14)	0.531
<Ba2—O>$_{12}$	2.98	1.87	B1—O6^{vi}	1.348 (14)	0.531
B2—O2	1.353(8)	1.047	B1—O7	1.378 (13)	0.489
B2—O13	1.383 9)	0.965	B1—O7^{vi}	1.378 (13)	0.489
B2—O9	1.416(8)	0.883	B1—O12	1.458 (9)	0.394
<B2—O>$_3$	1.38	2.90	B1—O12^{vi}	1.458 (9)	0.394
B4—O4	1.366(10)	1.011	<B1—O>$_6$	1.39	2.83
B4—O1	1.386(10)	0.958	B3—O3	1.354(11)	1.044
B4—O15	1.389(9)	0.950	B3—O14	1.356(11)	1.039
<B4—O>$_3$	1.38	2.92	B3—O8	1.370(9)	1.000
B5—O5	1.367(9)	1.008	<B3—O>$_3$	1.36	3.08
B5—O11	1.381(10)	0.971			
B5—O10	1.383(10)	0.965			
<B5—O>$_3$	1.38	2.94			

Bond valence sums (v.u.) were calculated according to (Brown & Altermatt, 1985)

Figure S1 The Rietveld refinement of the $Lu_5Ba_6B_9O_{27}$ crystal structure using powder X-ray diffraction data. The measured data is represented by a blue line, the refinement fit by a red line and the difference between the data and refinement fit by a gray line ($Lu_2Ba_3B_6O_{15}$ is marked with the circles).

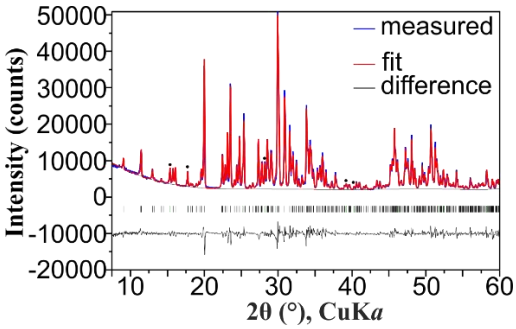

Figure S2 TG and DSC curves of $Lu_5Ba_6B_9O_{27}$ in the temperature range 40–1400 °C.