STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

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Monoclinic $SmAl_3(BO_3)_4$. Synthesis, structural and spectroscopic properties.

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Supporting information

Table S1 Main crystallographic parameters of monoclinic *Re*$Al_3(BO_3)_4$ compounds

Compound	Space group	Cell parameters, (Å, °)	Reference
$PrAl_3(BO_3)_4$	*C*2/*c*	*a* =7.283 (2) Å, *b* = 9.364 (7) Å, *c* = 11.144 (2) Å, *β* = 103.59 (2) °	Plachinda & Belokoneva, 2008
$NdAl_3(BO_3)_4$	*C*2/*c*	*a* = 7.246 (3) Å, *b* = 9.343 (3) Å, *c* = 11.1013 (4) Å, *β* = 103.38 (3) °	Wang *et al.*, 1991
$SmAl_3(BO_3)_4$	*C*2/*c*	*a* = 7.2386 (3) Å, *b* = 9.3412 (3) Å, *c* = 11.1013 (4) Å, *β* = 103.2240 (10) °	Present work
$EuAl_3(BO_3)_4$	*C*2/*c*	*a* = 7.22 Å, *b* = 9.327 Å, *c* = 11.074 Å, *β* = 103.17 °	Mazilkin *et al.*, 2019
$TbAl_3(BO_3)_4$	*C*2/*c*	*a* = 7.220 (3) Å, *b* = 9.312 (4) Å, *c* = 11.072 (4) Å, *β* = 103.20 (3) °	Plachinda & Belokoneva, 2008
$HoAl_3(BO_3)_4$	*C*2/*c*	*a* = 7.198 (3) Å, *b* = 9.300 (4) Å, *c* = 11.050 (4) Å, *β* = 103.11 (3) °	Plachinda & Belokoneva, 2008

Table S2 Main parameters of processing and refinement of the $SmAl_3(BO_3)_4$ sample

Compound	$SmAl_3(BO_3)_4$
Sp.Gr.	*C*2/*c*
a, Å	7.2446 (5)
b, Å	9.3455 (6)
c, Å	11.1013 (7)
β, º	103.225 (3)
V, Å^3	731.67 (8)
Z	4
2θ-interval, º	12-100
R_{wp}, %	3.82
R_p, %	2.91
R_{exp}, %	2.28
χ^2	1.68
R_B, %	2.15

Table S3 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Sm	0.5000	0.46392 (2)	0.7500	0.00459 (9)
Al1	0.44437 (12)	0.25008 (9)	0.47154 (8)	0.00380 (14)
Al2	0.5000	-0.08861 (12)	0.7500	0.00388 (18)
B1	0.7512 (4)	0.4709 (3)	0.5046 (3)	0.0043 (4)
B2	0.6929 (4)	0.1864 (3)	0.7220 (3)	0.0046 (4)
O1	0.9037 (3)	0.3968 (2)	0.57387 (18)	0.0048 (3)
O2	0.5944 (3)	0.4023 (2)	0.43632 (18)	0.0055 (3)
O3	0.8398 (3)	0.2634 (2)	0.79484 (18)	0.0050 (3)
O4	0.7499 (3)	0.6195 (2)	0.4973 (2)	0.0059 (3)
O5	0.5605 (3)	0.2595 (2)	0.63779 (18)	0.0058 (3)
O6	0.6883 (3)	0.0423 (2)	0.7411 (2)	0.0059 (3)

Table S4 The main bond lengths (Å) of compound $SmAl_3(BO_3)_4$

Sm—O6^{i}	2.353 (2)	Al2—O1^{x}	1.9245 (19)
Sm—O6^{ii}	2.353 (2)	Al2—O3^{vii}	1.941 (2)
Sm—O5^{iii}	2.374 (2)	Al2—O3^{x}	1.941 (2)
Sm—O5	2.374 (2)	Al2—O6	1.851 (2)
Sm—O2^{iv}	2.379 (2)	Al2—O6^{iii}	1.851 (2)
Sm—O2^{v}	2.379 (2)	Al2—O1^{vii}	1.9245 (19)
Al1—O5	1.847 (2)	B1—O2	1.371 (4)
Al1—O2	1.884 (2)	B1—O1	1.378 (3)
Al1—O1^{vi}	1.898 (2)	B1—O4	1.391 (3)
Al1—O4^{vii}	1.932 (2)	B2—O5	1.360 (3)
Al1—O3^{viii}	1.938 (2)	B2—O6	1.364 (3)
Al1—O4^{v}	1.951 (2)	B2—O3	1.382 (3)

Symmetry codes: (i) -*x*+3/2, *y*+1/2, -*z*+3/2; (ii) *x*-1/2, *y*+1/2, *z*; (iii) -*x*+1, *y*, -*z*+3/2; (iv) *x*, -*y*+1, *z*+1/2; (v) -*x*+1, -*y*+1, -*z*+1; (vi) -*x*+3/2, -*y*+1/2, -*z*+1; (vii) *x*-1/2, *y*-1/2, *z*; (viii) *x*-1/2, -*y*+1/2, *z*-1/2; (ix) -*x*+1, -*y*, -*z*+1; (x) -*x*+3/2, *y*-1/2, -*z*+3/2

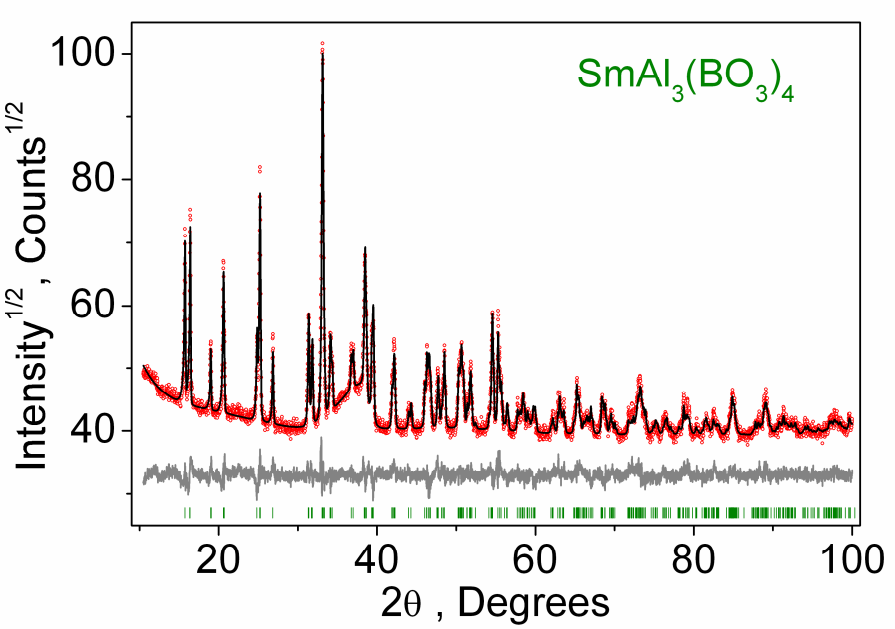

Figure S1 Difference X-ray powder patterns of $SmAl_3(BO_3)_4$

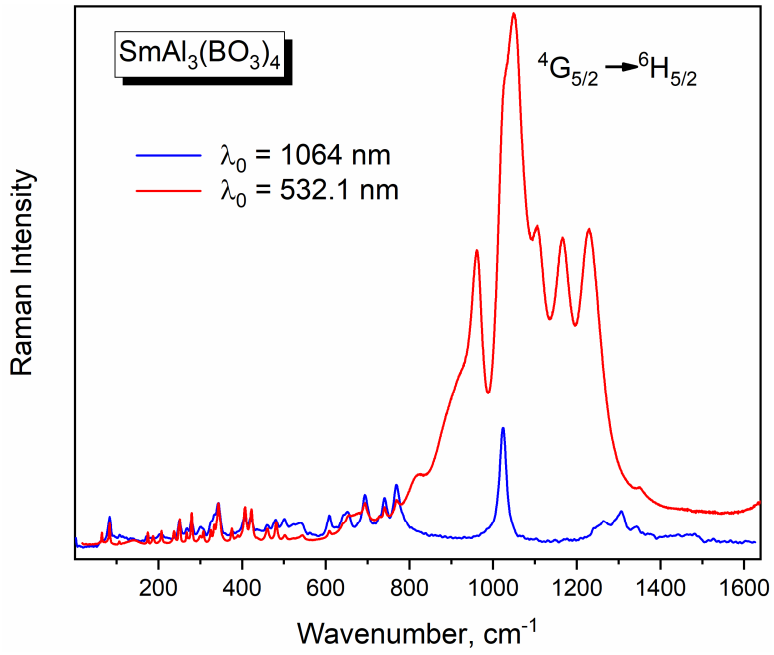

Figure S2 Raman spectra recorded with excitation at 532.1 and 1064 nm.

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