Systematic rare earth doping to adopt R32 huntite structure in $NdSc_3(BO_3)_4$ crystal.

Artem B. Kuznetsov[1], Konstantin A. Kokh[1], Ekaterina .V. Kaneva[2], Ammar Y. Jamous[1,3], Valery A. Svetlichnyi[3], Nadezda G. Kononova[1], Vyacheslav S. Shevchenko[1], Anastasia A. Goreiavcheva[1] and Aleksander E. Kokh[1]

[1]Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk 630090, Russia

[2]Vinogradov Institute of geochemistry SB RAS, Irkutsk 664033, Russia
[3]Tomsk State University, Tomsk 634050, Russia

KEYWORDS Rare earth borate, structure, crystal growth,

Abstract

Huntite borates with R32 crystal structure have great potential in photonics applications as nonlinear and self-doubling media. This study is focused on determining the type and quantity of impurities responsible for converting the structure of $NdSc_3(BO_3)_4$ to R32 polymorph. According to the single crystal X-ray diffraction of $R_xNd_ySc_z(BO_3)_4$ (R= Sm-Lu, x+y+z=4), the obtained compounds crystallize in the space group R32 (R = Eu, Er, Tm, Yb) and $P3_221$(R = Sm, Gd, Tb, Dy, Ho). Potential limitations to the future use of the crystals were identified, including compositional zonning and the possible presence of other polymorphic forms.

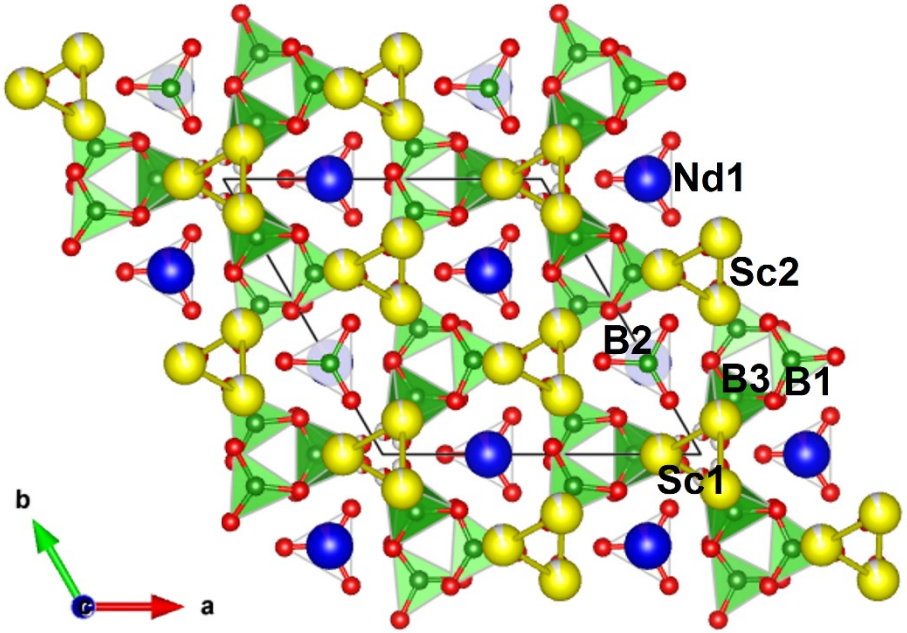

Figure S1. Crystal structure of $NdSc_3(BO_3)_4$:R (R = Sm, Gd, Tb, Dy, Ho, Lu) (sp. gr. $P3_221$) compound projected down the *c* axis. Nd and Sc cations are blue and yellow spheres, BO_3 groups are shown as green triangles (B – green spheres, O – red spheres).

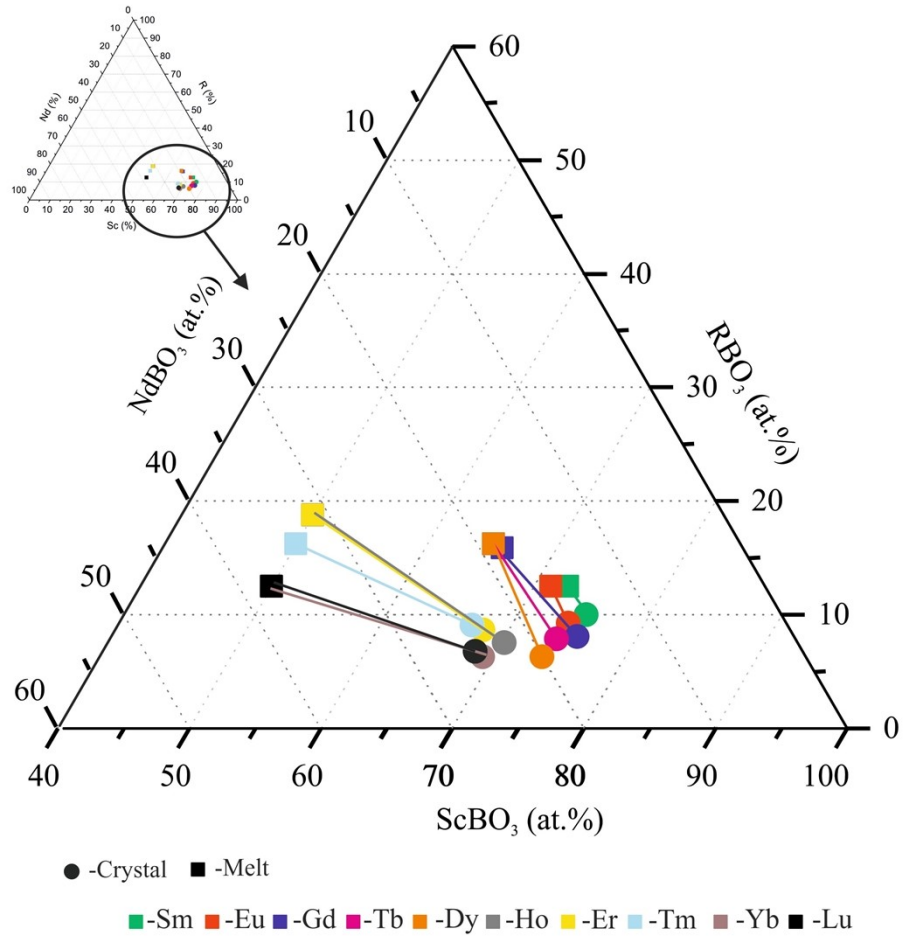

Figure S2. Relationship between the compositions in the melted batch and the compositions of the grown crystals.

Table S1. Selected bond distances (Å) for the coordination polyhedral of the studied $NdSc_3(BO_3)_4$:R (R = Eu, Er, Tm, Yb) samples (sp. gr. *R*32).

	R=Eu	**R=Er**	**R=Tm**	**R=Yb**
Nd-O1 $^{(\times 6)}$	2.43(2)	2.437(5)	2.440(2)	2.441(4)
m.a.n. (e^-)	*64.491*	*64.640*	*62.859*	*65.870*
Sc2-O1 $^{(\times 2)}$	2.110(2)	2.1243(6)	2.1271(4)	2.1192(6)
Sc2-O2 $^{(\times 2)}$	2.13(2)	2.142(6)	2.149(3)	2.142(5)
Sc2-O3 $^{(\times 2)}$	2.06(1)	2.069(4)	2.070(3)	2.065(4)
<Sc2-O>	2.10	2.112	2.115	2.109
m.a.n. (e^-)	*23.772*	*25.106*	*26.979*	*24.269*
B1-O1 $^{(\times 3)}$	1.374(7)	1.376(5)	1.378(3)	1.383(5)
B2-O2	1.36(3)	1.38(1)	1.366(6)	1.365(9)
B2-O3 $^{(\times 2)}$	1.36(1)	1.365(6)	1.368(3)	1.372(4)
<B2-O >	1.36	1.37	1.367	1.370
O1-B1-O1	120.0	120.0	120	120
O2-B2-O3	117.9(6)	117.9(3)	118.1(2)	118.1(2)
O2-B2-O3’	117.9(6)	117.9(3)	118.1(2)	118.1(2)
O3-B2-O3’	124.2(7)	124.3(6)	123.8(3)	123.9(3)

Table S2. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Eu)

	Nd1	**Sc2**	**B1**	**B2**	**Σ**
O1	$0.416^{(\times 6)}$	$0.482^{(\times 2)}$	$0.994^{(\times 3)}$	-	**1.892**
O2		$0.457^{(\times 2)[\times 2]}$	-	1.049	**1.963**
O3		$0.542^{(\times 2)[\times 2]}$		$1.023^{(\times 2)}$	**2.107**
Σ	**2.496**	**2.962**	**2.982**	**3.095**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S3. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Er)

	Nd1	**Sc2**	**B1**	**B2**	**Σ**
O1	$0.406^{(\times 6)}$	$0.467^{(\times 2)}$	$0.989^{(\times 3)}$	-	**1.862**
O2		$0.449^{(\times 2)[\times 2]}$	-	0.978	**1.876**
O3		$0.528^{(\times 2)[\times 2]}$		$1.020^{(\times 2)}$	**2.076**
Σ	**2.436**	**2.888**	**2.967**	**3.018**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S4. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Tm)

	Nd1	**Sc2**	**B1**	**B2**	**Σ**
O1	$0.403^{(\times 6)}$	$0.464^{(\times 2)}$	$0.983^{(\times 3)}$	-	**1.850**
O2		$0.442^{(\times 2)[\times 2]}$	-	1.017	**1.901**
O3		$0.526^{(\times 2)[\times 2]}$		$1.011^{(\times 2)}$	**2.063**
Σ	**2.418**	**2.864**	**2.949**	**3.039**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S5. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Yb)

	Nd1	**Sc2**	**B1**	**B2**	**Σ**
O1	$0.402^{(\times 6)}$	$0.472^{(\times 2)}$	$0.970^{(\times 3)}$	-	**1.844**
O2		$0.449^{(\times 2)[\times 2]}$	-	1.020	**1.918**
O3		$0.532^{(\times 2)[\times 2]}$		$1.000^{(\times 2)}$	**2.064**
Σ	**2.412**	**2.906**	**2.910**	**3.020**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S6. Selected data on single crystals, data collection and structure refinement parameters of the studied $NdSc_3(BO_3)_4$:R (R = Sm-Lu) samples.

	R=Sm	R=Eu	R=Gd	R=Tb	R=Dy	R=Ho	R=Er	R=Tm	R=Yb	R=Lu
Crystal data										
a (Å)	9.7768(3)	9.7610(3)	9.781(1)	9.7594(6)	9.7577(3)	9.7655(3)	9.7999(4)	9.8072(3)	9.804(1)	9.8013(4)
c (Å)	7.9305(3)	7.9185(2)	7.9407(8)	7.9234(5)	7.9240(3)	7.9374(2)	7.9735(3)	7.9928(3)	7.969(1)	7.9747(3)
V (Å^3)	656.48(2)	653.38(2)	657.87(7)	653.56(4)	653.39(2)	655.54(2)	663.08(2)	665.76(2)	663.26(8)	663.46(2)
Z	3	3	3	3	3	3	3	3	3	3
Crystal dimensions (mm)	0.26×0.24××0.15	0.31×0.30××0.10	0.22×0.19××0.09	0.24×0.22××0.09	0.30×0.19××0.11	0.25×0.22××0.10	0.19×0.18××0.16	0.18×0.17××0.04	0.19×0.12××0.05	0.22×0.10××0.07
Crystal density	3.794	4.181	3.972	3.865	4.023	4.064	4.231	4.264	4.208	4.049
Data collection										
Reflections measured	30027	5566	29162	31713	19846	88792	8635	9737	12042	19026
Independent reflections	2121	710	2128	2110	2111	2932	728	733	575	1697
$R_{merging}$ [$R_{(int)}$] (%)	6.2	4.8	4.9	4.5	5.7	6.1	4.2	4.6	3.6	4.4
h_{min}, h_{max}	-16, 16	-16, 16	-16, 16	-16, 16	-16, 16	-18, 17	-16, 16	-16, 16	-15, 15	-15, 15
k_{min}, k_{max}	-16, 16	-16, 15	-16, 16	-16, 16	-16, 16	-18, 18	-16, 16	-16, 16	-15, 15	-15, 15
l_{min}, l_{max}	-13, 13	-11, 13	-13, 13	-13, 13	-13, 13	-14, 14	-13, 13	-13, 13	-12, 12	-12, 12
Refinement										
Space group	$P3_221$	$R32$	$P3_221$	$P3_221$	$P3_221$	$P3_221$	$R32$	$R32$	$R32$	$P3_221$
Reflections used in the refinement ($I > 3\sigma_{(I)}$)	1963	701	1929	1995	1899	2582	724	731	573	1563
N. of refined parameters	102	44	107	106	107	107	44	44	44	107
R^a [on F] (%)	7.95	5.24	2.12	6.59	6.79	6.64	3.10	1.73	2.81	6.70
$R_w{}^b$ [on F] (%)	8.52	5.83	2.92	8.13	8.54	7.35	3.44	1.83	3.46	9.48
Goof^c	1.0269	1.0704	1.0560	1.0097	1.0248	1.1529	1.0808	1.0836	1.0240	0.9692
$\Delta\rho_{min}/\Delta\rho_{max}$ (e$^-$/Å^3)	-6.95/2.92	-5.60/2.50	-4.70/2.66	-4.53/2.64	-7.37/2.59	-3.89/2.44	-3.52/1.40	-1.90/0.90	-3.26/1.04	-4.92/2.36

[a] $R = \Sigma[|F_o| - |F_c|]/\Sigma|F_o|$.

[b] $R_w = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$; w = Chebyshev optimized weights.

[c] Goodness-of-fit = $[\Sigma[w(F_o^2-F_c^2)^2]/(N-p)]^{1/2}$, where N and p are the number of reflections and parameters, respectively.

Table S7. Selected bond distances (Å) for the coordination polyhedra of the studied $NdSc_3(BO_3)_4$:R (R = Sm, Gd, Tb, Dy, Ho, Lu) samples (sp. gr. $P3_221$).

	R=Sm	**R=Gd**	**R=Tb**	**R=Dy**	**R=Ho**	**R=Lu**
Nd1-O1 (×2)	2.422(6)	2.419(6)	2.415(6)	2.421(6)	2.424(6)	2.455(6)
Nd1-O2	2.802(5)	2.803(5)	2.791(4)	2.798(5)	2.820(5)	2.805(6)
Nd1-O3 (×2)	2.448(4)	2.447(3)	2.437(3)	2.441(3)	2.445(3)	2.453(4)
Nd1-O4 (×2)	3.009(5)	3.011(4)	2.999(4)	3.007(4)	3.002(4)	3.052(6)
Nd1-O5 (×2)	2.401(6)	2.401(6)	2.381(5)	2.401(6)	2.401(5)	2.438(7)
<Nd1-O>	2.596	2.595	2.584	2.593	2.596	2.622
m.a.n. (e^-)	*54.600*	*61.132*	*58.240*	*61.938*	*62.257*	*58.878*
Sc1-O2	2.026(8)	2.019(8)	2.023(7)	2.001(8)	2.005(8)	2.007(9)
Sc1-O2’	2.026(7)	2.019(7)	2.023(6)	2.002(7)	2.005(7)	2.007(8)
Sc1-O2’’	2.363(7)	2.365(7)	2.340(6)	2.366(7)	2.345(7)	2.432(8)
Sc1-O2’’’	2.363(6)	2.365(6)	2.340(6)	2.366(6)	2.346(6)	2.432(7)
Sc1-O5	2.121(5)	2.119(5)	2.130(4)	2.112(5)	2.103(4)	2.083(6)
Sc1-O5	2.122(7)	2.119(6)	2.131(5)	2.113(6)	2.103(6)	2.083(7)
Sc1-O6	2.148(4)	2.146(4)	2.136(4)	2.140(4)	2.148(4)	2.178(4)
Sc1-O6	2.148(4)	2.147(4)	2.136(4)	2.141(4)	2.148(4)	2.179(4)
<Sc1-O>	2.165	2.162	2.157	2.155	2.150	2.175
m.a.n. (e^-)	*19.194*	*20.013*	*18.837*	*20.286*	*21.126*	*20.916*
Sc2-O1	2.087(7)	2.093(7)	2.087(6)	2.094(7)	2.079(6)	2.097(7)
Sc2-O3	2.034(4)	2.031(3)	2.035(3)	2.033(3)	2.033(3)	2.038(4)
Sc2-O4	2.146(4)	2.154(4)	2.148(5)	2.149(4)	2.152(4)	2.157(5)
Sc2-O4’	2.161(6)	2.162(5)	2.148(4)	2.156(5)	2.159(5)	2.181(7)
Sc2-O7	2.105(4)	2.104(4)	2.096(3)	2.098(4)	2.096(3)	2.112(5)
Sc2-O7’	2.114(4)	2.119(4)	2.118(3)	2.118(4)	2.121(3)	2.126(4)
<Sc2-O>	2.108	2.111	2.105	2.108	2.107	2.119
m.a.n. (e^-)	*21.253*	*22.541*	*21.315*	*22.602*	*23.502*	*26.274*
B1-O3	1.363(8)	1.373(7)	1.362(7)	1.359(7)	1.347(7)	1.373(9)
B1-O4	1.362(5)	1.358(5)	1.362(5)	1.350(5)	1.359(5)	1.362(6)
B1-O5	1.362(9)	1.367(9)	1.369(8)	1.369(9)	1.397(8)	1.36(1)
<B1-O >	1.362	1.366	1.364	1.359	1.368	1.365

B2-O6	1.294(6)	1.318(5)	1.314(5)	1.304(5)	1.272(5)	1.307(6)
B2-O7 (×2)	1.401(8)	1.391(8)	1.392(7)	1.391(8)	1.410(7)	1.378(9)
<B2-O >	1.365	1.367	1.366	1.362	1.364	1.354
B3-O1 (×2)	1.339(6)	1.339(6)	1.337(5)	1.325(5)	1.351(5)	1.310(6)
B3-O2	1.533(9)	1.54(1)	1.532(9)	1.54(1)	1.514(9)	1.56(1)
B3-O2’	1.53(1)	1.54(1)	1.532(9)	1.54(1)	1.51(1)	1.56(1)
<B3-O >	1.404	1.406	1.402	1.468	1.458	1.393
O3-B1-O4	117.7(5)	116.9(4)	116.9(4)	117.3(4)	117.8(4)	115.7(5)
O3-B1-O5	125.2(5)	124.8(4)	125.5(4)	124.5(4)	124.7(4)	124.6(5)
O4-B1-O5	117.1(5)	118.3(4)	117.6(4)	118.1(4)	117.4(4)	119.8(5)
O6-B2-O7	123.1(4)	122.0(4)	122.4(5)	122.5(5)	123.4(5)	120.8(5)
O6-B2-O7’	123.1(5)	122.0(5)	122.4(5)	122.5(5)	123.4(5)	120.8(5)
O7-B2-O7’	113.8(5)	115.9(4)	115.3(4)	115.1(5)	113.1(4)	118.3(5)
O1-B3-O1’	124.9(8)	125.4(7)	124.5(7)	124.9(7)	122.7(7)	128.2(9)
O1-B3-O2	106.0(4)	105.8(4)	105.7(3)	106.2(4)	107.4(3)	105.8(4)
O1’-B3-O2	124.8(5)	124.5(4)	125.6(4)	124.3(4)	125.5(4)	121.1(5)

Table S8. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Sm)

	Nd1	**Sc1**	**Sc2**	**B1**	**B2**	**B3**	**Σ**
O1	$0.423^{(\times 2)}$	-	0.507	-	-	$1.097^{(\times 2)}$	**2.027**
O2	0.152	$0.580^{(\times 2)}$ $0.275^{(\times 2)}$	-	-	-	0.637/0.642	**1.644/1.649**
O3	$0.395^{(\times 2)}$	-	0.776	1.026	-	-	**2.179**
O4	$0.087^{(\times 2)}$	-	0.445 0.430	1.028	-	-	**1.990**
O5	$0.448^{(\times 2)}$	0.470/0.469	-	1.028	-	-	**1.945/1.946**
O6	-	$0.443^{(\times 2)\,[\times 2]}$	-	-	1.244	-	**2.130**
O7	-	-	0.487 0.478	-	$0.922^{(\times 2)}$	-	**1.887**
Σ	**2.858**	**2.375/2.985**	**3.132**	**3.082**	**3.088**	**2.831/2.836**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S9. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Gd)

	Nd1	**Sc1**	**Sc2**	**B1**	**B2**	**B3**	**Σ**
O1	$0.427^{(\times 2)}$	-	0.500	-	-	$1.097^{(\times 2)}$	**2.024**
O2	0.152	$0.589^{(\times 2)}$ $0.274^{(\times 2)}$	-	-	-	0.625	**1.640**
O3	$0.396^{(\times 2)}$	-	0.574	0.997	-	-	**1.967**
O4	$0.087^{(\times 2)}$	-	0.437 0.430	1.040	-	-	**1.994**
O5	$0.448^{(\times 2)}$	$0.472^{(\times 2)}$	-	1.014	-	-	**1.934**
O6	-	$0.445^{(\times 2)[\times 2]}$	-	-	1.163	-	**2.053**
O7	-	-	0.488 0.472	-	$0.948^{(\times 2)}$	-	**1.908**
Σ	**2.868**	**2.382/3.012**	**2.901**	**3.051**	**3.059**	**2.819**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S10. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Tb)

	Nd1	**Sc1**	**Sc2**	**B1**	**B2**	**B3**	**Σ**
O1	$0.431^{(\times 2)}$	-	0.507	-	-	$1.103^{(\times 2)}$	**2.041**
O2	0.157	$0.584^{(\times 2)}$ $0.290^{(\times 2)}$	-	-	-	0.639	**1.670**
O3	$0.406^{(\times 2)}$	-	0.569	1.028	-	-	**2.003**
O4	$0.089^{(\times 2)}$	-	$0.443^{(\times 2)[\times 2]}$	1.028	-	-	**2.003**
O5	$0.473^{(\times 2)}$	0.460/0.461	-	1.008	-	-	**1.941/1.942**
O6	-	$0.455^{(\times 2)[\times 2]}$	-	-	1.176	-	**2.086**
O7	-	-	0.497 0.473	-	$0.946^{(\times 2)}$	-	**1.916**
Σ	**2.955**	**2.411/2.999**	**2.932**	**3.064**	**3.068**	**2.845**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S11. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Dy)

	Nd1	**Sc1**	**Sc2**	**B1**	**B2**	**B3**	**Σ**
O1	$0.424^{(\times 2)}$	-	0.499	-	-	$1.141^{(\times 2)}$	**2.064**
O2	0.154	0.613/0.612 $0.273^{(\times 2)}$	-	-	-	0.625	**1.664/1.665**
O3	$0.402^{(\times 2)}$	-	0.571	1.037	-	-	**2.010**
O4	$0.087^{(\times 2)}$	-	0.442 0.435	1.064	-	-	**2.028**
O5	$0.448^{(\times 2)}$	0.480/0.479	-	1.008	-	-	**1.935/1.936**
O6	-	0.451 0.450	-	-	1.210	-	**2.111**
O7	-	-	0.495 0.473	-	$0.948^{(\times 2)}$	-	**1.916**
Σ	**2.876**	**2.406/3.085**	**2.915**	**3.109**	**3.106**	**2.391**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S12. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Ho)

	Nd1	Sc1	Sc2	B1	B2	B3	Σ
O1	0.421$^{(\times 2)}$	-	0.516	-	-	1.061$^{(\times 2)}$	**2.064**
O2	0.145	0.608$^{(\times 2)}$ 0.287/0.286	-	-	-	0.672/0.679	**1.71/1.72**
O3	0.398$^{(\times 2)}$	-	0.571	1.073	-	-	**2.042**
O4	0.089$^{(\times 2)}$	-	0.439 0.432	1.037	-	-	**1.997**
O5	0.448$^{(\times 2)}$	0.489$^{(\times 2)}$	-	0.932	-	-	**1.869**
O6	-	0.443$^{(\times 2)[\times 2]}$	-	-	1.323	-	**2.209**
O7	-	-	0.497 0.470	-	0.899$^{(\times 2)}$	-	**1.866**
Σ	**2.857**	**2.438/3.080**	**2.925**	**3.042**	**3.121**	**2.794/2.801**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S13. Valence balance calculation for studied sample $NdSc_3(BO_3)_4$:R (R = Lu)

	Nd1	Sc1	Sc2	B1	B2	B3	Σ
O1	0.387$^{(\times 2)}$	-	0.496	-	-	1.190$^{(\times 2)}$	**2.073**
O2	0.151$^{(\times 2)}$	0.605$^{(\times 2)}$ 0.236$^{(\times 2)}$	-	-	-	0.591	**1.583**
O3	0.389$^{(\times 2)}$	-	0.565	0.997	-	-	**1.951**
O4	0.077$^{(\times 2)}$	-	0.434 0.412	1.028	-	-	**1.951**
O5	0.405$^{(\times 2)}$	0.512$^{(\times 2)}$	-	1.034	-	-	**1.951**
O6	-	0.415 0.414	-	-	1.200	-	**2.029**
O7	-	-	0.480 0.465	-	0.983$^{(\times 2)}$	-	**1.928**
Σ	**2.818**	**2.325/3.063**	**2.852**	**3.059**	**3.166**	**2.971**	

$^{(\times 2)}$ – valence strengths doubled in the calculation of valence balance at the cations

$^{[\times 2]}$ – valence strengths doubled in the calculation of valence balance at the anions

Table S14. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Sm).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66725(5)	0.66725(5)	0.5	0.910(1)	0.0001	0.0002(2)	0.0002(2)	-0.0005(2)	-0.00020(6)	0.00020(6)	-0.0002(1)
Sc1	0	0.8744(3)	5/6	0.914(1)	0.0406	0.0019(6)	0.0010(5)	0.1190(9)	0.0022(4)	0.0044(7)	0.0010(3)
Sc2	0.2150(2)	0.6708(1)	0.4973(1)	0.891(1)	0.0007	0.0040(4)	0.001(4)	-0.0040(3)	-0.0006(3)	-0.0016(3)	0.0011(3)
Sm2	0.2150(2)	0.6708(1)	0.4973(1)	0.0410(9)	0.0007	0.0040(4)	0.001(4)	-0.0040(3)	-0.0006(3)	-0.0016(3)	0.0011(3)
O1	0.6576(6)	0.8606(6)	0.6829(7)	1	0.0179	0.0082(9)	0.0092(9)	0.0352(9)	0.0029(9)	0.0158(9)	0.0036(8)
O2	0.9628(7)	0.9155(7)	0.4005(8)	0.5	0.0046	0.0036(9)	-0.0001(9)	0.0093(9)	-0.0003(9)	0.0001(9)	0.0002(9)
O3	0.4506(5)	0.4785(5)	0.3212(5)	1	0.0008	0.0017(8)	0.0003(8)	0.0008(8)	0.0000(7)	-0.0011(7)	0.0009(7)
O4	0.3555(5)	0.6008(5)	0.6451(5)	1	0.0035	0.0078(8)	-0.0003(8)	0.0016(8)	-0.0003(8)	-0.0001(8)	0.0008(7)
O5	0.6721(6)	0.8668(6)	0.3195(6)	1	0.0154	0.0135(9)	0.0247(9)	0.0133(9)	-0.0144(8)	-0.0128(8)	0.0135(8)
O6	0.8025(6)	0.8025(6)	0	1	0.0360	0.0058(6)	0.058(6)	0.010(1)	0.0034(7)	-0.0034(7)	0.0055(8)
O7	0.6612(5)	0.5226(5)	0.0008(5)	1	0.0013	0.0055(8)	-0.0007(8)	-0.0010(8)	0.0009(7)	-0.0013(8)	0.0012(7)
B1	0.8866(6)	0.5439(6)	0.6731(6)	1	0.0009	0.0003(8)	0.0000(8)	0.0004(9)	0.0002(8)	-0.0002(8)	0.0015(8)
B2	0.6701(6)	0.6701(6)	0	1	0.0038	0.0023(6)	0.0023(6)	0.0049(9)	-0.0020(6)	0.0020(6)	0.0004(8)
B3	0.7906(8)	0	2/3	1	0.0393	0.0039(9)	0.0125(9)	0.104(1)	0.0006(9)	0.0003(4)	0.0062(4)

Table S15. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Eu).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0	0	0	0.952(2)	0.0012	0.0012(4)	0.0012(4)	0.0013(5)	0.0000(1)	0.0000(1)	0.0006(2)
Eu1	0	0	0	0.117(2)	0.0012	0.0012(4)	0.0012(4)	0.0013(5)	0.0000(1)	0.0000(1)	0.0006(2)
Sc2	0.5449(5)	0	0	0.808(3)	0.0080	0.0051(9)	0.005(1)	0.014(1)	0.0024(9)	0.0012(4)	0.0023(5)
Eu2	0.5449(5)	0	0	0.108(2)	0.0080	0.0051(9)	0.005(1)	0.014(1)	0.0024(9)	0.0012(4)	0.0023(5)
O1	0.8592(14)	0	0.5	1	0.0041	0.001(2)	0.004(2)	0.008(2)	0.0000(1)	0.0000(1)	0.001(1)
O2	0.592(2)	0	0.5	1	0.0496	0.022(2)	0.066(2)	0.075(2)	-0.061(2)	-0.031(1)	0.033(1)
O3	0.4587(15)	0.1419(13)	0.5152(15)	1	0.0081	0.012(2)	0.003(2)	0.007(2)	0.000(2)	0.003(2)	0.002(2)
B1	0	0	0.5	1	0.0018	0.0000(1)	0.0000(1)	0.005(2)	0	0	0.0000(1)
B2	0.4532(18)	0	0.5	1	0.0070	0.001(2)	0.005(2)	0.016(2)	-0.002(2)	-0.001(1)	0.003(1)

Table S16. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Gd).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66727(4)	0.66727(4)	0.5	0.909(1)	0.0045	0.0042(1)	0.0042(1)	0.0046(2)	-0.00012(5)	0.00012(5)	0.0017(1)
Gd1	0.66727(4)	0.66727(4)	0.5	0.103(1)	0.0045	0.0042(1)	0.0042(1)	0.0046(2)	-0.00012(5)	0.00012(5)	0.0017(1)
Sc1	0	0.8747(2)	5/6	0.953(1)	0.0321	0.0009(5)	-0.0002(4)	0.0957(9)	0.0008(3)	0.0017(6)	0.0003(3)
Sc2	0.2139(1)	0.6701(1)	0.49740(7)	0.871(1)	0.0011	0.0037(3)	0.0019(3)	-0.0026(3)	-0.0006(2)	-0.0015(2)	0.0012(2)
Gd2	0.2139(1)	0.6701(1)	0.49740(7)	0.0664(9)	0.0011	0.0037(3)	0.0019(3)	-0.0026(3)	-0.0006(2)	-0.0015(2)	0.0012(2)
O1	0.6586(6)	0.8604(6)	0.6831(7)	1	0.0212	0.0068(8)	0.0094(9)	0.0461(9)	-0.018(9)	0.0072(9)	0.0031(8)
O2	0.9627(7)	0.9161(7)	0.4013(7)	0.5	0.0078	0.0034(9)	0.0001(9)	0.0192(9)	-0.0005(9)	0.0000(9)	0.0004(8)
O3	0.4527(4)	0.4791(4)	0.3194(4)	1	0.0026	0.0034(8)	0.0000(8)	0.0047(8)	0.0002(7)	-0.0017(7)	0.0011(7)
O4	0.3555(5)	0.6013(4)	0.6447(5)	1	0.0066	0.0101(8)	0.0020(7)	0.0084(8)	-0.0034(7)	-0.0035(8)	0.0035(7)
O5	0.6734(5)	0.8676(6)	0.3202(6)	1	0.0131	0.0112(8)	0.0193(9)	0.0137(8)	-0.0081(8)	-0.0077(8)	0.0112(7)
O6	0.8029(6)	0.8029(6)	0	1	0.0411	0.0089(6)	0.0089(6)	0.1088(10)	0.0048(7)	-0.0048(7)	0.0068(8)
O7	0.6624(4)	0.5232(5)	0.0001(4)	1	0.0015	0.0053(8)	-0.0005(8)	-0.0001(8)	-0.0002(6)	-0.0010(7)	0.0013(6)
B1	0.8850(5)	0.5433(5)	0.6722(5)	1	0.0005	0.0001(8)	0.0012(8)	-0.0003(8)	0.0004(7)	0.0006(8)	0.0019(7)
B2	0.6682(5)	0.6682(5)	0	1	0.0023	0.0020(6)	0.0020(6)	0.0011(9)	-0.0007(5)	0.0007(5)	-0.0003(8)
B3	0.7913(8)	0	2/3	1	0.0349	0.0082(9)	0.0295(9)	0.0743(10)	0.0212(9)	0.0106(4)	0.0148(4)

Table S17. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Tb).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66735(4)	0.66735(4)	0.5	0.884(1)	0.0043	0.0041(1)	0.0041(1)	0.0041(2)	-0.00012(5)	0.00012(5)	0.0016(1)
Tb1	0.66735(4)	0.66735(4)	0.5	0.080(1)	0.0043	0.0041(1)	0.0041(1)	0.0041(2)	-0.00012(5)	0.00012(5)	0.0016(1)
Sc1	0	0.8752(2)	5/6	0.897(1)	0.0341	0.0018(5)	0.0002(4)	0.1003(9)	0.0008(3)	0.0015(6)	0.0005(3)
Sc2	0.2145(2)	0.67030(9)	0.49728(7)	1.015(1)	0.0008	0.0031(3)	0.0017(3)	-0.0031(3)	-0.0004(2)	-0.0015(2)	0.0008(2)
O1	0.6578(5)	0.8607(6)	0.6824(7)	1	0.0265	0.0122(8)	0.0126(9)	0.0546(9)	0.0030(9)	0.0207(8)	0.0060(7)
O2	0.9614(6)	0.9156(6)	0.3993(7)	0.5	0.0091	0.0031(9)	0.0032(9)	0.0226(9)	-0.0011(9)	-0.0002(9)	0.0029(8)
O3	0.4533(4)	0.4793(4)	0.3197(4)	1	0.0051	0.0079(8)	0.0032(8)	0.0052(8)	-0.0002(7)	-0.0036(7)	0.0035(7)
O4	0.3559(4)	0.6019(4)	0.6434(4)	1	0.0062	0.0086(8)	0.0040(7)	0.0071(8)	-0.0036(7)	-0.0009(7)	0.0039(7)
O5	0.6727(5)	0.8663(5)	0.3217(5)	1	0.0168	0.0154(8)	0.0246(9)	0.0177(8)	-0.0177(8)	-0.0162(8)	0.0155(7)
O6	0.8038(6)	0.8038(6)	0	1	0.0522	0.0078(6)	0.0078(6)	0.1430(10)	0.0037(7)	-0.0037(7)	0.0054(8)
O7	0.6624(4)	0.5233(4)	-0.0008(3)	1	0.0030	0.0096(8)	-0.0002(7)	0.0002(8)	0.0003(6)	-0.0009(7)	0.0027(6)
B1	0.8856(5)	0.5432(5)	0.6723(5)	1	0.0007	0.0002(8)	0.0035(8)	0.0011(8)	0.0004(7)	0.0000(8)	0.0030(7)
B2	0.6692(5)	0.6692(5)	0	1	0.0040	0.0021(6)	0.0021(6)	0.0053(9)	-0.0014(5)	0.0014(5)	-0.0009(8)
B3	0.7912(7)	0	2/3	1	0.0401	0.0010(9)	0.0045(8)	0.1159(10)	0.0007(9)	0.0003(4)	0.0023(4)

Table S18. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Dy).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66732(4)	0.66732(4)	0.5	0.919(1)	0.0039	0.0039(2)	0.0039(2)	0.0031(2)	-0.00014(5)	0.00014(5)	0.0014(1)
Dy1	0.66732(4)	0.66732(4)	0.5	0.103(1)	0.0039	0.0039(2)	0.0039(2)	0.0031(2)	-0.00014(5)	0.00014(5)	0.0014(1)
Sc1	0	0.8751(3)	5/6	0.966(1)	0.0330	0.0012(6)	-0.0004(4)	0.0984(9)	0.0008(3)	0.0016(7)	0.0004(3)
Sc2	0.2142(2)	0.6703(1)	0.49734(7)	0.850(1)	0.0009	0.0035(3)	0.0020(3)	-0.0031(3)	-0.0005(2)	-0.0015(2)	0.0012(2)
Dy2	0.2142(2)	0.6703(1)	0.49734(7)	0.072(1)	0.0009	0.0035(3)	0.0020(3)	-0.0031(3)	-0.0005(2)	-0.0015(2)	0.0012(2)
O1	0.6595(5)	0.8618(6)	0.6833(7)	1	0.0207	0.0068(8)	0.0115(9)	0.0419(9)	-0.0025(9)	0.0153(8)	0.0033(8)
O2	0.9632(7)	0.9167(7)	0.4027(8)	0.5	0.0093	0.0041(9)	-0.0003(9)	0.0242(9)	-0.0004(9)	0.0001(9)	0.0010(8)
O3	0.4530(4)	0.4787(4)	0.3194(4)	1	0.0016	0.0031(8)	0.0000(8)	0.0018(8)	0.0001(7)	-0.0012(7)	0.0008(7)
O4	0.3551(5)	0.6008(4)	0.6448(5)	1	0.0045	0.0076(8)	0.0001(7)	0.0045(8)	-0.0005(7)	-0.0003(8)	0.0009(7)
O5	0.6738(5)	0.8685(6)	0.3201(6)	1	0.0121	0.0092(8)	0.0205(9)	0.0110(9)	-0.0096(8)	-0.0092(8)	0.0108(7)
O6	0.8030(6)	0.8030(6)	0	1	0.0463	0.0050(6)	0.0050(6)	0.1299(10)	0.0074(7)	-0.0074(7)	0.0033(8)
O7	0.6623(4)	0.5234(5)	-0.0004(4)	1	0.0011	0.0059(8)	-0.0010(8)	-0.0008(8)	0.0004(6)	0.0012(7)	0.0018(7)
B1	0.8853(5)	0.5428(5)	0.6723(5)	1	0.0013	0.0005(8)	0.0006(8)	-0.0004(8)	0.0006(7)	0.0001(8)	0.0028(7)
B2	0.6694(5)	0.6694(5)	0	1	0.0016	0.0006(6)	0.0006(6)	0.0026(9)	-0.0012(6)	0.0012(6)	-0.0005(8)
B3	0.7914(8)	0	2/3	1	0.0353	0.0016(9)	0.0058(8)	0.0999(10)	0.0006(9)	0.0003(4)	0.0029(4)

Table S19. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Ho).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66722(4)	0.66722(4)	0.5	0.936(1)	0.0113	0.0122(1)	0.0122(1)	0.0087(1)	-0.00026(4)	0.00026(4)	0.0055(1)
Ho1	0.66722(4)	0.66722(4)	0.5	0.091(1)	0.0113	0.0122(1)	0.0122(1)	0.0087(1)	-0.00026(4)	0.00026(4)	0.0055(1)
Sc1	0	0.8754(2)	5/6	1.006(1)	0.0353	0.0070(5)	0.0065(4)	0.0926(9)	0.0006(3)	0.0012(6)	0.0035(2)
Sc2	0.2137(1)	0.67005(9)	0.49742(5)	0.832(1)	0.0068	0.0107(3)	0.0092(2)	0.0002(2)	-0.0008(2)	-0.0016(1)	0.0046(2)
Ho2	0.2137(1)	0.67005(9)	0.49742(5)	0.090(1)	0.0068	0.0107(3)	0.0092(2)	0.0002(2)	-0.0008(2)	-0.0016(1)	0.0046(2)
O1	0.6569(5)	0.8607(5)	0.6827(7)	1	0.0280	0.0192(8)	0.0171(8)	0.0459(9)	0.0068(8)	0.0223(8)	0.0078(8)
O2	0.9645(7)	0.9175(7)	0.3987(7)	0.5	0.0164	0.0086(9)	0.0070(9)	0.0315(9)	-0.0035(9)	0.0020(9)	0.0024(8)
O3	0.4528(4)	0.4784(4)	0.3195(4)	1	0.0102	0.0151(8)	0.0113(8)	0.0065(7)	-0.0008(6)	-0.0027(6)	0.0083(6)
O4	0.3560(5)	0.6017(4)	0.6443(4)	1	0.0130	0.0194(8)	0.0118(7)	0.0099(7)	-0.0042(7)	-0.0035(7)	0.0093(7)
O5	0.6752(5)	0.8679(5)	0.3188(5)	1	0.0224	0.0294(8)	0.0343(9)	0.0154(8)	-0.0131(8)	-0.0139(7)	0.0248(7)
O6	0.8021(6)	0.8021(6)	0	1	0.0495	0.0137(6)	0.0137(6)	0.1218(10)	0.0057(7)	-0.0057(7)	0.0072(8)
O7	0.6618(4)	0.5227(4)	-0.0003(3)	1	0.0081	0.0145(8)	0.0073(8)	0.0045(7)	0.0003(6)	-0.0035(6)	0.0070(6)
B1	0.8862(5)	0.5424(5)	0.6718(4)	1	0.0059	0.0088(8)	0.0105(8)	0.0040(7)	0.0010(7)	0.0020(7)	0.0089(7)
B2	0.6718(5)	0.6718(5)	0	1	0.0083	0.0062(6)	0.0062(6)	0.0087(9)	-0.0049(5)	0.0049(5)	0.0001(8)
B3	0.7929(7)	0	2/3	1	0.0473	0.0090(9)	0.0288(9)	0.1107(10)	0.0076(9)	0.0038(4)	0.0144(4)

Table S20. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Er).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0	0	0	0.964(1)	0.0046	0.0046(1)	0.0046(1)	0.0045(2)	0.0000(1)	0.0000(1)	0.0023(7)
Er1	0	0	0	0.100(1)	0.0046	0.0046(1)	0.0046(1)	0.0045(2)	0.0000(1)	0.0000(1)	0.0023(7)
Sc2	0.5440(1)	0	0	0.658(1)	0.0062	0.0037(3)	0.0035(3)	0.0111(4)	0.0017(2)	0.0009(1)	0.0017(2)
Er2	0.5440(1)	0	0	0.166(1)	0.0062	0.0037(3)	0.0035(3)	0.0111(4)	0.0017(2)	0.0009(1)	0.0017(2)
O1	0.8596(5)	0	0.5	1	0.0064	0.0024(9)	0.0072(10)	0.0113(11)	-0.0009(9)	-0.0004(5)	0.0036(5)
O2	0.5935(8)	0	0.5	1	0.0690	0.024(1)	0.088(1)	0.116(1)	-0.094(1)	-0.0471(5)	0.0443(6)
O3	0.4588(5)	0.1415(5)	0.5144(5)	1	0.0102	0.0156(10)	0.0042(9)	0.0088(10)	0.0001(8)	0.0033(9)	0.0035(8)
B1	0	0	0.5	1	0.0027	0.0025(8)	0.0025(8)	0.0030(12)	0	0	0.0013(4)
B2	0.4531(7)	0	0.5	1	0.0101	0.0056(10)	0.009(1)	0.017(1)	-0.009(1)	-0.0046(5)	0.0048(5)

Table S21. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Tm).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0	0	0	0.897(1)	0.0077	0.00746(8)	0.00746(8)	0.0082(1)	0.0000(1)	0.0000(1)	0.00373(4)
Tm1	0	0	0	0.131(1)	0.0077	0.00746(8)	0.00746(8)	0.0082(1)	0.0000(1)	0.0000(1)	0.00373(4)
Sc2	0.54377(6)	0	0	0.782(1)	0.0081	0.0056(1)	0.0052(2)	0.0133(2)	0.0016(1)	0.00081(5)	0.00251(8)
Tm2	0.54377(6)	0	0	0.153(1)	0.0081	0.0056(1)	0.0052(2)	0.0133(2)	0.0016(1)	0.00081(5)	0.00251(8)
O1	0.8595(3)	0	0.5	1	0.0087	0.0045(5)	0.0084(7)	0.0145(8)	-0.0010(6)	-0.0005(3)	0.0042(3)
O2	0.5930(4)	0	0.5	1	0.0697	0.0223(7)	0.0834(10)	0.124(1)	-0.0916(9)	-0.0458(5)	0.0417(5)
O3	0.4588(3)	0.1415(2)	0.5144(3)	1	0.0127	0.0175(7)	0.0068(6)	0.0121(6)	0.0004(5)	0.0033(6)	0.0048(5)
B1	0	0	0.5	1	0.0060	0.0053(6)	0.0053(6)	0.0074(10)	0	0	0.0026(3)
B2	0.4537(4)	0	0.5	1	0.0136	0.0077(7)	0.0145(9)	0.0208(9)	-0.0102(9)	-0.0051(4)	0.0072(5)

Table S22. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Yb).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0	0	0	0.966(1)	0.0050	0.0051(2)	0.0051(2)	0.0048(2)	0.0000(1)	0.0000(1)	0.00253(8)
Yb1	0	0	0	0.113(1)	0.0050	0.0051(2)	0.0051(2)	0.0048(2)	0.0000(1)	0.0000(1)	0.00253(8)
Sc2	0.5449(1)	0	0	0.659(1)	0.0051	0.0027(3)	0.0023(3)	0.0103(5)	0.0017(2)	0.0008(1)	0.0012(2)
Yb2	0.5449(1)	0	0	0.149(1)	0.0051	0.0027(3)	0.0023(3)	0.0103(5)	0.0017(2)	0.0008(1)	0.0012(2)
O1	0.8589(5)	0	0.5	1	0.0061	0.0027(9)	0.0043(9)	0.0118(10)	-0.0004(9)	-0.0002(4)	0.0021(4)
O2	0.5925(7)	0	0.5	1	0.0602	0.0190(10)	0.0723(10)	0.107(1)	-0.0776(10)	-0.0388(5)	0.0362(5)
O3	0.4584(5)	0.1419(5)	0.5152(5)	1	0.0096	0.0127(9)	0.0048(9)	0.0085(9)	0.0001(8)	0.0044(9)	0.0023(8)
B1	0	0	0.5	1	0.0037	0.0032(7)	0.0032(7)	0.0047(11)	0	0	0.0016(4)
B2	0.4533(6)	0	0.5	1	0.0099	0.0033(9)	0.0109(10)	0.0180(10)	-0.0102(10)	-0.0051(5)	0.0054(5)

Table S23. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of $NdSc_3(BO_3)_4$:R (R = Lu).

Site	x/a	y/b	z/c	Occ.	Ueq	U11	U22	U33	U23	U13	U12
Nd1	0.66687(5)	0.66687(5)	0.5	0.889(1)	0.0059	0.0059(2)	0.0059(2)	0.0054(3)	-0.00024(7)	0.00024(7)	0.0026(2)
Lu1	0.66687(5)	0.66687(5)	0.5	0.078(1)	0.0059	0.0059(2)	0.0059(2)	0.0054(3)	-0.00024(7)	0.00024(7)	0.0026(2)
Sc1	0	0.8745(3)	5/6	0.996(1)	0.0280	-0.0001(6)	-0.0024(5)	0.0871(9)	0.0004(3)	0.0008(7)	-0.0001(3)
Sc2	0.2130(2)	0.6698(1)	0.49795(7)	0.886(1)	0.0008	0.0034(3)	0.0015(3)	-0.0030(3)	-0.0002(3)	-0.0021(2)	0.0008(2)
Lu2	0.2130(2)	0.6698(1)	0.49795(7)	0.108(1)	0.0008	0.0034(3)	0.0015(3)	-0.0030(3)	-0.0002(3)	-0.0021(2)	0.0008(2)
O1	0.6616(6)	0.8626(6)	0.6879(7)	1	0.0230	0.0076(9)	0.0068(9)	0.0478(9)	-0.0027 (9)	0.0164(9)	-0.0016(8)
O2	0.9645(8)	0.9150(8)	0.4081(8)	0.5	0.0176	0.0104(9)	-0.0007(9)	0.0424(9)	0.0001(9)	-0.0004(9)	0.0018(9)
O3	0.4540(5)	0.4781(5)	0.3182(5)	1	0.0048	0.0052(8)	0.0057(8)	0.0040(8)	-0.0003(8)	0.0018(8)	0.0032(7)
O4	0.3525(6)	0.5992(6)	0.6495(5)	1	0.0134	0.0245(9)	0.0067(9)	0.0054(8)	0.0018(8)	-0.0025(9)	0.0052(8)
O5	0.6775 (6)	0.8720(7)	0.3182(6)	1	0.0201	0.0200(9)	0.0367(9)	0.0171(9)	-0.0193(9)	-0.0151(8)	0.0243(8)
O6	0.7987(6)	0.7987 (6)	0	1	0.0408	0.0045(6)	0.0045(6)	0.1167(10)	0.0005(7)	-0.0005(7)	0.0048(9)
O7	0.6630(5)	0.5236(6)	-0.0004(4)	1	0.0026	0.0074(9)	-0.0006(8)	-0.0018(9)	0.0009(7)	-0.0005(8)	0.0023(7)
B1	0.8848(6)	0.5456(6)	0.6717(6)	1	0.0021	0.0017(9)	0.0038(9)	0.0006(9)	0.0010(8)	0.0004(9)	0.0013(8)
B2	0.6654(6)	0.6654(6)	0	1	0.0047	0.0039(6)	0.0039(6)	0.0038(9)	-0.0013(6)	0.0013(6)	-0.0001(9)
B3	0.7887(9)	0	2/3	1	0.0374	0.0178(9)	0.0297(8)	0.0688(10)	0.0281(8)	0.0140(4)	0.0149(4)