

Supporting Information

NIR-to-NIR ratiometric and lifetime based luminescence thermometer on a structural phase transition in $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3\text{:Yb}^{3+}$

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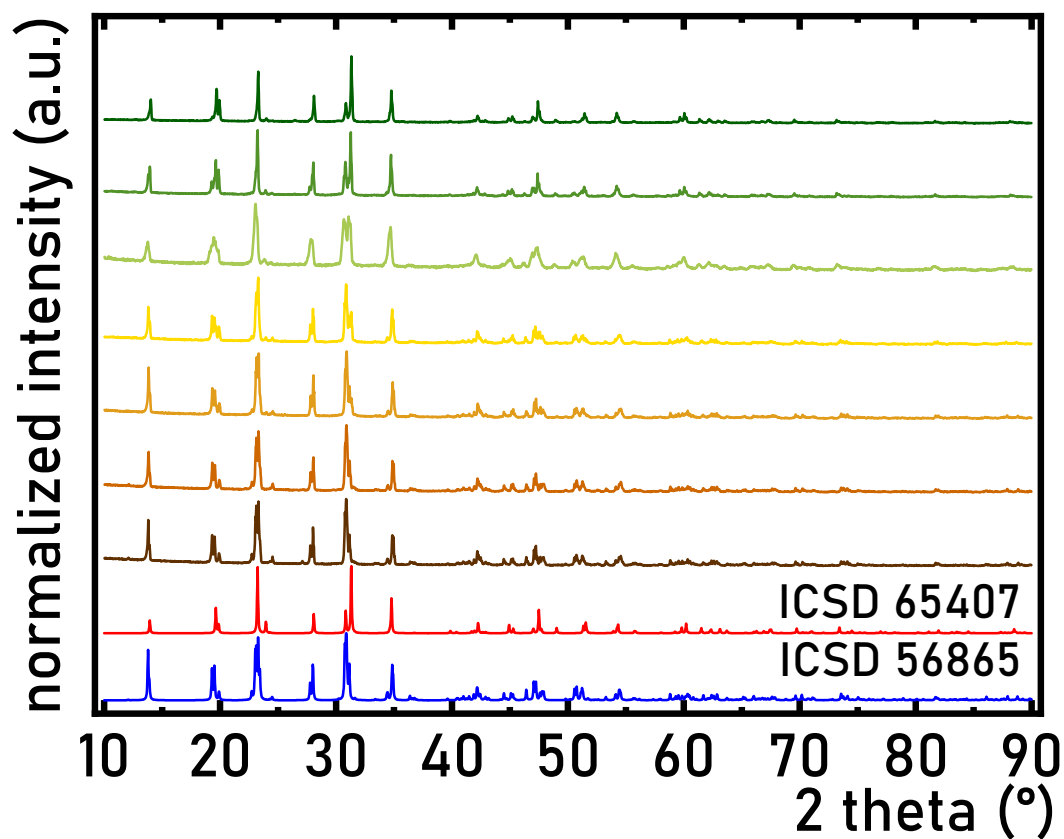


Figure S1. XRD patterns of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:\text{Yb}^{3+}$ for different Yb^{3+} concentration.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 298K

Global Parameters

Number of used phases:	1
Number of variables:	15
Number of constraints:	0
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,105(1)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,85300
R (profile)/ %:	5,58234
R (weighted profile)/ %:	7,33104
GOF:	6,60278
d-statistic:	0,82478
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000

Asymmetry 2: 0,000000
 Shape Type: Shape Individual
 Shape 1 Left: 0,600000
 Shape 2 Left: 0,000000
 Shape 3 Left: 0,000000
 Shape 1 Right: 0,600000
 Shape 2 Right: 0,000000
 Shape 3 Right: 0,000000
 K a1/a2 intensity ratio: 0,500000
 K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Structure and profile data:
 Formula sum: Na_{12,00}P_{12,00}Sc_{8,00}O_{48,00}
 Formula mass/ g/mol: 1775,1820
 Density (calculated)/ g/cm³: 2,8281
 F(000): 864,0000
 Weight fraction/ %: 100,000000
 Space group (No.): C 1 c 1 (9)
 Lattice parameters:
 a/ Å: 15,3938(4)
 b/ Å: 8,9203(2)
 c/ Å: 9,1011(2)
 alpha/ °: 90
 beta/ °: 123,498(2)
 gamma/ °: 90
 V/ 10⁶ pm³: 1042,16900
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,058(5)
 V Left: -0,050(4)
 W Left: 0,0180(9)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,63(2)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 5,21245

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291

O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

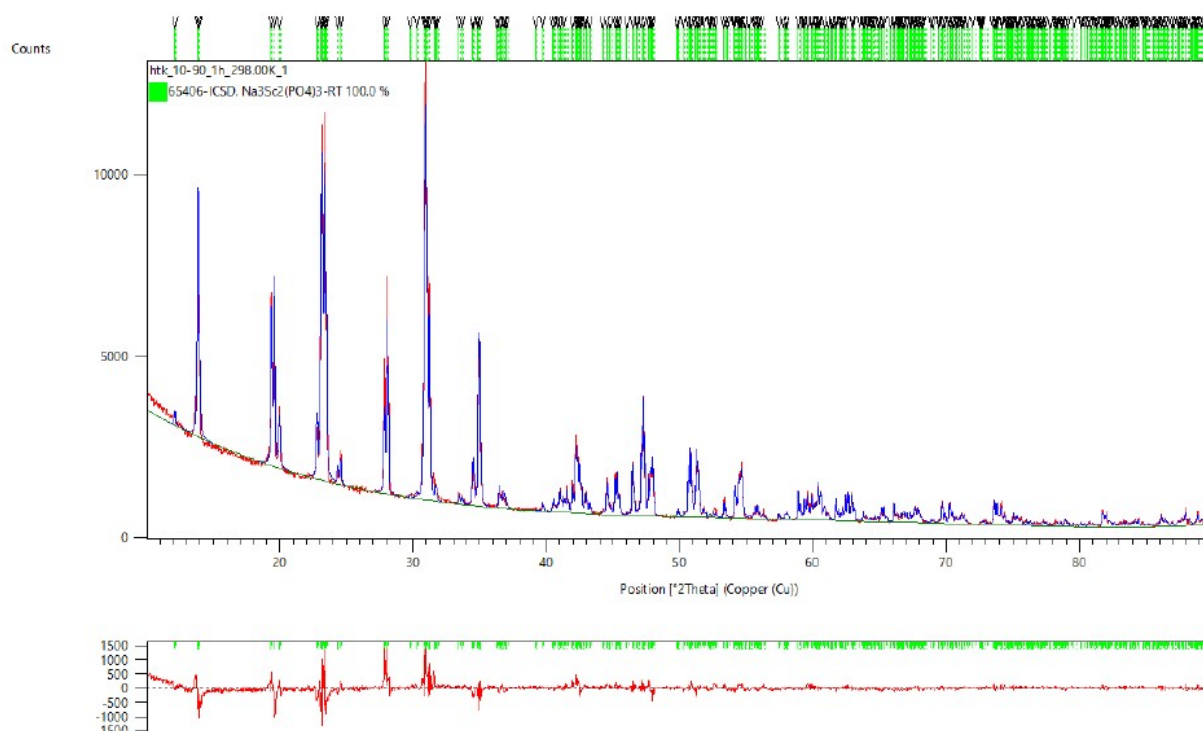


Figure S2. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 298K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 303K

Global Parameters

Number of used phases:	1
Number of variables:	15
Number of constraints:	0
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,334(1)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,84608
R (profile)/ %:	5,81598
R (weighted profile)/ %:	7,53607
GOF:	7,01123
d-statistic:	0,70321
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000

U Left: 0,000000
 V Left: 0,000000
 W Left: 0,010000
 U Right: 0,000000
 V Right: 0,000000
 W Right: 0,010000
 Asymmetry Type: No Asymmetry Function
 Asymmetry 1: 0,000000
 Asymmetry 2: 0,000000
 Shape Type: Shape Individual
 Shape 1 Left: 0,600000
 Shape 2 Left: 0,000000
 Shape 3 Left: 0,000000
 Shape 1 Right: 0,600000
 Shape 2 Right: 0,000000
 Shape 3 Right: 0,000000
 K a1/a2 intensity ratio: 0,500000
 K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 65406-ICSD, Na3Sc2(PO4)3-RT

Structure and profile data:
 Formula sum: $\text{Na}_{12,00}\text{P}_{12,00}\text{Sc}_{8,00}\text{O}_{48,00}$
 Formula mass/ g/mol: 1775,1820
 Density (calculated)/ g/cm³: 2,8309
 F(000): 864,0000
 Weight fraction/ %: 100,000000
 Space group (No.): C 1 c 1 (9)
 Lattice parameters:
 a/ Å: 15,3891(5)
 b/ Å: 8,9174(2)
 c/ Å: 9,0982(3)
 alpha/ °: 90
 beta/ °: 123,502(2)
 gamma/ °: 90
 V/ 10⁶ pm³: 1041,12700
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,059(5)
 V Left: -0,050(4)
 W Left: 0,0181(9)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,63(2)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 5,54814

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na3Sc2(PO4)3-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255

P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

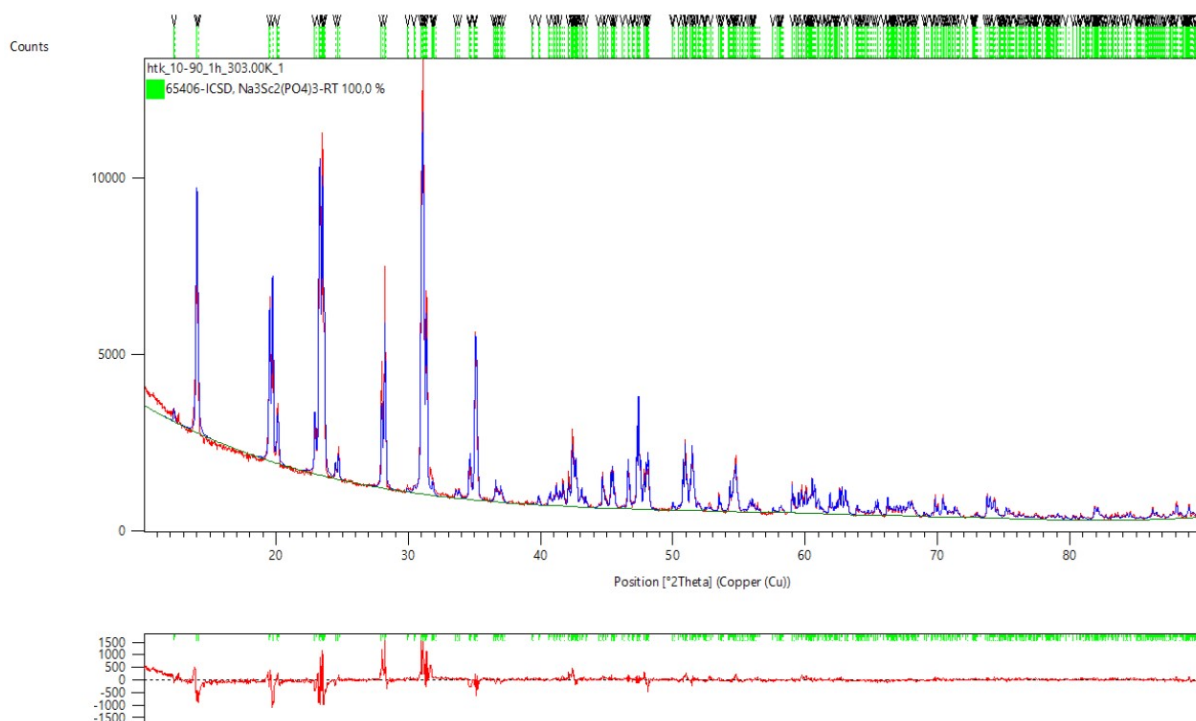


Figure S3. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 303K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 313K

Global Parameters

Number of used phases:	1
Number of variables:	15
Number of constraints:	0
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,403(1)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,84114
R (profile)/ %:	5,74436

R (weighted profile)/ %:	7,44430
GOF:	6,86533
d-statistic:	0,71516
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000
K alpha/beta intensity ratio:	0,000000
Crystal Shape Factor K:	1,0000
Instrumental FWHM Curve Type:	Caglioti function
Instr. Gauss Curve Coefficient A:	0,0045(5)
Instr. Gauss Curve Coefficient B:	-0,0032(9)
Instr. Gauss Curve Coefficient C:	0,0046(3)
Instr. Lorentz Curve Coefficient A:	0,0062(7)
Instr. Lorentz Curve Coefficient B:	-0,004(1)
Instr. Lorentz Curve Coefficient C:	0,0064(5)

Relevant parameters of 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Structure and profile data:	
Formula sum:	Na _{12,00} P _{12,00} Sc _{8,00} O _{48,00}
Formula mass/ g/mol:	1775,1820
Density (calculated)/ g/cm ³	2,8317
F(000):	864,0000
Weight fraction/ %:	100,000000
Space group (No.):	C 1 c 1 (9)
Lattice parameters:	
a/ Å:	15,3893(5)
b/ Å:	8,9168(2)
c/ Å:	9,0972(3)
alpha/ °:	90
beta/ °:	123,513(2)
gamma/ °:	90
V/ 10 ⁶ pm ³	1040,83400
Overall displacement parameter:	0,000000
Extinction:	0,000000
Flat Plate Absorption Correction:	0,000000
Porosity:	0,000000
Roughness:	0,000000
Fitting mode:	Structure Fit
U Left:	0,059(5)
V Left:	-0,050(4)
W Left:	0,0182(9)
Preferred orientation direction/ hkl:	0,00 0,00 1,00
Preferred orientation parameter:	1,000000
Asymmetry parameter 1:	0,000000
Asymmetry parameter 2:	0,000000
Peak shape:	
parameter 1 Left:	0,63(2)
parameter 2 Left:	0,000000
parameter 3 Left:	0,000000
R (Bragg)/ %:	5,30466

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

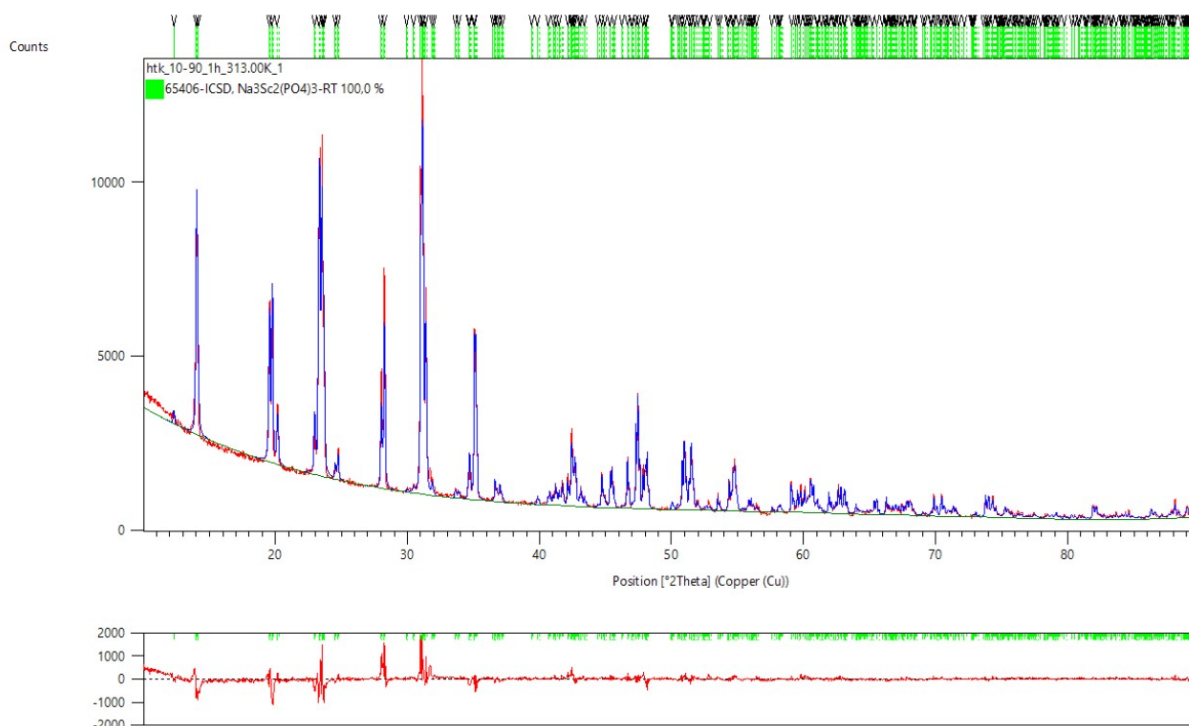


Figure S4. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 313K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 323K

Global Parameters

Number of used phases: 1
Number of variables: 15

Number of constraints:	0
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,341(1)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,85363
R (profile)/ %:	5,88617
R (weighted profile)/ %:	7,60888
GOF:	7,10961
d-statistic:	0,74630
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000
K alpha/beta intensity ratio:	0,000000
Crystal Shape Factor K:	1,0000
Instrumental FWHM Curve Type:	Caglioti function
Instr. Gauss Curve Coefficient A:	0,0045(5)
Instr. Gauss Curve Coefficient B:	-0,0032(9)
Instr. Gauss Curve Coefficient C:	0,0046(3)
Instr. Lorentz Curve Coefficient A:	0,0062(7)
Instr. Lorentz Curve Coefficient B:	-0,004(1)
Instr. Lorentz Curve Coefficient C:	0,0064(5)

Relevant parameters of 65406-ICSD, Na3Sc2(PO4)3-RT

Structure and profile data:	
Formula sum:	Na _{12,00} P _{12,00} Sc _{8,00} O _{48,00}
Formula mass/ g/mol:	1775,1820
Density (calculated)/ g/cm ³	2,8308
F(000):	864,0000
Weight fraction/ %:	100,000000
Space group (No.):	C 1 c 1 (9)
Lattice parameters:	
a/ Å:	15,3923(5)
b/ Å:	8,9181(2)
c/ Å:	9,0980(3)
alpha/ °:	90
beta/ °:	123,522(2)
gamma/ °:	90
V/ 10 ⁶ pm ³	1041,16000
Overall displacement parameter:	0,000000
Extinction:	0,000000
Flat Plate Absorption Correction:	0,000000
Porosity:	0,000000
Roughness:	0,000000
Fitting mode:	Structure Fit
U Left:	0,058(5)
V Left:	-0,050(4)
W Left:	0,0182(9)
Preferred orientation direction/ hkl:	0,00 0,00 1,00
Preferred orientation parameter:	1,000000
Asymmetry parameter 1:	0,000000
Asymmetry parameter 2:	0,000000
Peak shape:	

parameter 1 Left: 0,64(2)
parameter 2 Left: 0,000000
parameter 3 Left: 0,000000
R (Bragg)/ %: 5,36151

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

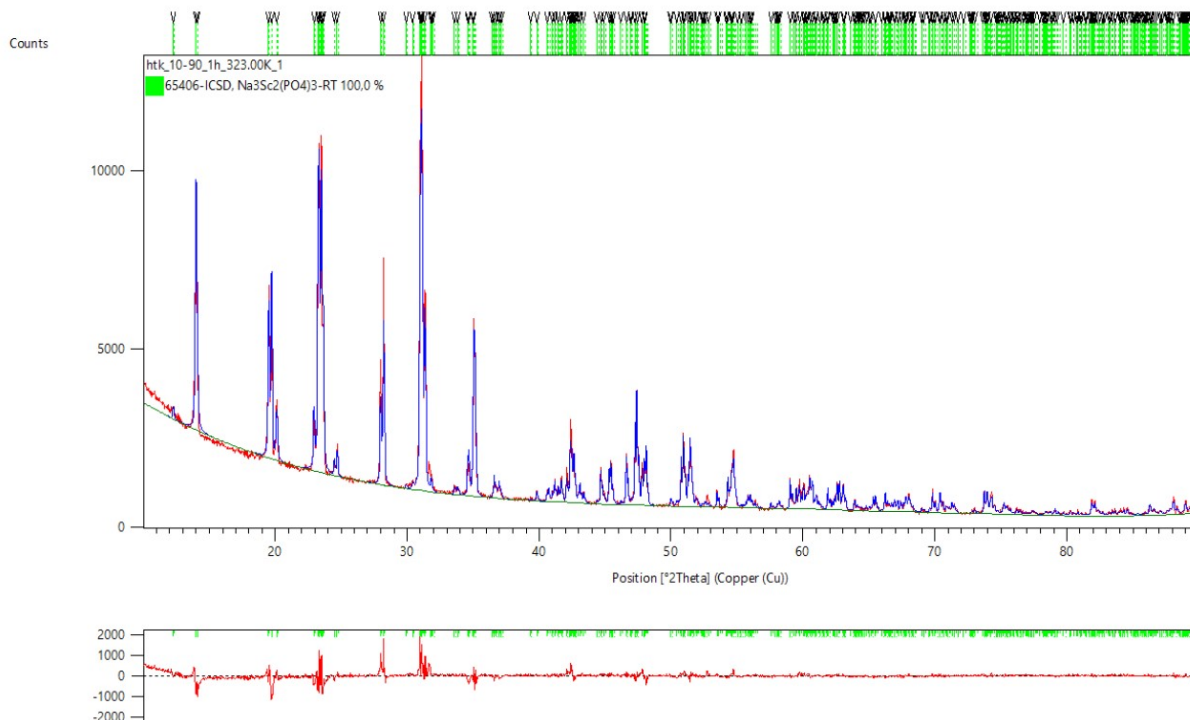


Figure S5. Rietveld refinement of XRD pattern of Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 323K.

Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 333K

Global Parameters

Number of used phases:	1
Number of variables:	15
Number of constraints:	0
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,231(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,86235
R (profile)/ %:	5,89180
R (weighted profile)/ %:	7,67277
GOF:	7,18554
d-statistic:	0,72158
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000
K alpha/beta intensity ratio:	0,000000
Crystal Shape Factor K:	1,0000
Instrumental FWHM Curve Type:	Caglioti function
Instr. Gauss Curve Coefficient A:	0,0045(5)
Instr. Gauss Curve Coefficient B:	-0,0032(9)
Instr. Gauss Curve Coefficient C:	0,0046(3)
Instr. Lorentz Curve Coefficient A:	0,0062(7)
Instr. Lorentz Curve Coefficient B:	-0,004(1)
Instr. Lorentz Curve Coefficient C:	0,0064(5)

Relevant parameters of 65406-ICSD, Na3Sc2(PO4)3-RT

Structure and profile data:	
Formula sum:	Na _{12,00} P _{12,00} Sc _{8,00} O _{48,00}
Formula mass/ g/mol:	1775,1820
Density (calculated)/ g/cm ³	2,8292
F(000):	864,0000
Weight fraction/ %:	100,000000
Space group (No.):	C 1 c 1 (9)
Lattice parameters:	
a/ Å:	15,3963(5)
b/ Å:	8,9199(3)
c/ Å:	9,1000(3)
alpha/ °:	90
beta/ °:	123,532(2)
gamma/ °:	90
V/ 10 ⁶ pm ³	1041,75000
Overall displacement parameter:	0,000000
Extinction:	0,000000
Flat Plate Absorption Correction:	0,000000
Porosity:	0,000000
Roughness:	0,000000
Fitting mode:	Structure Fit
U Left:	0,059(5)
V Left:	-0,049(5)
W Left:	0,018(1)

Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,65(2)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 5,47393

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

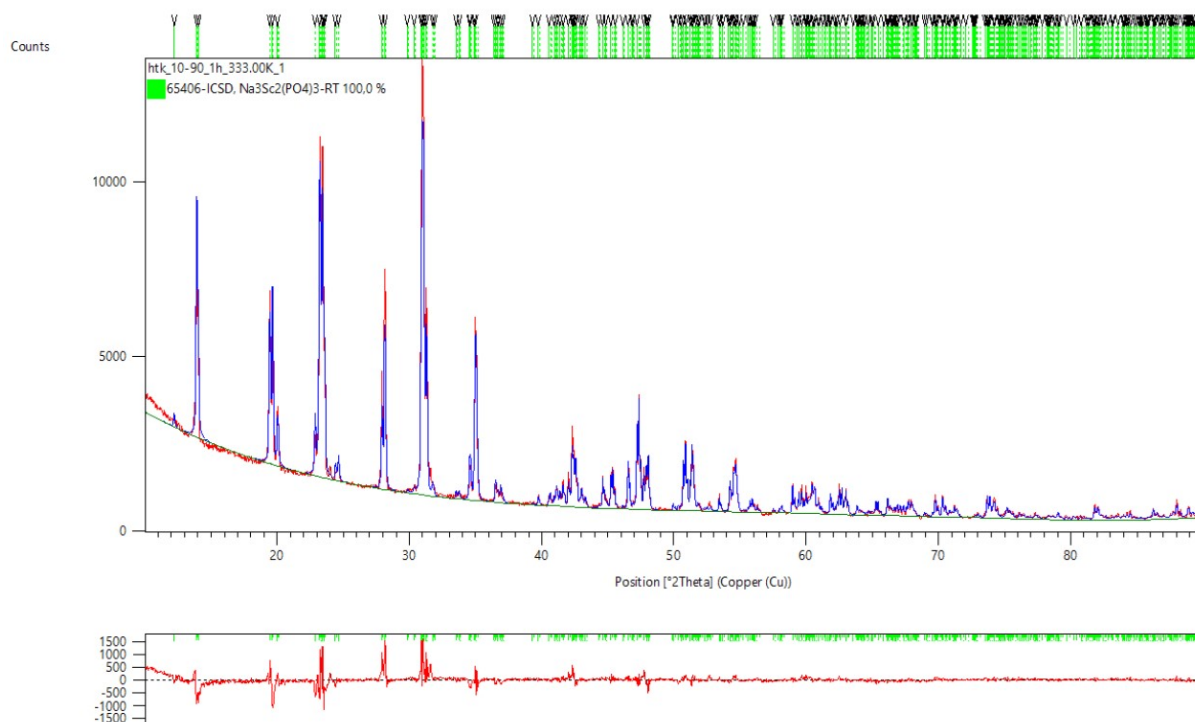


Figure S6. Rietveld refinement of XRD pattern of Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 333K.

Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 343K

Global Parameters

Number of used phases:	2
Number of variables:	22
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,220(3)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,85714
R (profile)/ %:	7,56578
R (weighted profile)/ %:	10,70992
GOF:	14,05108
d-statistic:	0,35010
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000
K alpha/beta intensity ratio:	0,000000
Crystal Shape Factor K:	1,0000
Instrumental FWHM Curve Type:	Caglioti function
Instr. Gauss Curve Coefficient A:	0,0045(5)
Instr. Gauss Curve Coefficient B:	-0,0032(9)
Instr. Gauss Curve Coefficient C:	0,0046(3)
Instr. Lorentz Curve Coefficient A:	0,0062(7)
Instr. Lorentz Curve Coefficient B:	-0,004(1)
Instr. Lorentz Curve Coefficient C:	0,0064(5)

Relevant parameters of 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Structure and profile data:	
Formula sum:	Na _{12,00} P _{12,00} Sc _{8,00} O _{48,00}
Formula mass/ g/mol:	1775,1820
Density (calculated)/ g/cm ³	2,8283
F(000):	864,0000
Weight fraction/ %:	45(1)
Space group (No.):	C 1 c 1 (9)
Lattice parameters:	
a/ Å:	15,394(2)
b/ Å:	8,9206(9)
c/ Å:	9,1038(9)
alpha/ °:	90
beta/ °:	123,536(7)
gamma/ °:	90
V/ 10 ⁶ pm ³	1042,07400
Overall displacement parameter:	0,000000
Extinction:	0,000000
Flat Plate Absorption Correction:	0,000000

Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,07(3)
 V Left: -0,05(2)
 W Left: 0,018(4)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,63(9)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 8,65094

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,6001
 F(000): 1176,8040
 Weight fraction/ %: 55(1)
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9217(4)
 b/ Å: 8,9217(4)
 c/ Å: 22,359(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1541,24900
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,33(2)
 V Left: -0,25(2)
 W Left: 0,049(3)

Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,60(5)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 11,77228

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

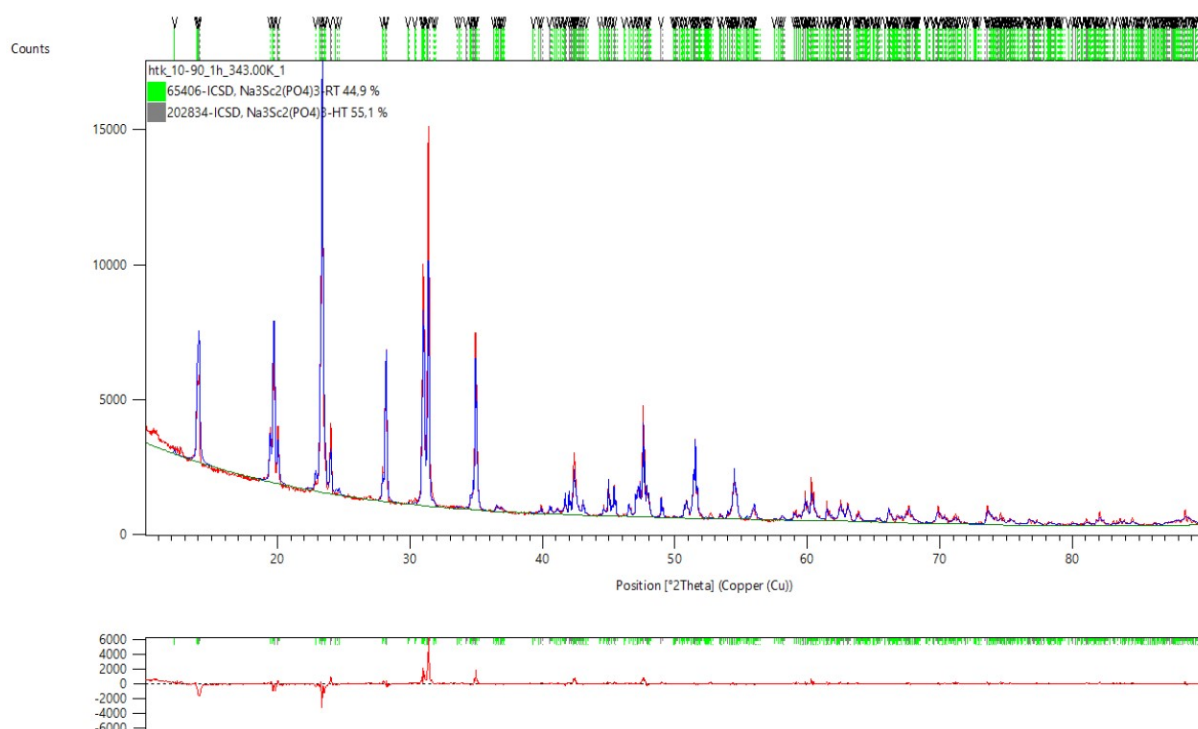


Figure S7. Rietveld refinement of XRD pattern of Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 343K.

Na₃Sc₂(PO₄)₃:1%Yb³⁺ measured at 353K

Global Parameters

Number of used phases: 2
 Number of variables: 22
 Number of constraints: 1
 Zero shift/ °2Theta: 0,000000
 Specimen displacement/ mm : -0,241(2)
 Profile function: Pseudo Voigt
 Background: Polynomial

R (expected)/ %:	2,86023
R (profile)/ %:	8,07976
R (weighted profile)/ %:	11,75570
GOF:	16,89255
d-statistic:	0,28409
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000
K alpha/beta intensity ratio:	0,000000
Crystal Shape Factor K:	1,0000
Instrumental FWHM Curve Type:	Caglioti function
Instr. Gauss Curve Coefficient A:	0,0045(5)
Instr. Gauss Curve Coefficient B:	-0,0032(9)
Instr. Gauss Curve Coefficient C:	0,0046(3)
Instr. Lorentz Curve Coefficient A:	0,0062(7)
Instr. Lorentz Curve Coefficient B:	-0,004(1)
Instr. Lorentz Curve Coefficient C:	0,0064(5)

Relevant parameters of 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Structure and profile data:	
Formula sum:	Na _{12,00} P _{12,00} Sc _{8,00} O _{48,00}
Formula mass/ g/mol:	1775,1820
Density (calculated)/ g/cm ³	2,8247
F(000):	864,0000
Weight fraction/ %:	32(1)
Space group (No.):	C 1 c 1 (9)
Lattice parameters:	
a/ Å:	15,399(3)
b/ Å:	8,922(1)
c/ Å:	9,112(1)
alpha/ °:	90
beta/ °:	123,54(1)
gamma/ °:	90
V/ 10 ⁶ pm ³	1043,41900
Overall displacement parameter:	0,000000
Extinction:	0,000000
Flat Plate Absorption Correction:	0,000000
Porosity:	0,000000
Roughness:	0,000000
Fitting mode:	Structure Fit
U Left:	0,07(4)
V Left:	-0,05(3)
W Left:	0,017(6)
Preferred orientation direction/ hkl:	0,00 0,00 1,00
Preferred orientation parameter:	1,000000
Asymmetry parameter 1:	0,000000
Asymmetry parameter 2:	0,000000
Peak shape:	
parameter 1 Left:	0,7(1)
parameter 2 Left:	0,000000
parameter 3 Left:	0,000000
R (Bragg)/ %:	9,18134

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na3Sc2(PO4)3-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

Relevant parameters of 202834-ICSD, Na3Sc2(PO4)3-HT

Structure and profile data:

Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}

Formula mass/ g/mol: 2413,6550

Density (calculated)/ g/cm³: 2,5974

F(000): 1176,8040

Weight fraction/ %: 68(1)

Space group (No.): R -3 c (167)

Lattice parameters:

a/ Å: 8,9226(3)

b/ Å: 8,9226(3)

c/ Å: 22,377(1)

alpha/ °: 90

beta/ °: 90

gamma/ °: 120

V/ 10⁶ pm³: 1542,82600

Overall displacement parameter: 0,000000

Extinction: 0,000000

Flat Plate Absorption Correction: 0,000000

Porosity: 0,000000

Roughness: 0,000000

Fitting mode: Structure Fit

U Left: 0,16(1)

V Left: -0,12(1)

W Left: 0,030(2)

Preferred orientation direction/ hkl: 0,00 0,00 1,00

Preferred orientation parameter: 1,000000

Asymmetry parameter 1: 0,000000

Asymmetry parameter 2: 0,000000

Peak shape:

parameter 1 Left: 0,58(4)

parameter 2 Left: 0,000000

parameter 3 Left: 0,000000

R (Bragg)/ %: 13,72114

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na3Sc2(PO4)3-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000

O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

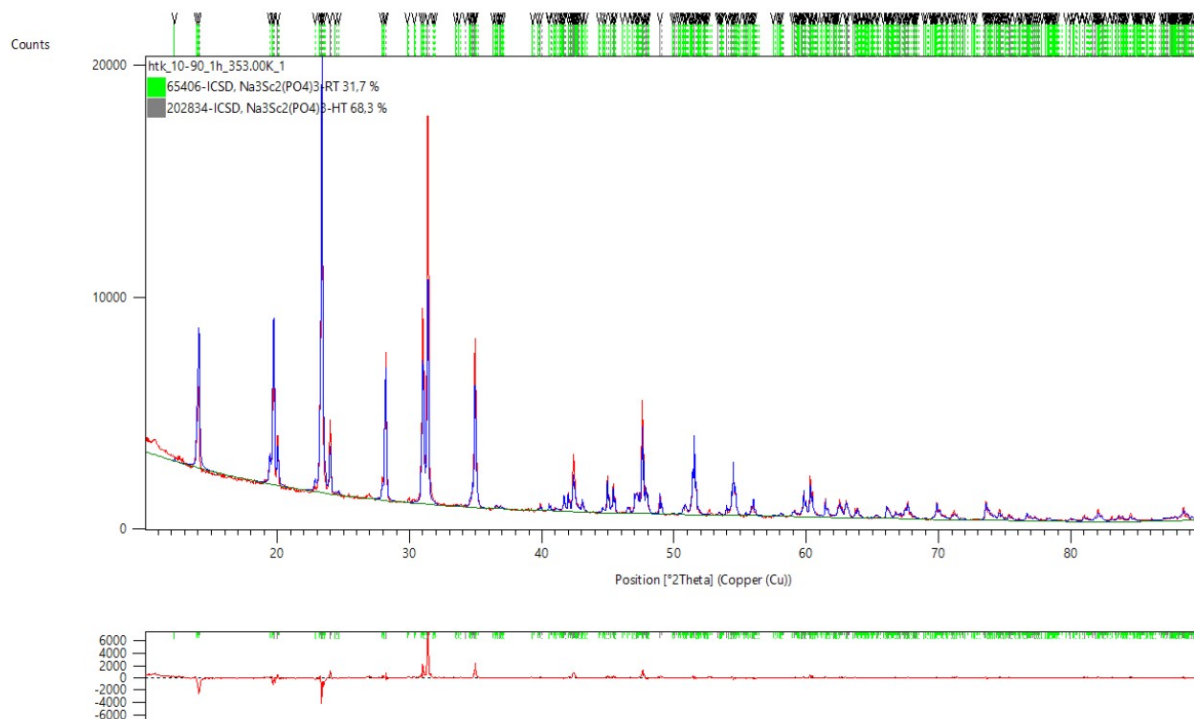


Figure S8. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 353K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 363K

Global Parameters

Number of used phases:	2
Number of variables:	22
Number of constraints:	1
Zero shift/ $^{\circ}\text{2Theta}$:	0,000000
Specimen displacement/ mm :	-0,276(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,86506
R (profile)/ %:	8,31528
R (weighted profile)/ %:	12,08455
GOF:	17,79073
d-statistic:	0,26067
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000

Asymmetry 2: 0,000000
 Shape Type: Shape Individual
 Shape 1 Left: 0,600000
 Shape 2 Left: 0,000000
 Shape 3 Left: 0,000000
 Shape 1 Right: 0,600000
 Shape 2 Right: 0,000000
 Shape 3 Right: 0,000000
 K a1/a2 intensity ratio: 0,500000
 K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Structure and profile data:
 Formula sum: Na_{12,00}P_{12,00}Sc_{8,00}O_{48,00}
 Formula mass/ g/mol: 1775,1820
 Density (calculated)/ g/cm³: 2,8232
 F(000): 864,0000
 Weight fraction/ %: 27(1)
 Space group (No.): C 1 c 1 (9)
 Lattice parameters:
 a/ Å: 15,405(3)
 b/ Å: 8,921(2)
 c/ Å: 9,116(2)
 alpha/ °: 90
 beta/ °: 123,56(1)
 gamma/ °: 90
 V/ 10⁶ pm³: 1043,96800
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,09(6)
 V Left: -0,05(4)
 W Left: 0,016(7)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,7(2)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 9,52414

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na₃Sc₂(PO₄)₃-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291

O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456
O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

Relevant parameters of 202834-ICSD, Na3Sc2(PO4)3-HT

Structure and profile data:

Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}

Formula mass/ g/mol: 2413,6550

Density (calculated)/ g/cm³ 2,5960

F(000): 1176,8040

Weight fraction/ %: 73(1)

Space group (No.): R -3 c (167)

Lattice parameters:

a/ Å: 8,9222(3)

b/ Å: 8,9222(3)

c/ Å: 22,392(1)

alpha/ °: 90

beta/ °: 90

gamma/ °: 120

V/ 10⁶ pm³ 1543,69000

Overall displacement parameter: 0,000000

Extinction: 0,000000

Flat Plate Absorption Correction: 0,000000

Porosity: 0,000000

Roughness: 0,000000

Fitting mode: Structure Fit

U Left: 0,16(1)

V Left: -0,12(1)

W Left: 0,029(2)

Preferred orientation direction/ hkl: 0,00 0,00 1,00

Preferred orientation parameter: 1,000000

Asymmetry parameter 1: 0,000000

Asymmetry parameter 2: 0,000000

Peak shape:

parameter 1 Left: 0,54(4)

parameter 2 Left: 0,000000

parameter 3 Left: 0,000000

R (Bragg)/ %: 14,12986

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na3Sc2(PO4)3-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

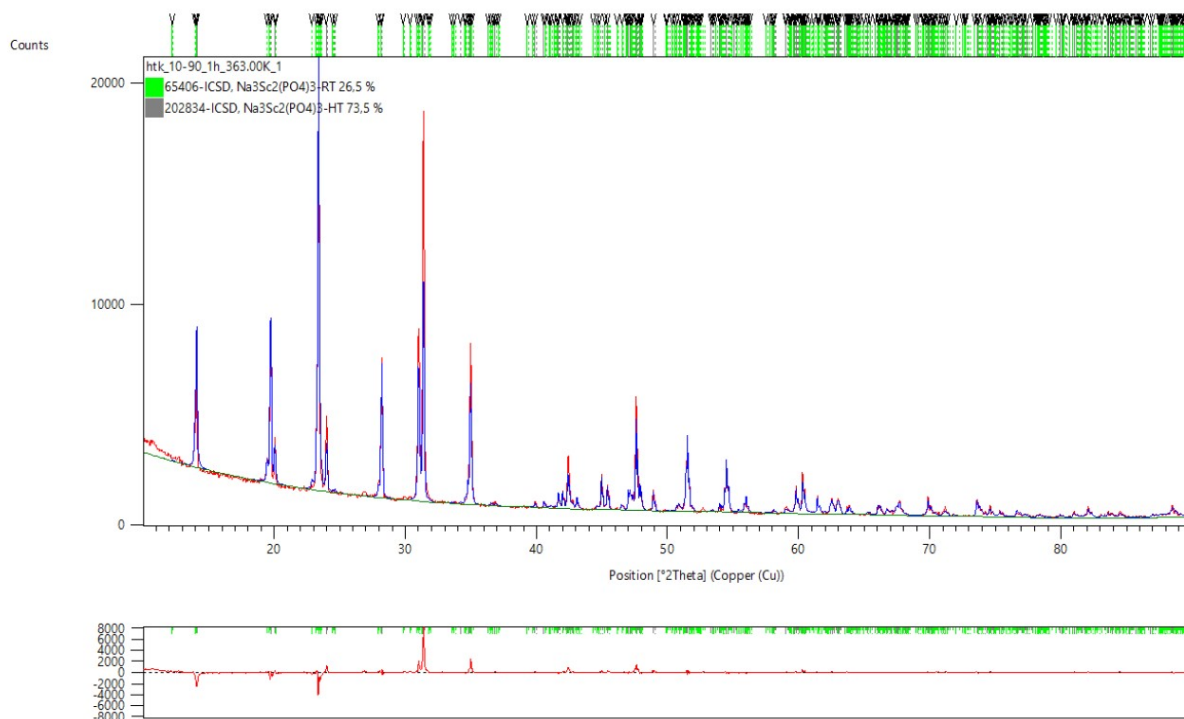


Figure S9. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 363K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 373K

Global Parameters

Number of used phases:	2
Number of variables:	22
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,277(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,87330
R (profile)/ %:	8,37464
R (weighted profile)/ %:	12,19211
GOF:	18,00515
d-statistic:	0,24164
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 65406-ICSD, Na3Sc2(PO4)3-RT

Structure and profile data:
 Formula sum: Na_{12,00}P_{12,00}Sc_{8,00}O_{48,00}
 Formula mass/ g/mol: 1775,1820
 Density (calculated)/ g/cm³: 2,8218
 F(000): 864,0000
 Weight fraction/ %: 23(1)
 Space group (No.): C 1 c 1 (9)
 Lattice parameters:
 a/ Å: 15,411(4)
 b/ Å: 8,922(2)
 c/ Å: 9,120(2)
 alpha/ °: 90
 beta/ °: 123,59(2)
 gamma/ °: 90
 V/ 10⁶ pm³: 1044,47600
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,09(7)
 V Left: -0,05(5)
 W Left: 0,015(8)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,8(2)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 9,44304

Occupancy, atomic fract. coordinates and Biso for 65406-ICSD, Na3Sc2(PO4)3-RT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Na1	4a	1,000000	0,225700	0,151300	0,704900	3,979423
Na2	4a	1,000000	0,422200	0,390700	0,021100	2,787175
Na3	4a	1,000000	0,091500	0,574900	0,453600	2,613470
P1	4a	1,000000	0,060500	0,108400	0,000399	0,813255
P2	4a	1,000000	0,275700	0,608400	0,020400	0,813255
P3	4a	1,000000	0,421700	0,045300	0,012000	0,821151
Sc1	4a	1,000000	0,318200	0,246200	0,207000	0,647446
Sc2	4a	1,000000	0,017100	0,247700	0,309700	0,647446
O1	4a	1,000000	0,272900	0,437200	0,042800	1,073812
O2	4a	1,000000	0,066300	0,061200	0,479800	1,073812
O3	4a	1,000000	0,483100	0,050400	0,676300	1,113291
O4	4a	1,000000	0,386900	0,051000	0,346000	1,113291
O5	4a	1,000000	0,163600	0,181500	0,054300	1,421222
O6	4a	1,000000	0,172000	0,323100	0,472700	1,421222
O7	4a	1,000000	0,035600	0,128600	0,138500	1,934441
O8	4a	1,000000	0,295700	0,366900	0,376300	1,934441
O9	4a	1,000000	0,473400	0,318600	0,325600	1,176456
O10	4a	1,000000	0,361000	0,679200	0,195000	1,176456

O11	4a	1,000000	0,344300	0,149500	0,020800	1,334370
O12	4a	1,000000	0,000000	0,641900	0,000000	1,334370

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:

Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}

Formula mass/ g/mol: 2413,6550

Density (calculated)/ g/cm³ 2,5942

F(000): 1176,8040

Weight fraction/ %: 77(1)

Space group (No.): R -3 c (167)

Lattice parameters:

a/ Å: 8,9221(4)

b/ Å: 8,9221(4)

c/ Å: 22,407(1)

alpha/ °: 90

beta/ °: 90

gamma/ °: 120

V/ 10⁶ pm³ 1544,74300

Overall displacement parameter: 0,000000

Extinction: 0,000000

Flat Plate Absorption Correction: 0,000000

Porosity: 0,000000

Roughness: 0,000000

Fitting mode: Structure Fit

U Left: 0,16(1)

V Left: -0,12(1)

W Left: 0,029(2)

Preferred orientation direction/ hkl: 0,00 0,00 1,00

Preferred orientation parameter: 1,000000

Asymmetry parameter 1: 0,000000

Asymmetry parameter 2: 0,000000

Peak shape:

parameter 1 Left: 0,55(4)

parameter 2 Left: 0,000000

parameter 3 Left: 0,000000

R (Bragg)/ %: 14,05946

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

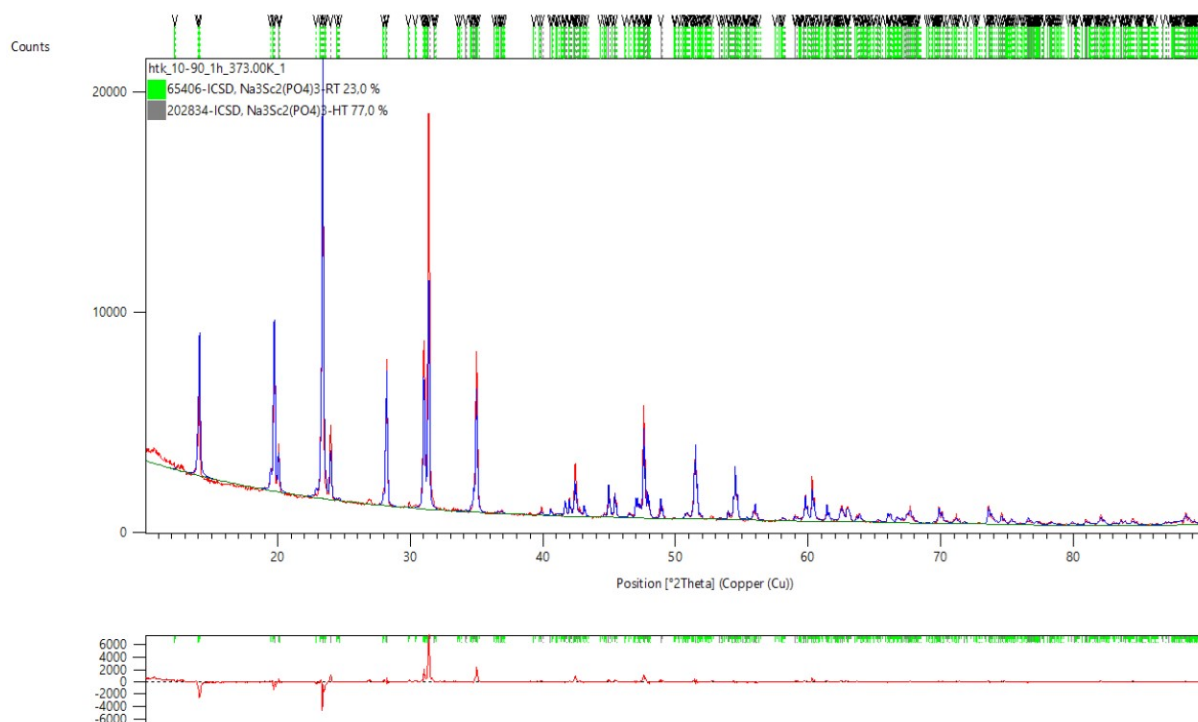


Figure S10. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 373K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 383K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,114(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,87887
R (profile)/ %:	9,31326
R (weighted profile)/ %:	13,57703
GOF:	22,24162
d-statistic:	0,30847
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5907
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9235(4)
 b/ Å: 8,9235(4)
 c/ Å: 22,431(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1546,84800
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,17(2)
 V Left: -0,12(1)
 W Left: 0,029(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,82(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,21758

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

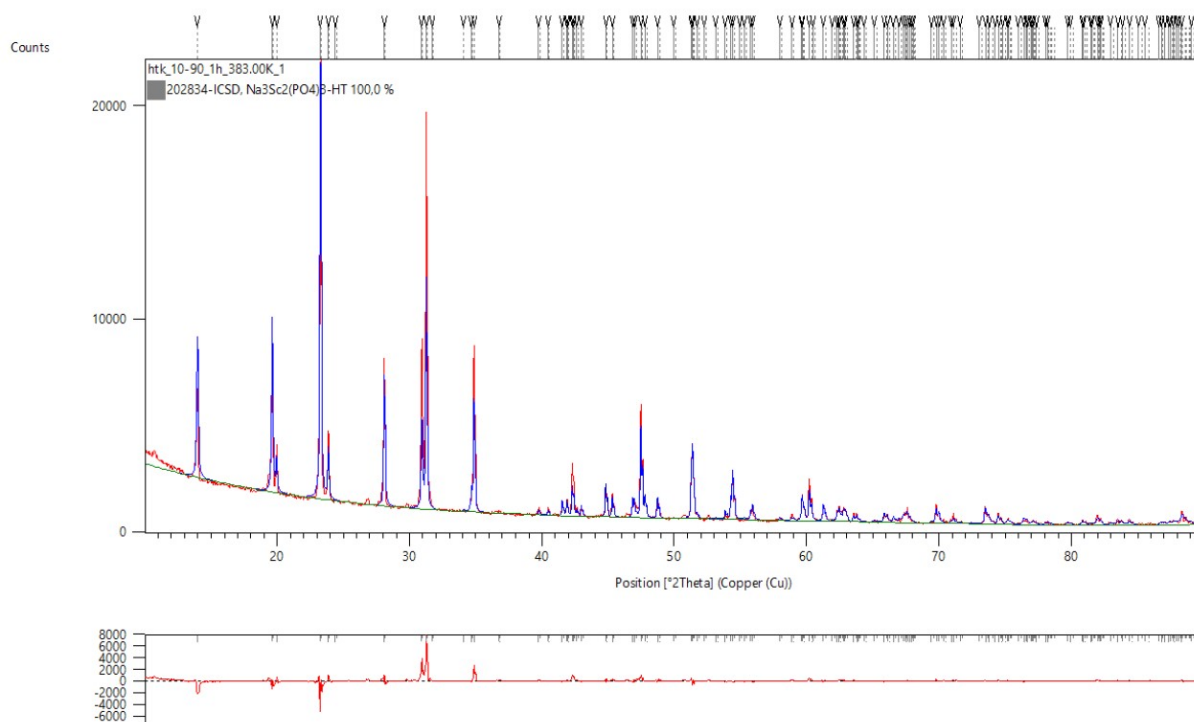


Figure S11. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 383K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 393K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,115(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,87755
R (profile)/ %:	9,21781
R (weighted profile)/ %:	13,42425
GOF:	21,76372
d-statistic:	0,32585
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5890
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9234(4)
 b/ Å: 8,9234(4)
 c/ Å: 22,446(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1547,85300
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,17(2)
 V Left: -0,12(1)
 W Left: 0,029(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,78(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,13162

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

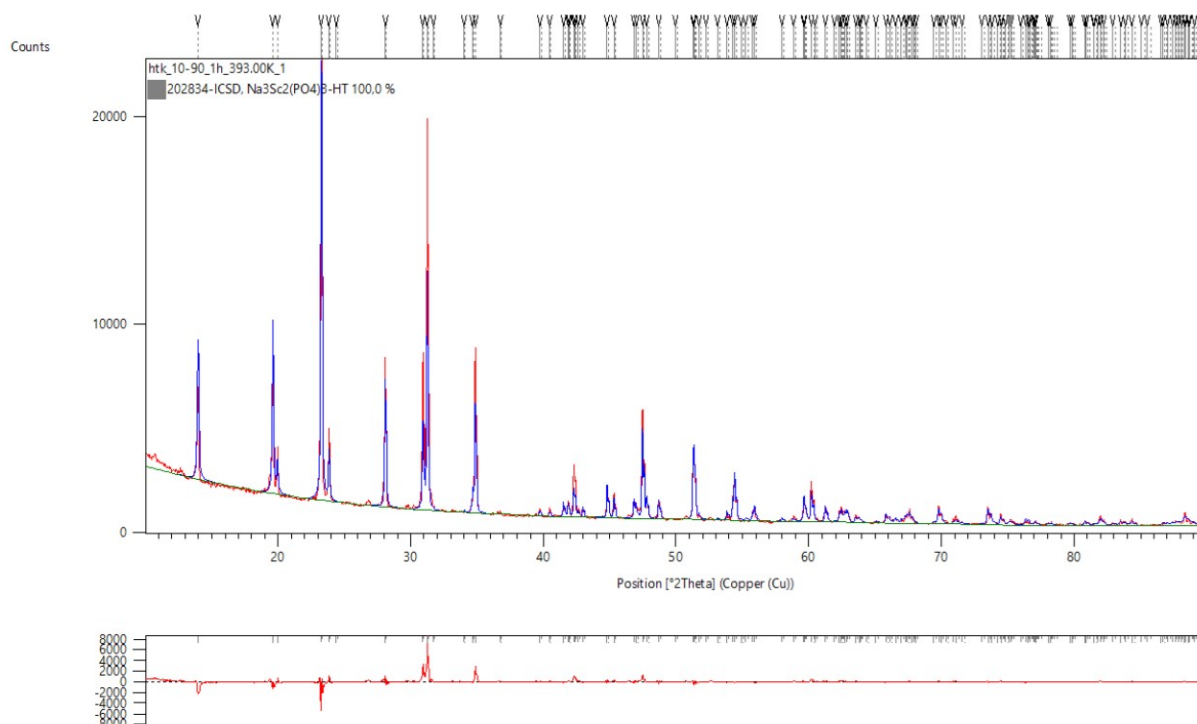


Figure S12. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 393K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 403K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,118(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,87874
R (profile)/ %:	9,19360
R (weighted profile)/ %:	13,31011
GOF:	21,37758
d-statistic:	0,26957
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5870
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9235(4)
 b/ Å: 8,9235(4)
 c/ Å: 22,463(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1549,06300
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,17(2)
 V Left: -0,13(1)
 W Left: 0,030(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,73(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,23629

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

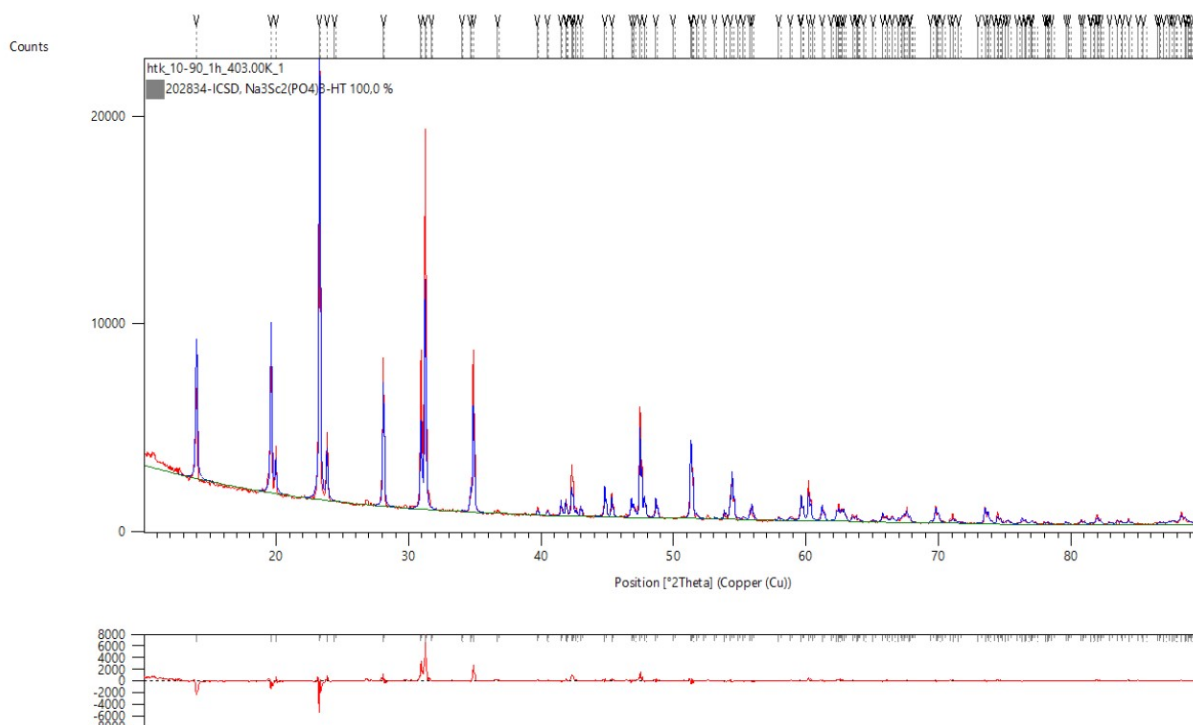


Figure S13. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 403K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 413K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,441(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88785
R (profile)/ %:	9,24160
R (weighted profile)/ %:	13,36863
GOF:	21,43019
d-statistic:	0,24308
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5888
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9191(4)
 b/ Å: 8,9191(4)
 c/ Å: 22,469(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1547,99900
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,17(2)
 V Left: -0,12(1)
 W Left: 0,030(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,70(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,58223

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

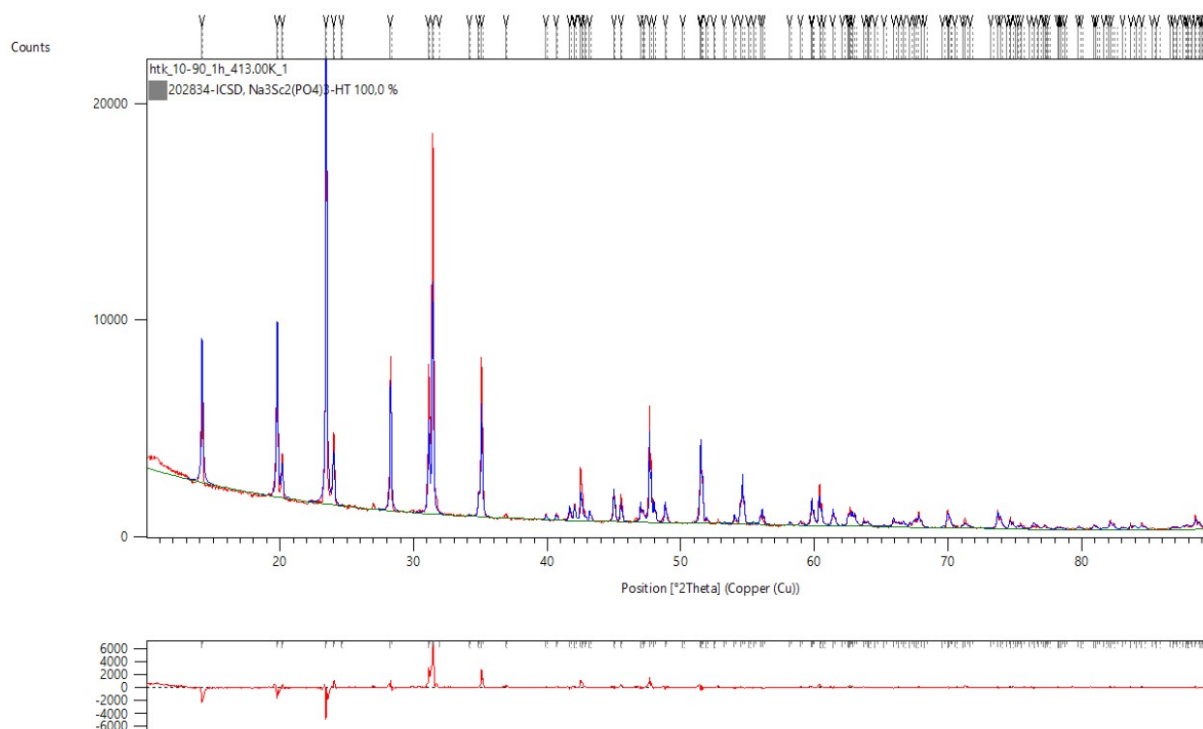


Figure S14. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 413K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 423K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,409(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88851
R (profile)/ %:	9,28042
R (weighted profile)/ %:	13,47285
GOF:	21,75560
d-statistic:	0,25336
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5861
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9193(4)
 b/ Å: 8,9193(4)
 c/ Å: 22,492(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1549,56600
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,18(2)
 V Left: -0,13(1)
 W Left: 0,031(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,68(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,41998

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

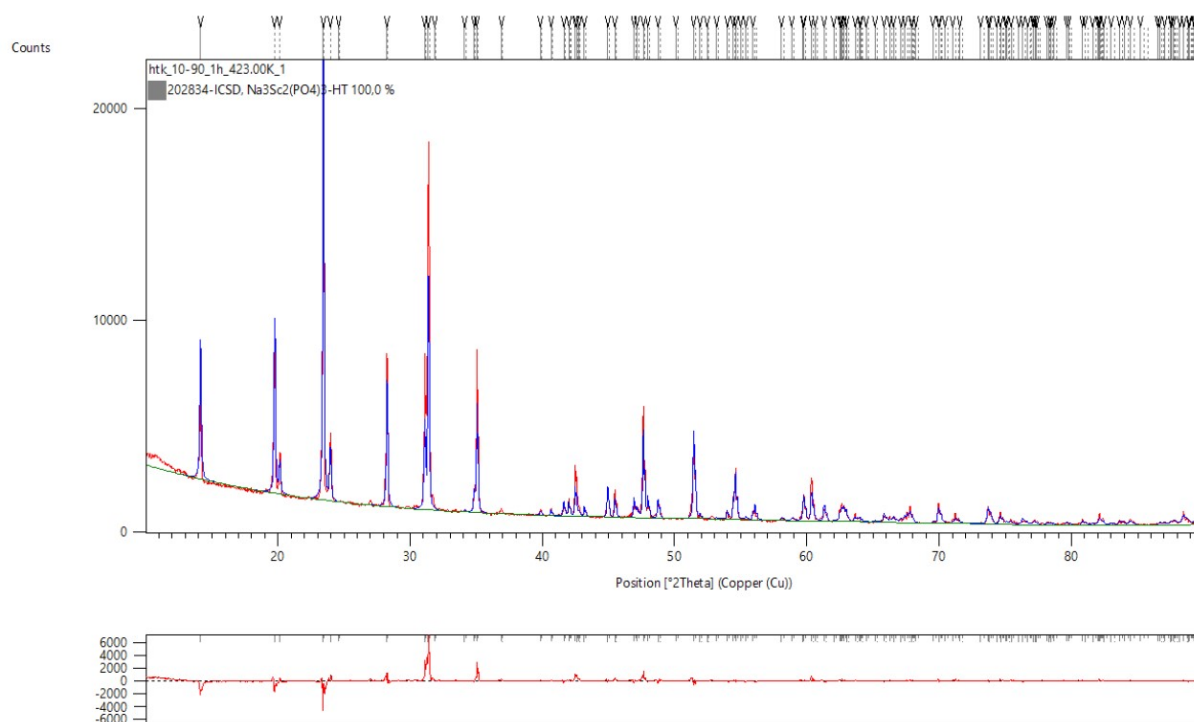


Figure S15. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 423K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 433K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,129(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88806
R (profile)/ %:	9,37117
R (weighted profile)/ %:	13,83650
GOF:	22,95312
d-statistic:	0,27505
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5776
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9229(4)
 b/ Å: 8,9229(4)
 c/ Å: 22,548(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1554,69700
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,22(2)
 V Left: -0,14(1)
 W Left: 0,032(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,64(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,60008

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

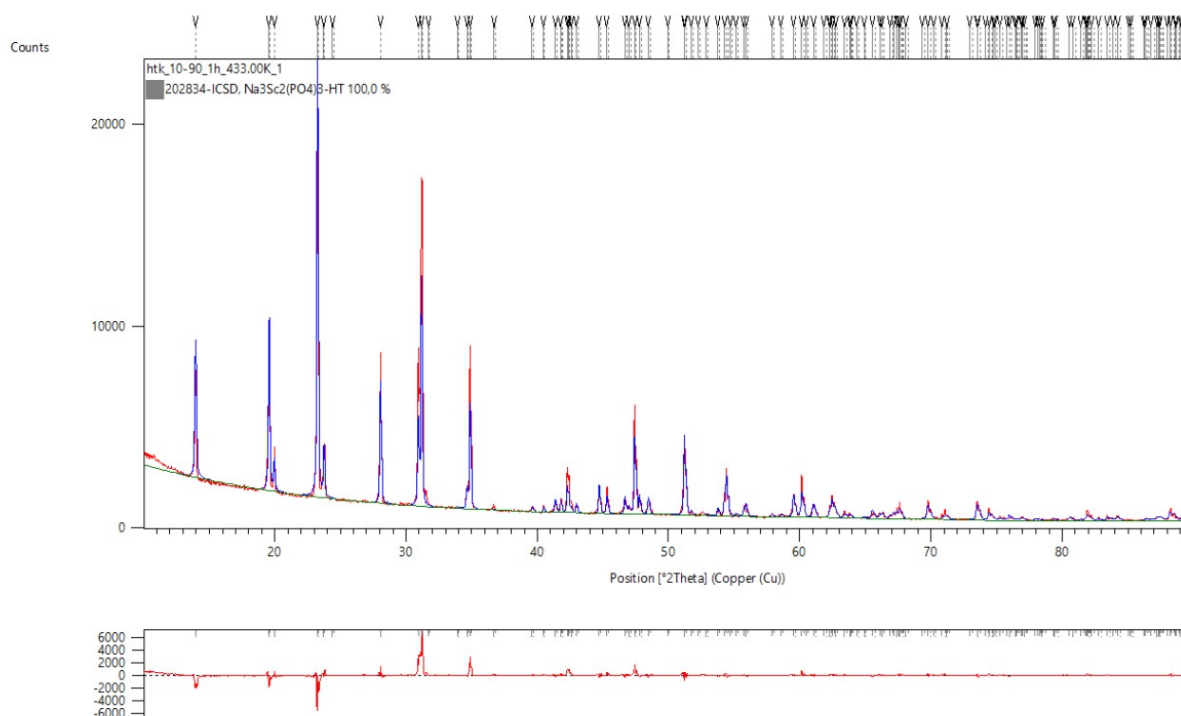


Figure S16. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 433K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 443K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,128(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88527
R (profile)/ %:	9,03181
R (weighted profile)/ %:	13,34765
GOF:	21,40110
d-statistic:	0,26071
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5747
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9229(4)
 b/ Å: 8,9229(4)
 c/ Å: 22,573(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1556,46100
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,19(2)
 V Left: -0,14(1)
 W Left: 0,032(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,63(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,72811

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

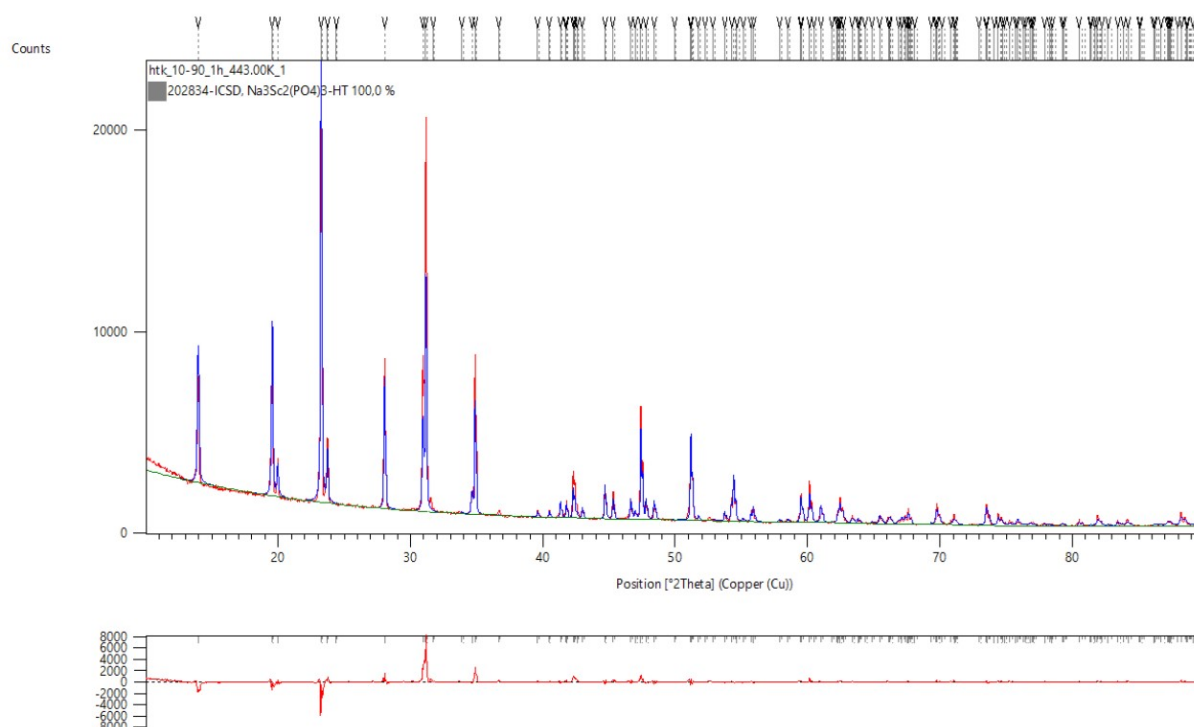


Figure S17. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 443K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 453K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,475(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88238
R (profile)/ %:	9,09203
R (weighted profile)/ %:	13,22509
GOF:	21,05208
d-statistic:	0,24730
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5770
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9184(3)
 b/ Å: 8,9184(3)
 c/ Å: 22,576(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1555,06400
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,18(1)
 V Left: -0,13(1)
 W Left: 0,031(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,62(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,73016

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

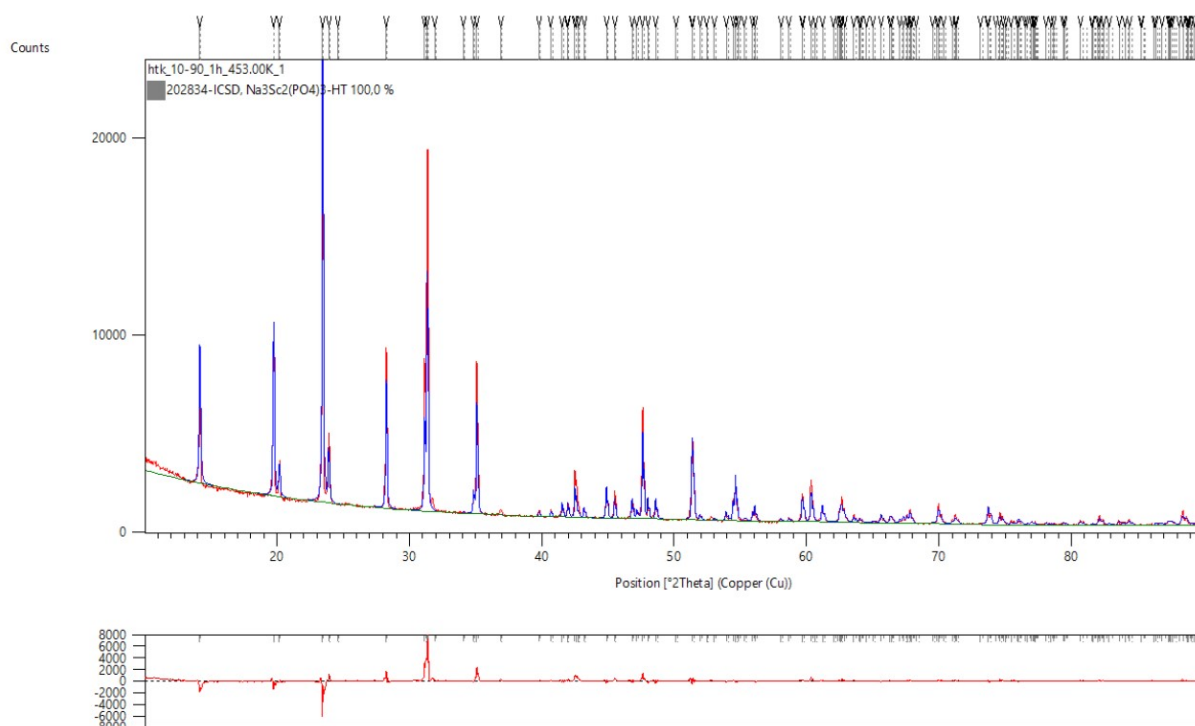


Figure S18. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 453K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 463K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,136(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88567
R (profile)/ %:	9,07447
R (weighted profile)/ %:	13,45562
GOF:	21,74275
d-statistic:	0,31947
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5716
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9230(3)
 b/ Å: 8,9230(3)
 c/ Å: 22,600(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1558,35700
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,18(1)
 V Left: -0,13(1)
 W Left: 0,030(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,64(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,76294

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

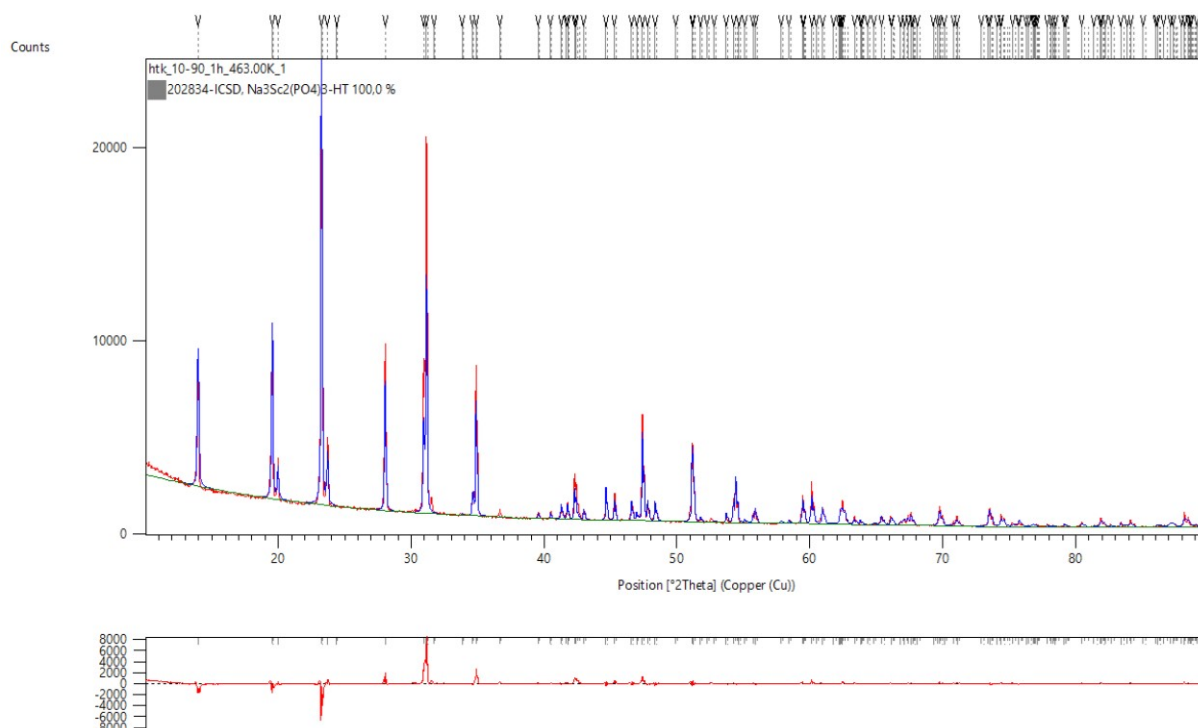


Figure S19. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 463K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 473K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,138(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,88250
R (profile)/ %:	9,09876
R (weighted profile)/ %:	13,35207
GOF:	21,45645
d-statistic:	0,28824
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5703
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9231(3)
 b/ Å: 8,9231(3)
 c/ Å: 22,611(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1559,14400
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,18(1)
 V Left: -0,13(1)
 W Left: 0,030(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,62(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,79295

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

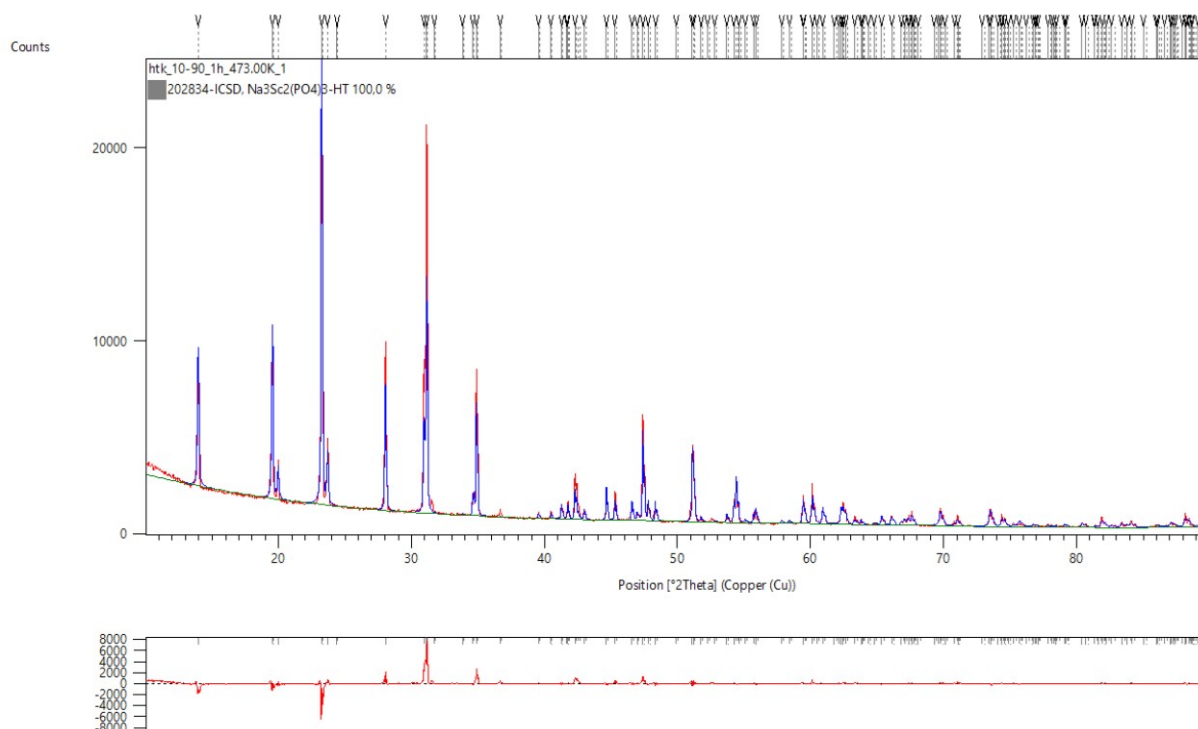


Figure S20. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 473K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 503K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,148(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,89828
R (profile)/ %:	9,04362
R (weighted profile)/ %:	13,41603
GOF:	21,42734
d-statistic:	0,33987
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5668
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9234(3)
 b/ Å: 8,9234(3)
 c/ Å: 22,640(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1561,23600
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,16(1)
 V Left: -0,12(1)
 W Left: 0,027(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,59(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,90019

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

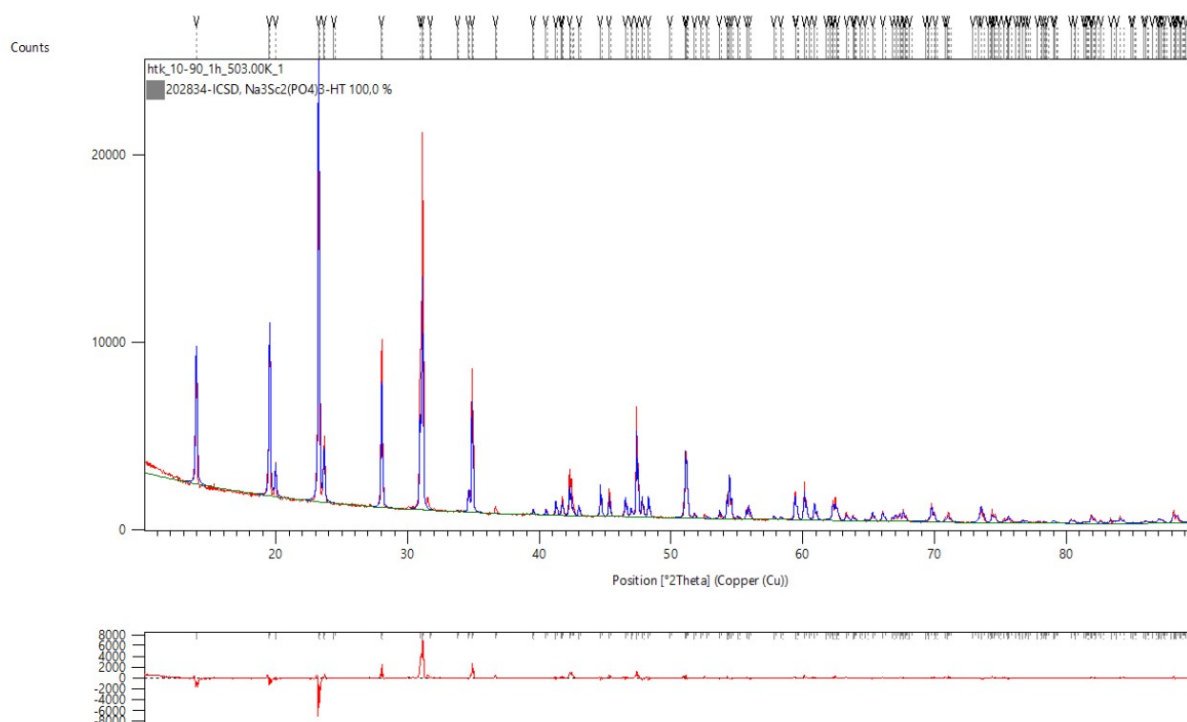


Figure S21. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 503K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 533K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,160(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,89463
R (profile)/ %:	9,15345
R (weighted profile)/ %:	13,20446
GOF:	20,80914
d-statistic:	0,29405
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5634
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9242(3)
 b/ Å: 8,9242(3)
 c/ Å: 22,666(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1563,30100
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,15(1)
 V Left: -0,111(9)
 W Left: 0,027(2)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,60(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,67010

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

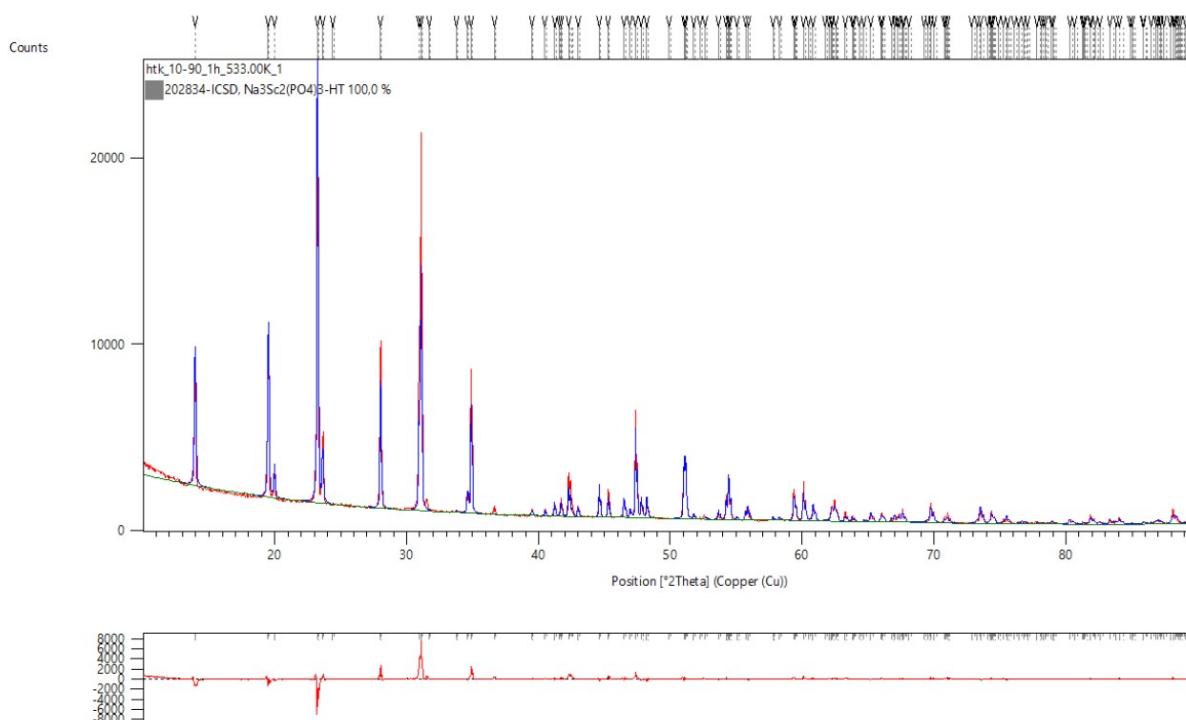


Figure S22. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 533K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 563K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,171(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,89224
R (profile)/ %:	8,97361
R (weighted profile)/ %:	13,26356
GOF:	21,03062
d-statistic:	0,32526
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5608
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9247(3)
 b/ Å: 8,9247(3)
 c/ Å: 22,687(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1564,92100
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,14(1)
 V Left: -0,104(8)
 W Left: 0,025(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,61(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 14,79207

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

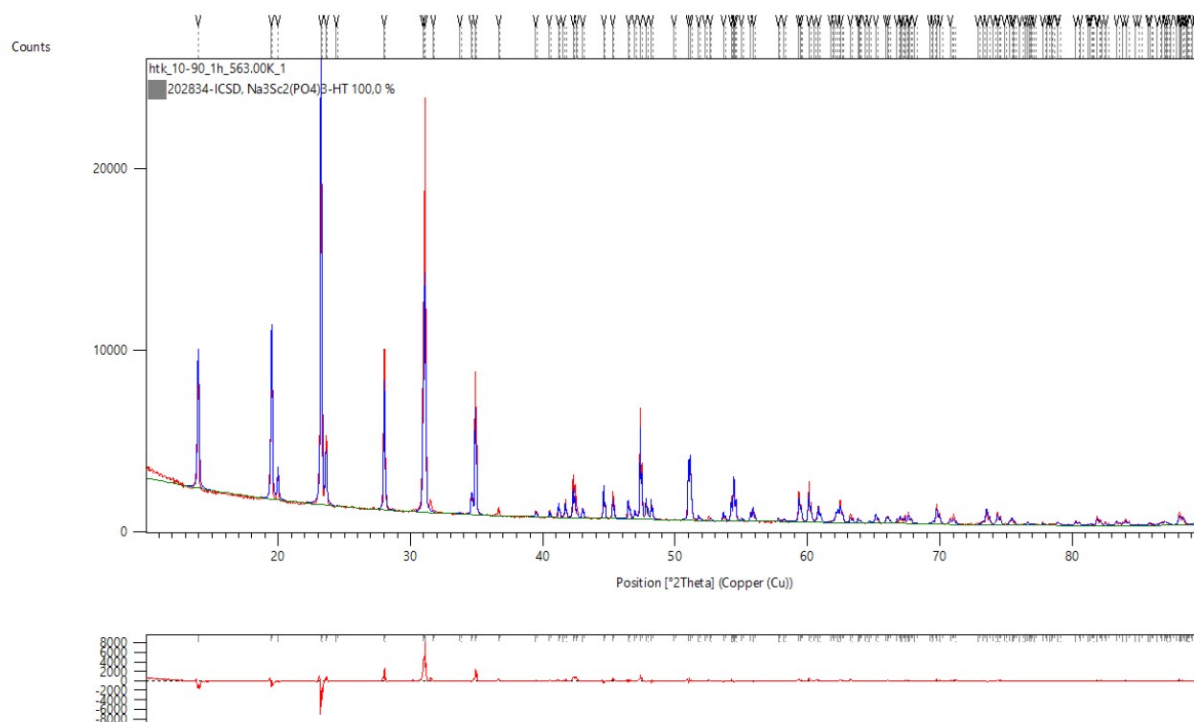


Figure S23. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 563K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 593K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,179(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,89600
R (profile)/ %:	9,35050
R (weighted profile)/ %:	13,55675
GOF:	21,91369
d-statistic:	0,27560
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5584
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9251(3)
 b/ Å: 8,9251(3)
 c/ Å: 22,706(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1566,37600
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,14(1)
 V Left: -0,101(8)
 W Left: 0,025(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,59(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,47104

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

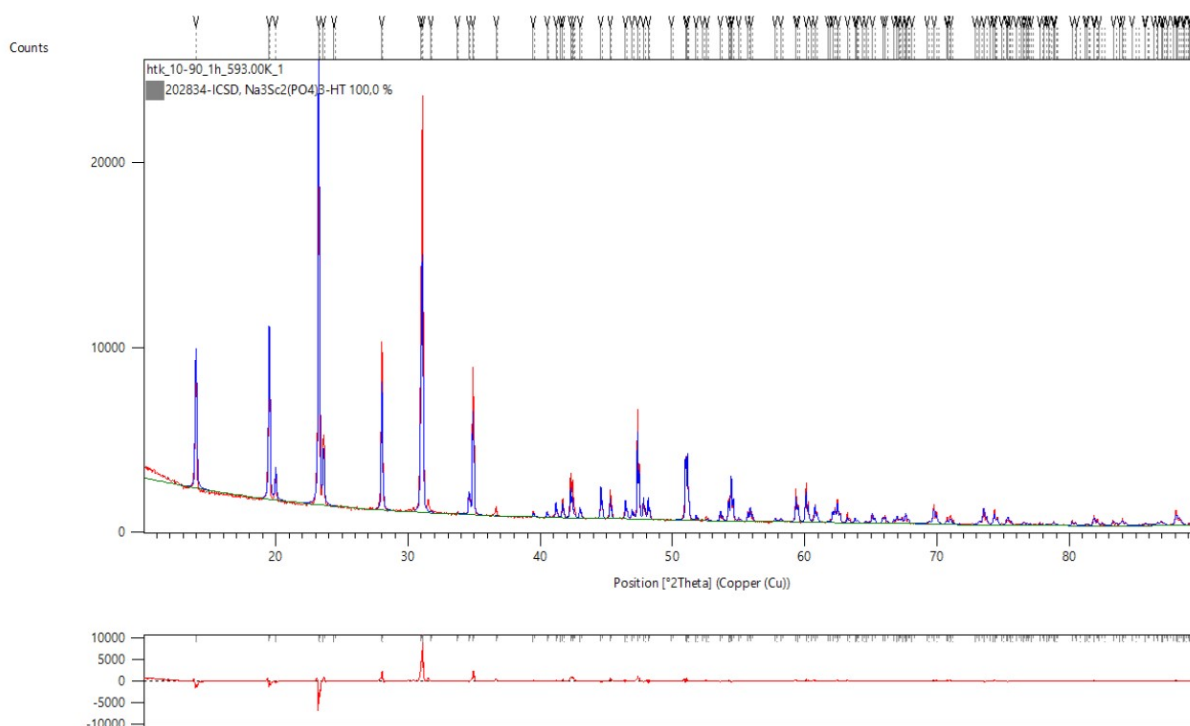


Figure S24. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 593K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 623K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,463(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,90218
R (profile)/ %:	9,26581
R (weighted profile)/ %:	13,43628
GOF:	21,43427
d-statistic:	0,27755
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5594
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9220(3)
 b/ Å: 8,9220(3)
 c/ Å: 22,713(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1565,73900
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,13(1)
 V Left: -0,098(8)
 W Left: 0,025(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,60(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,39925

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

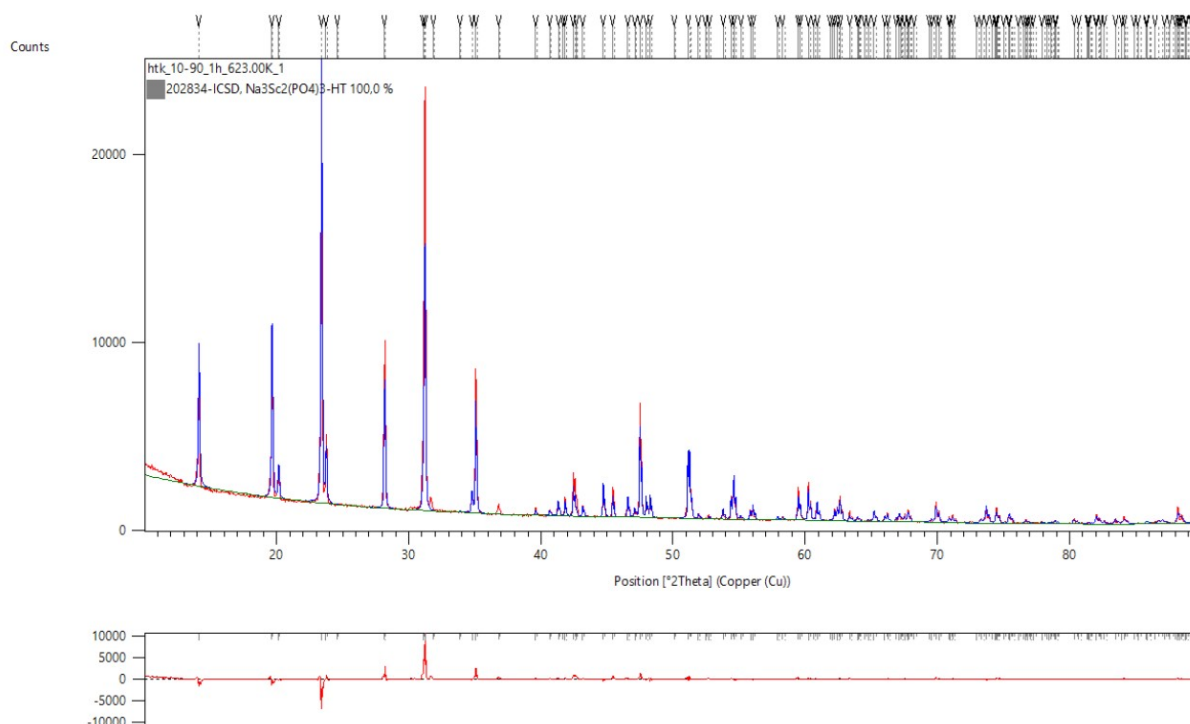


Figure S25. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 623K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 653K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,199(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,90681
R (profile)/ %:	9,26869
R (weighted profile)/ %:	13,57613
GOF:	21,81323
d-statistic:	0,30144
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5541
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9263(3)
 b/ Å: 8,9263(3)
 c/ Å: 22,737(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1568,97500
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,12(1)
 V Left: -0,093(8)
 W Left: 0,024(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,58(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,46780

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

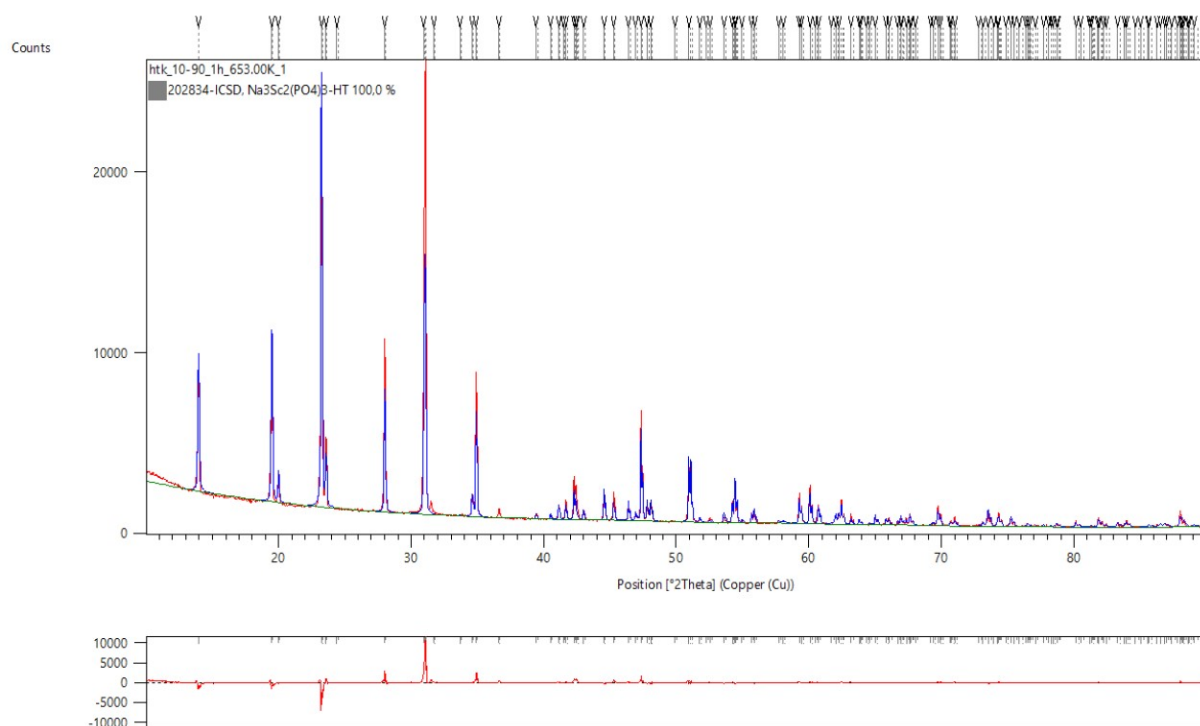


Figure S26. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 653K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 683K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,208(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,92289
R (profile)/ %:	9,16905
R (weighted profile)/ %:	13,68019
GOF:	21,90578
d-statistic:	0,37185
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5524
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9268(3)
 b/ Å: 8,9268(3)
 c/ Å: 22,751(1)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1570,05500
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,12(1)
 V Left: -0,090(7)
 W Left: 0,023(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,58(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,49614

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

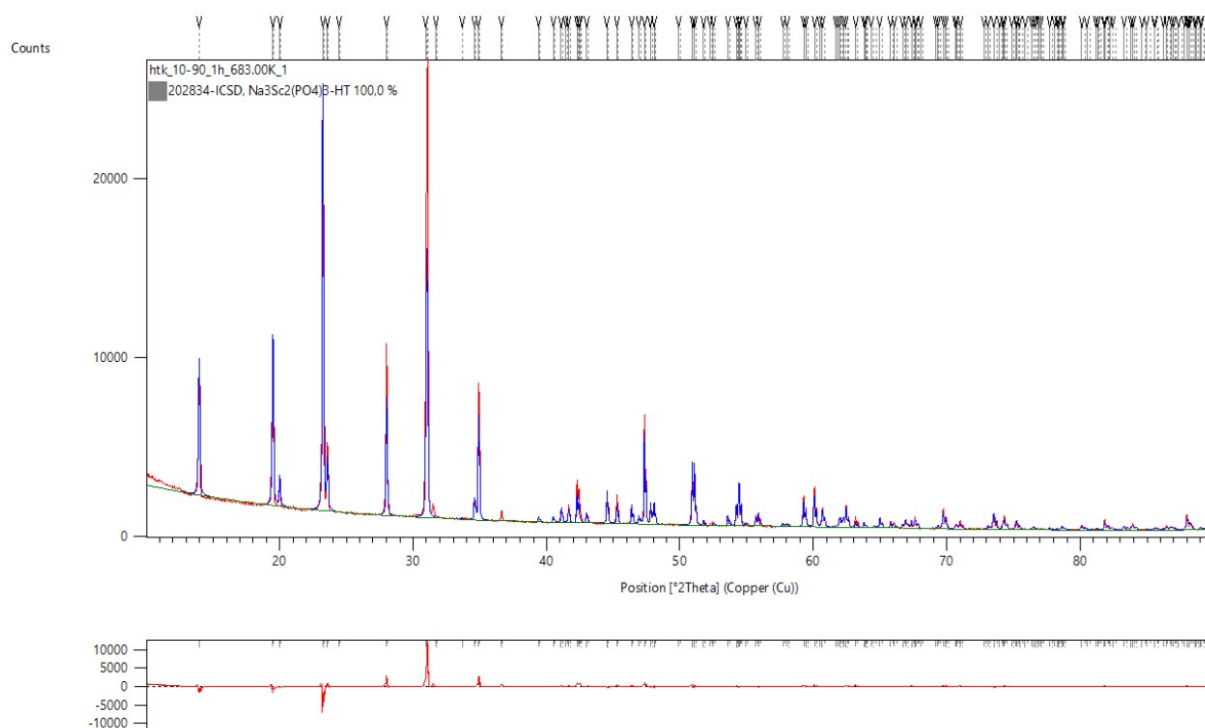


Figure S27. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 683K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 713K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,219(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,90969
R (profile)/ %:	9,26467
R (weighted profile)/ %:	13,55227
GOF:	21,69350
d-statistic:	0,32804
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5504
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9276(3)
 b/ Å: 8,9276(3)
 c/ Å: 22,7643(9)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1571,28400
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,114(9)
 V Left: -0,089(7)
 W Left: 0,023(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,59(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,60316

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

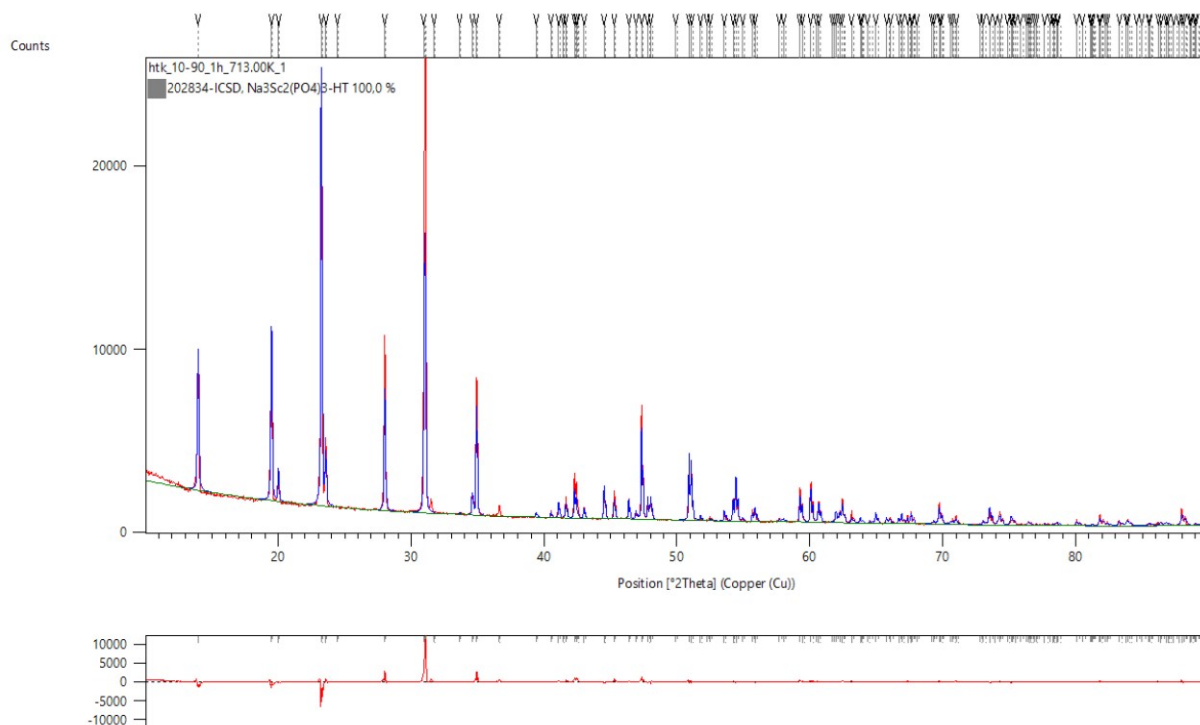


Figure S28. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 713K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 743K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ $^{\circ}2\theta$:	0,000000
Specimen displacement/ mm :	-0,231(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,90843
R (profile)/ %:	9,47695
R (weighted profile)/ %:	13,74076
GOF:	22,32046
d-statistic:	0,31599
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5484
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9285(3)
 b/ Å: 8,9285(3)
 c/ Å: 22,7772(9)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1572,49100
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,110(9)
 V Left: -0,087(7)
 W Left: 0,023(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,57(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,76183

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

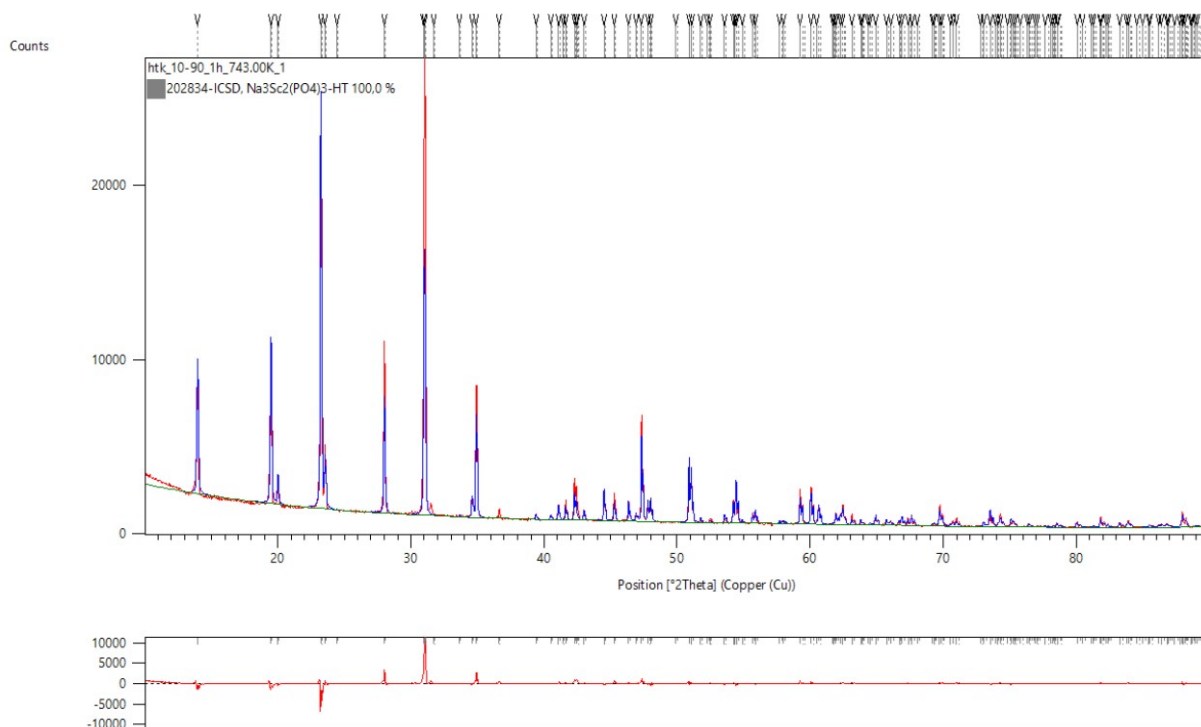


Figure S29. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 743K.

$\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 773K

Global Parameters

Number of used phases:	1
Number of variables:	13
Number of constraints:	1
Zero shift/ °2Theta:	0,000000
Specimen displacement/ mm :	-0,242(2)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (expected)/ %:	2,90700
R (profile)/ %:	9,30386
R (weighted profile)/ %:	13,59104
GOF:	21,85820
d-statistic:	0,30995
U standard:	0,000000
V standard:	0,000000
W standard:	0,010000
U Left:	0,000000
V Left:	0,000000
W Left:	0,010000
U Right:	0,000000
V Right:	0,000000
W Right:	0,010000
Asymmetry Type:	No Asymmetry Function
Asymmetry 1:	0,000000
Asymmetry 2:	0,000000
Shape Type:	Shape Individual
Shape 1 Left:	0,600000
Shape 2 Left:	0,000000
Shape 3 Left:	0,000000
Shape 1 Right:	0,600000
Shape 2 Right:	0,000000
Shape 3 Right:	0,000000
K a1/a2 intensity ratio:	0,500000

K alpha/beta intensity ratio: 0,000000
 Crystal Shape Factor K: 1,0000
 Instrumental FWHM Curve Type: Caglioti function
 Instr. Gauss Curve Coefficient A: 0,0045(5)
 Instr. Gauss Curve Coefficient B: -0,0032(9)
 Instr. Gauss Curve Coefficient C: 0,0046(3)
 Instr. Lorentz Curve Coefficient A: 0,0062(7)
 Instr. Lorentz Curve Coefficient B: -0,004(1)
 Instr. Lorentz Curve Coefficient C: 0,0064(5)

Relevant parameters of 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Structure and profile data:
 Formula sum: Sc_{12,00}P_{18,00}O_{72,00}Na_{7,16}
 Formula mass/ g/mol: 2413,6550
 Density (calculated)/ g/cm³: 2,5467
 F(000): 1176,8040
 Weight fraction/ %: 100,000000
 Space group (No.): R -3 c (167)
 Lattice parameters:
 a/ Å: 8,9292(3)
 b/ Å: 8,9292(3)
 c/ Å: 22,7891(9)
 alpha/ °: 90
 beta/ °: 90
 gamma/ °: 120
 V/ 10⁶ pm³: 1573,57200
 Overall displacement parameter: 0,000000
 Extinction: 0,000000
 Flat Plate Absorption Correction: 0,000000
 Porosity: 0,000000
 Roughness: 0,000000
 Fitting mode: Structure Fit
 U Left: 0,110(9)
 V Left: -0,087(7)
 W Left: 0,023(1)
 Preferred orientation direction/ hkl: 0,00 0,00 1,00
 Preferred orientation parameter: 1,000000
 Asymmetry parameter 1: 0,000000
 Asymmetry parameter 2: 0,000000
 Peak shape:
 parameter 1 Left: 0,59(3)
 parameter 2 Left: 0,000000
 parameter 3 Left: 0,000000
 R (Bragg)/ %: 15,67015

Occupancy, atomic fract. coordinates and Biso for 202834-ICSD, Na₃Sc₂(PO₄)₃-HT

Atom	Wyck.	s.o.f.	x	y	z	B/ 10 ⁴ pm ²
Sc1	12c	1,000000	0,000000	0,000000	0,148700	0,000000
P1	18e	1,000000	0,295100	0,000000	0,250000	0,000000
O1	36f	1,000000	0,023500	0,209100	0,194600	0,000000
O2	36f	1,000000	0,192170	0,172830	0,088730	0,000000
Na1	18e	0,347000	0,637200	0,000000	0,250000	0,000000
Na2	6b	0,153000	0,000000	0,000000	0,000000	0,000000

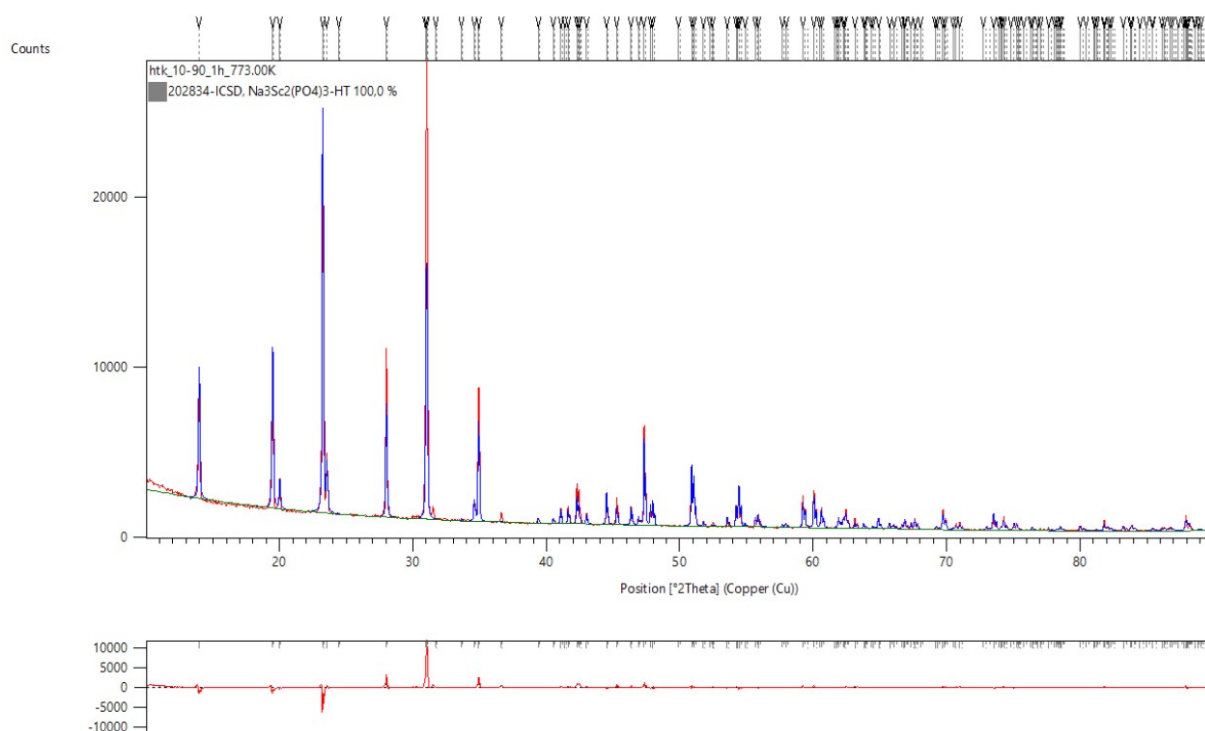


Figure S30. Rietveld refinement of XRD pattern of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 773K.

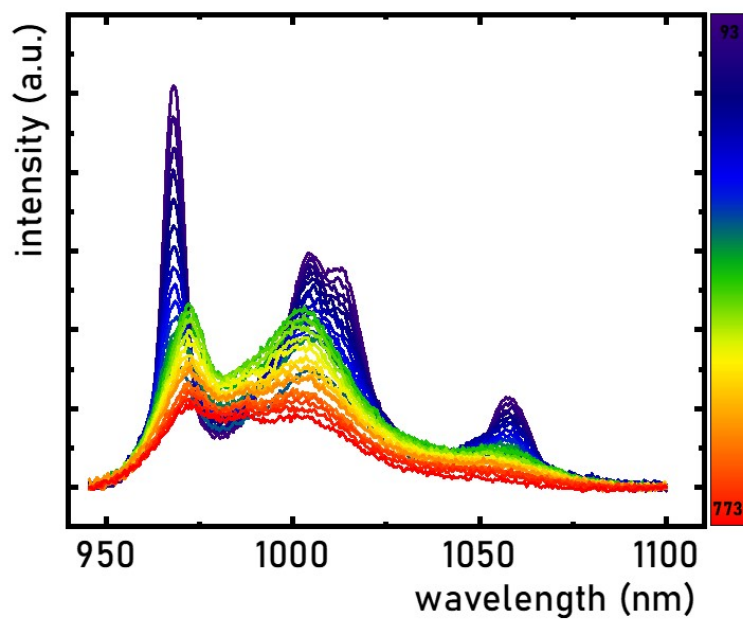


Figure S31. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:0.1\%\text{Yb}^{3+}$ measured as a function of temperature.

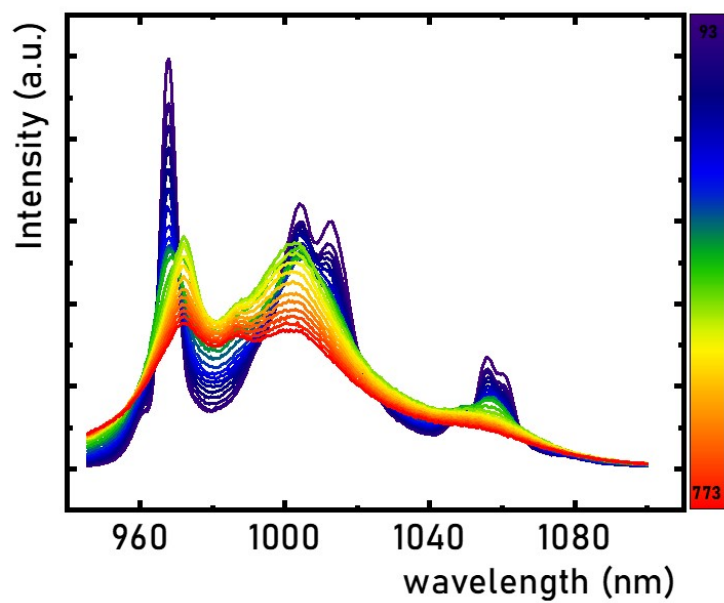


Figure S32. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured as a function of temperature.

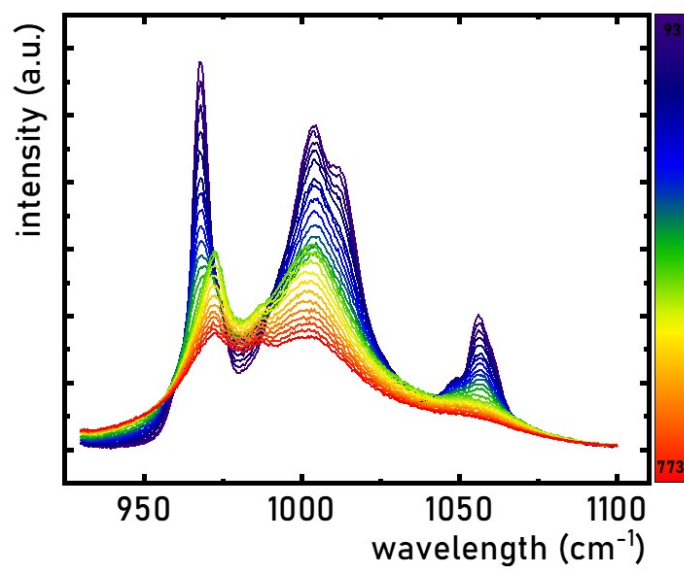


Figure S33. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:2\%\text{Yb}^{3+}$ measured as a function of temperature.

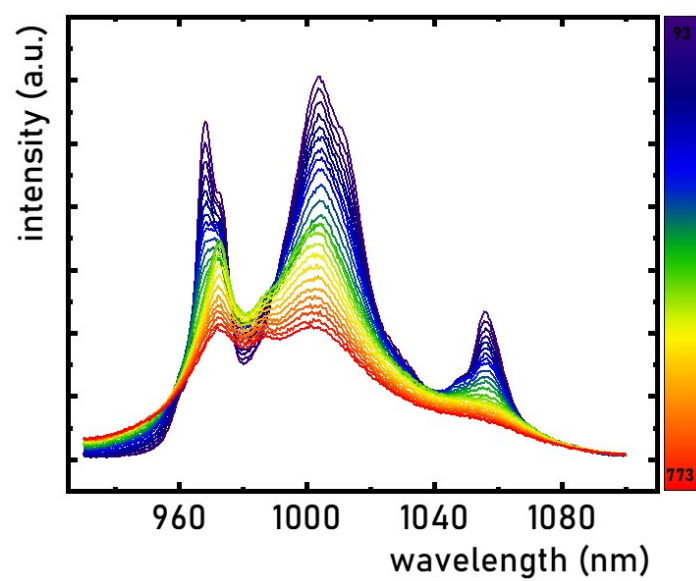


Figure S34. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:5\%\text{Yb}^{3+}$ measured as a function of temperature.

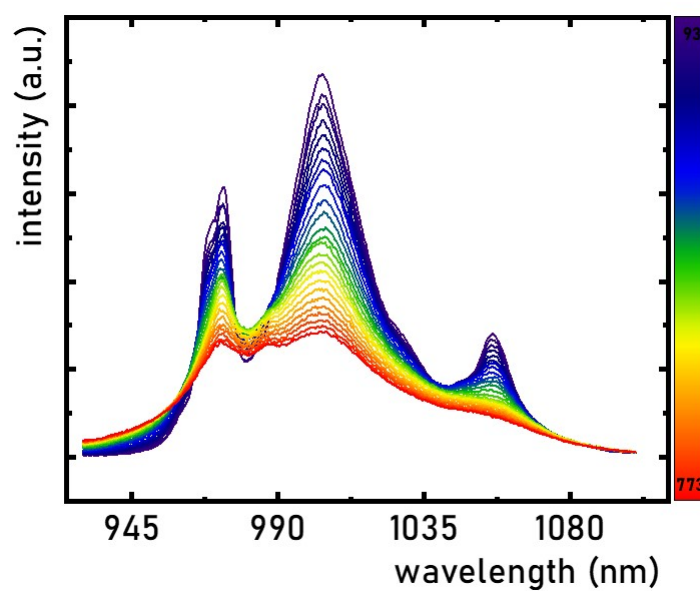


Figure S35. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:10\%\text{Yb}^{3+}$ measured as a function of temperature.

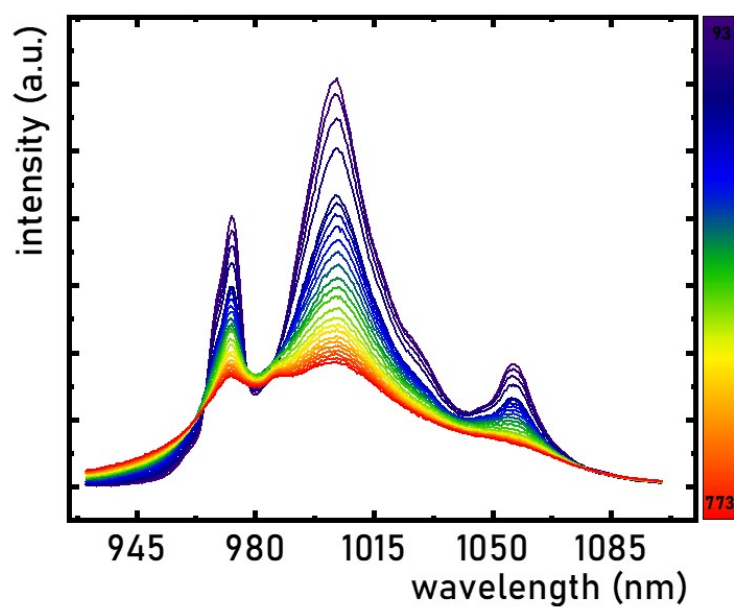


Figure S36. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:15\%\text{Yb}^{3+}$ measured as a function of temperature.

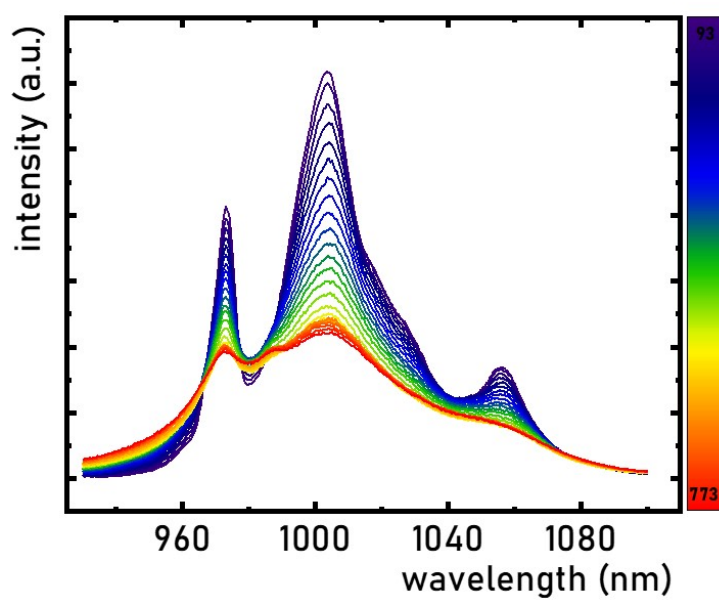


Figure S37. Emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:20\%\text{Yb}^{3+}$ measured as a function of temperature.

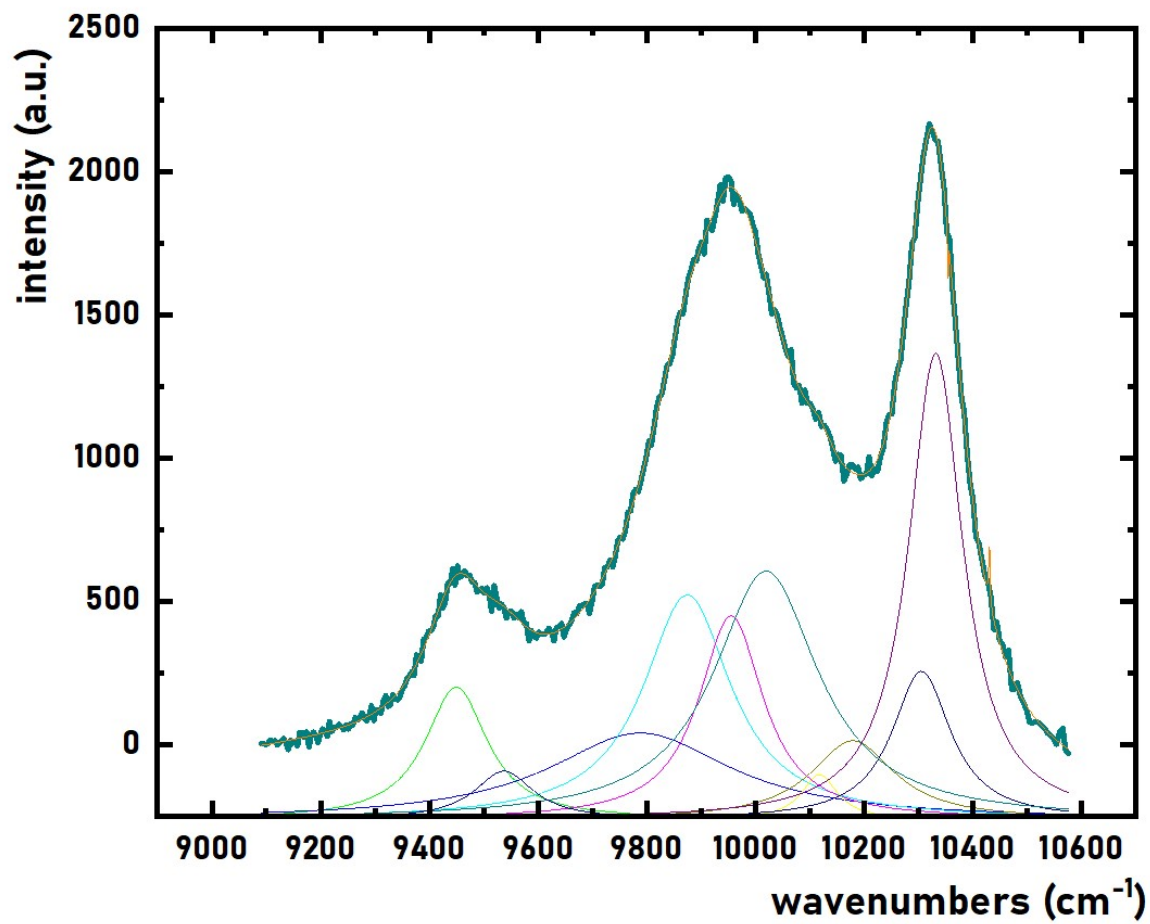


Figure S38. Representative deconvolution of emission spectra of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured at 313K.

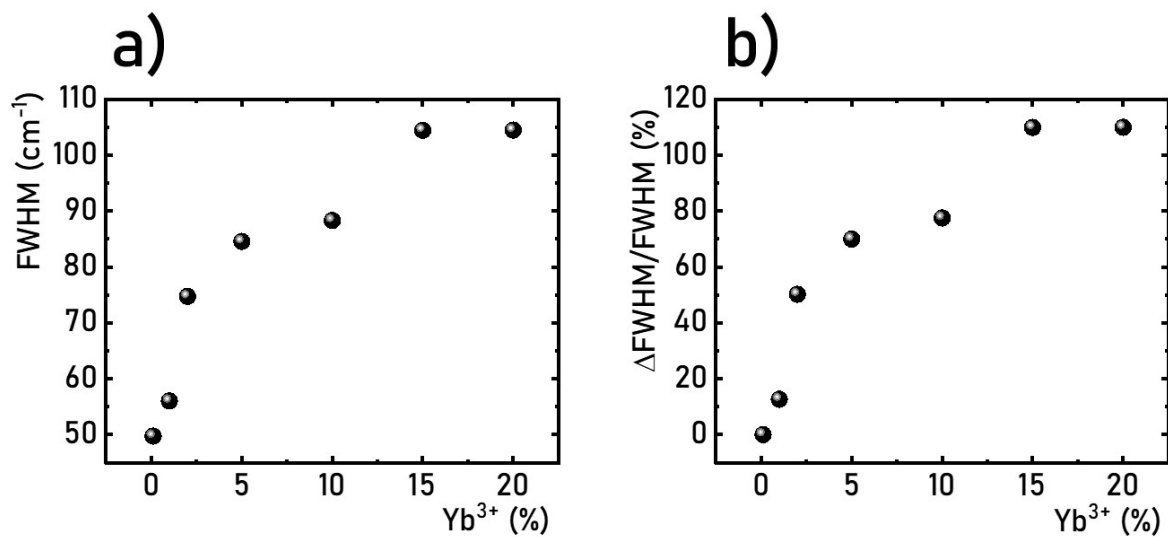


Figure S39. The influence of the Yb^{3+} ions concentration on the FWHM of the $5 \rightarrow 1$ line of Yb^{3+} ions in $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:\text{Yb}^{3+}$ -a) and the change of FWHM in respect to the one obtained for 0.1% Yb^{3+} dopant concentration-b) calculated based on the deconvolution of the emission spectra measured at 313K.

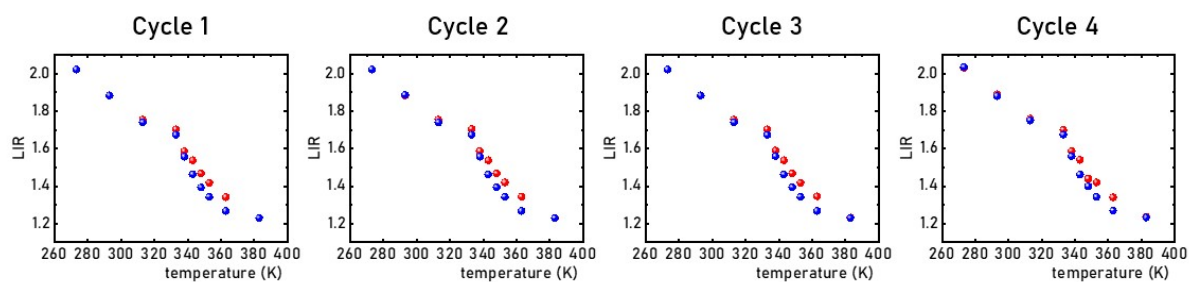


Figure S40. Thermal dependence of LIR_2 measured for $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:0.1\%\text{Yb}^{3+}$ within 4 heating (red dots) - cooling (blue dots) cycles.

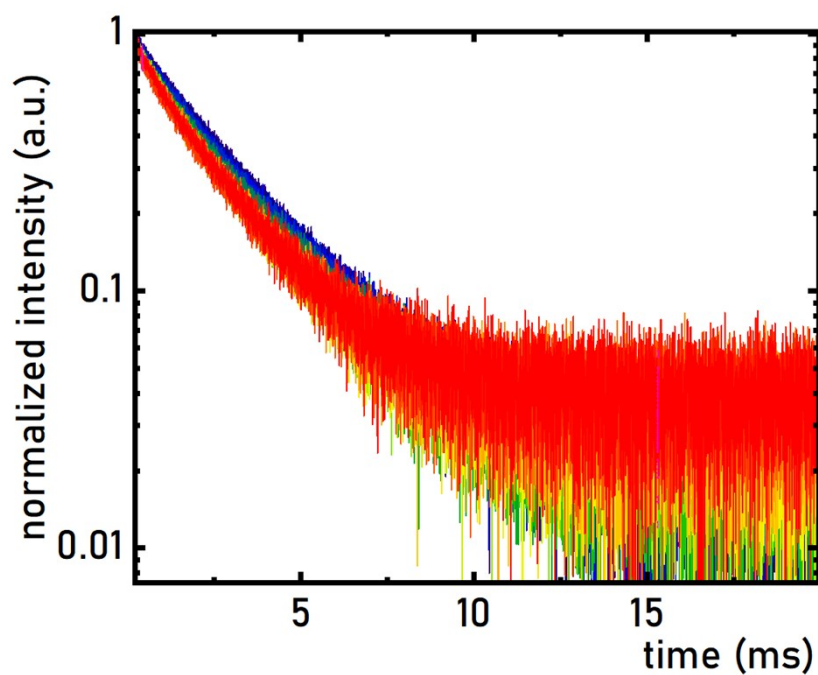


Figure S41. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:0.1\%\text{Yb}^{3+}$ measured as a function of temperature.

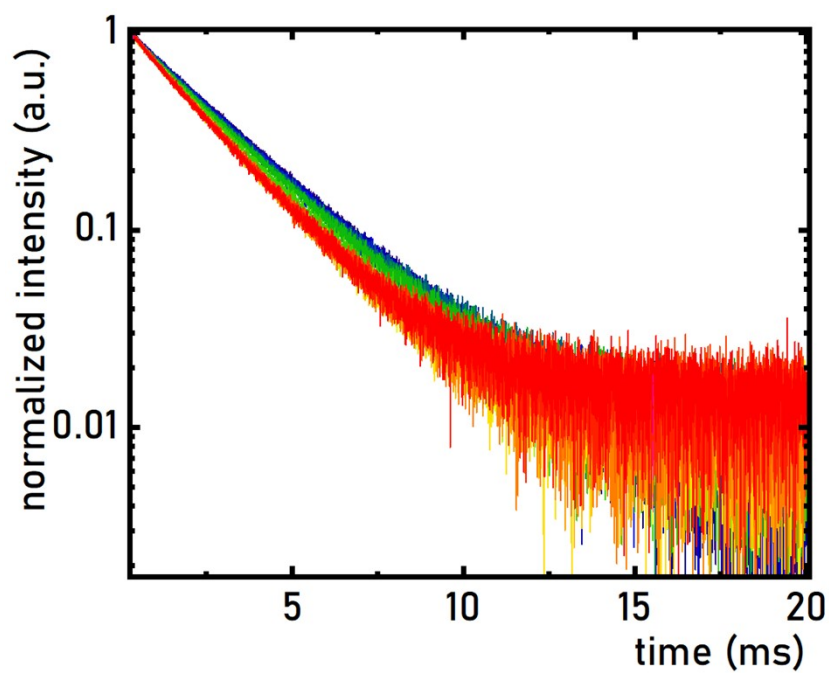


Figure S42. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:1\%\text{Yb}^{3+}$ measured as a function of temperature.

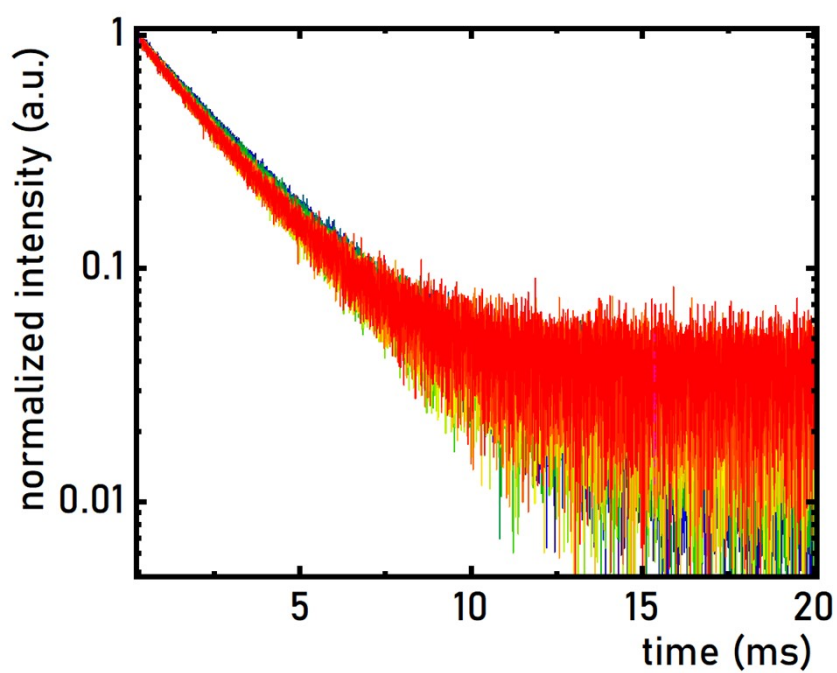


Figure S43. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:2\%\text{Yb}^{3+}$ measured as a function of temperature.

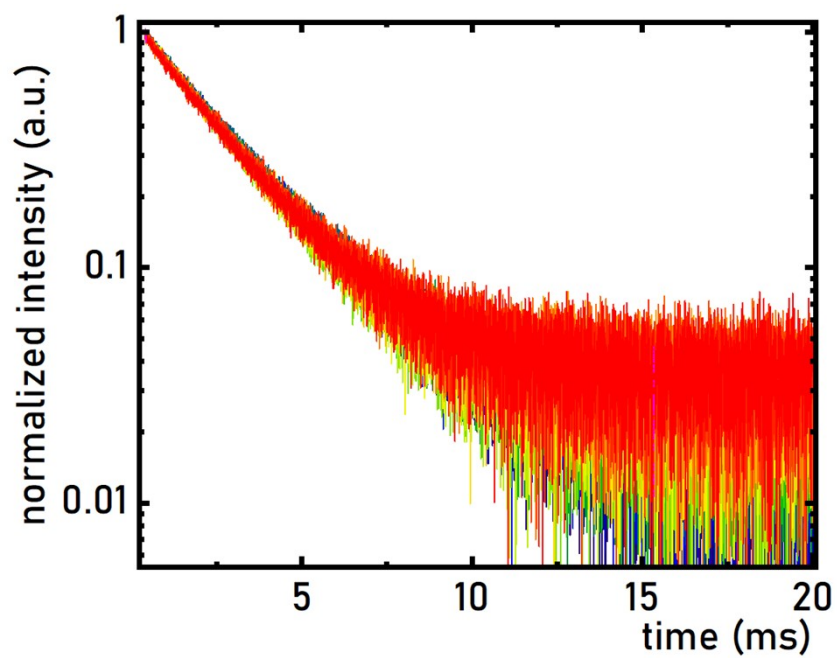


Figure S44. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:5\%\text{Yb}^{3+}$ measured as a function of temperature.

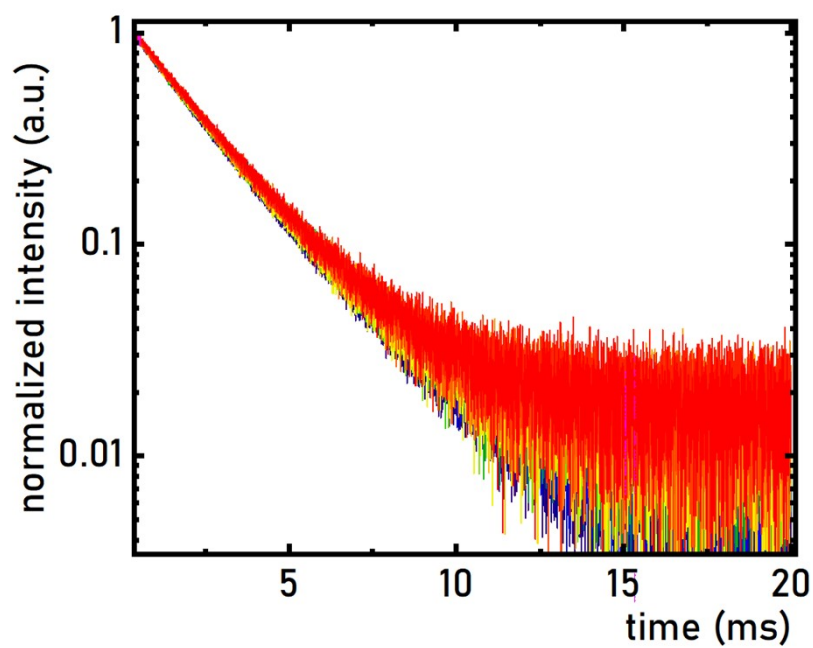


Figure S45. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:10\%\text{Yb}^{3+}$ measured as a function of temperature.

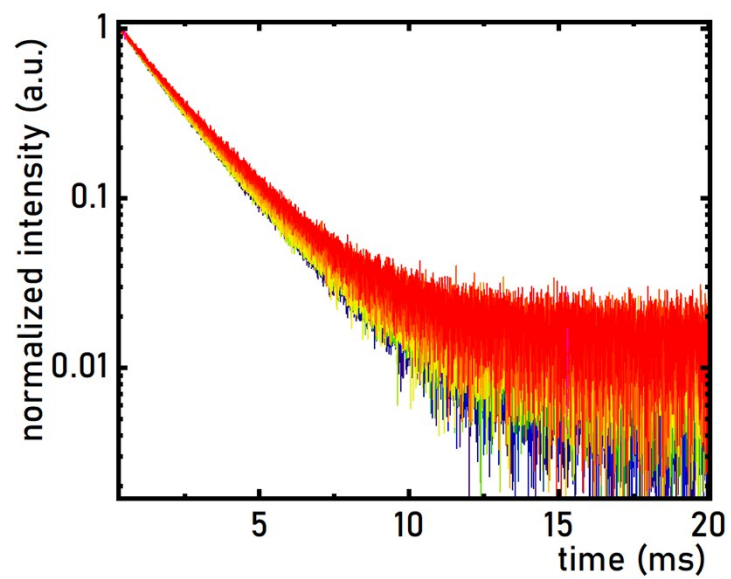


Figure S46. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:15\%\text{Yb}^{3+}$ measured as a function of temperature.

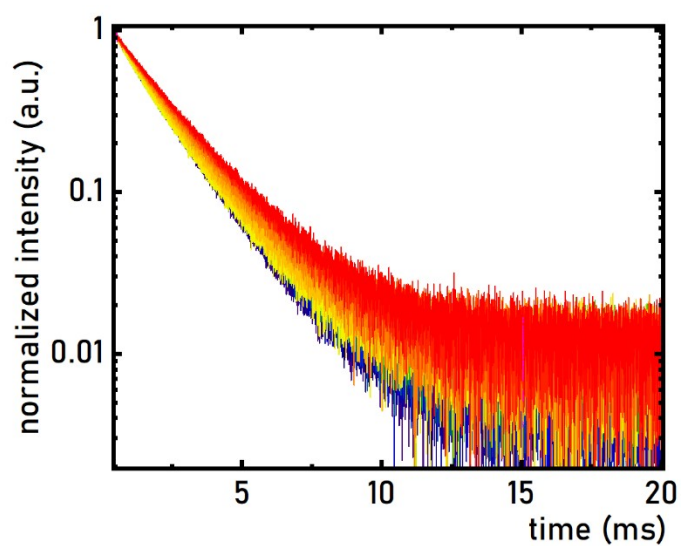


Figure S47. Luminescence decay profiles of $\text{Na}_3\text{Sc}_2(\text{PO}_4)_3:20\%\text{Yb}^{3+}$ measured as a function of temperature.