Supplementary Information:
XRD Rietveld refinement

Understanding the structure and mechanism of Na^+ diffusion in NASICON solid-state electrolytes and the effect of Sc- and Al/Y- substitution

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XRD Rietveld refinements details

Table 1: Global parameters and XRD setup summary

Experimental setup		Global instrument parameters fixed for refinement	
Method	XRD	**Sample Displacement [mm]**	-0.034579
Instrument geometry	Reflection	**Profile Asymmetry**	
Radiation source	Cu-$K_{\alpha 2}/K_{\alpha 1}$	**Finger-Cox-Jephcoat**	0.027861
Wavelength [Å]	1.540598	**S/L = D/L**	
Kβ-Filter	Ni	**$K\alpha_2/K\alpha_1$-ratio**	0.460779
Thickness [mm]	0.02		
Data collection Range [°2θ]	10 – 130	**Calculated Peak width FWHM**	90
Step size [°]	0.026		
Time per step [s]	246.84	**11-coefficients form factors**	Yes
Detector	PIXcel	**Ionic form factors**	Yes

The following section provides the complete list of refined parameter values of the diffraction data. All refinements were carried out using starting values for asymmetry correction as well as the $K_{\alpha 2}/K_{\alpha 1}$ ratio was refined on a sample of CeO_2 powder (NIST-674b SRM) measured with the same experimental setup conditions as the samples. The refined values for $K_{\alpha 2}/K_{\alpha 1}$ ratio, Sample Displacement and Finger-Cox-Jephcoat (FCJ)-Asymmetry[1] parameters D/L and S/L were then used as fixed values for the Rietveld-refinements of the samples. The refined parameters and their corresponding standard uncertainties are listed below. Refinements were carried out using the HighScore software package[2] with Thomson-Cox-Hastings (TCH) type pseudo-Voigt profile functions, as Rietveld-fit as implemented in the software.

Refinement procedure:

Rhombohedral $R\bar{3}c$ f^3e^2cb-structure model:

The refinement procedure started with the refinement of the 25 °C NaZr ($Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$) sample. We call this the “reference data sample”. We tested variuos refinements on this data set before we applied the following procedure on the refinement of all data sets with all structure models. As a starting point, we used the single-crystal structure determination of rhombohedral $R\bar{3}c$ f^3e^2cb model of $Na_{3.35}Zr_2Si_{2.35}P_{0.65}O_{12}$ from Boilot et al. ICSD-#62386.[3] First, only the scale factor and an increasing number of polynomial Chebyshev-type background parameters (added one by one) were refined until no improvement in R_{wp} was observed.

In some refinements it was necessary to include one or two small Gaussian peaks at ≈14.09 °2θ and 15.39 °2θ, to account for some anisotropic shape in the background, probably originating from residual grease or the capillary quartz-glass material.

In the next step lattice parameters were added to the refinement, followed by profile parameters U and Y. Finally, the site coordinate parameters were then added one by one starting with Zr z-coordinate, Si/P x-coordinates, O1 and O2 (x, y, and z). Finally, the three Na positions were refined, including their relative occupancy. The last parameter added to the refinements was the combined parameter for the thermal displacement $B_{overall}$. For the reference data sample it was also tested to use individual atomic site thermal displacement parameters, but this resulted in unstable refinements and gave no further improvement in overall fit quality. Additionally, anisotropic thermal displacement for the Na-atoms was tested, but these often refined to unphysical values or became excessively large.

The refinement procedure was carried out with standard neutral atomic form factors and ionic form factors as well as with the 9- and 11-coefficient form factor parametrizations. The refinement with ionic form factors and 11-coefficients for the reference data sample gave the overall best results (in terms of refined Na-content R_{wp}, R_{Bragg}) and was thus subsequently used in all refinements.

An unexpected problem encountered was, that there is no ionic form factor tabulated for P^{5+}. Since the material investigated here should feature a mixed Si/P site it became apparent that using the neutral atom form factor for P while using the Si^{4+} form factor for Si would introduce a large mismatch for the mixed site occupancy. Therefore, only the Si^{4+} form factor was used in the refinements and the site occupancy was fixed to 1 instead of 0.8/0.2 as would be the expected value from the stoichiometric formula. In the listed tables below, however, the expected mixed site occupancy of 0.8/0.2 is listed.

Another notable observation is that the refined total sodium content in most structure models deviates from the nominal composition. The best fit is generally achieved using the f^{11} or f^{12} monoclinic models. However, a more surprising finding is the significant deviation in the refined sodium content for the Al/Y-doped sample. The unusually high values suggest the possibility of some Y^{3+} atoms being disordered on the Na sites. This disorder could also account for the pronounced decrease in total conductivity, as the presence of Y^{3+} on Na sites would likely obstruct the free movement of Na^{+} ions within the structure.

Table 2: Atomic form factors used in the refinements as provided by HighScore, according to the 11-coefficient scattering functions provided by Waasmeier and Kirfel[4] and HighScore software suite v5[2]. Anomalous dispersion coefficients according to International Tables for Crystallography Volume A, section 4.2.6.8.

Atom	A1 B1	A2 B2	A3 B3	A4 B4	A5 B5	C	f'	f''
Na^{+}	3.14869 2.594987	4.073989 6.046925	0.76789 0.070139	0.99561 14.12266	0.96825 0.21700	0.04530	0.1353	0.1239
Zr^{4+}	6.802956 0.096228	17.69925 1.296127	10.65065 11.24072	-0.24811 -0.21926	0.25034 -0.21900	0.82790	-0.1862	2.2449
Si^{4+}	3.676722 1.446851	3.82850 3.013144	1.258033 0.06440	0.41902 0.20625	0.72042 5.97000	0.09727	0.2541	0.3302
O^{2-}	3.990247 0.108493	16.63996 1.907882	2.300563 47.29971	5.63682 1.16708	0.60720 0.37900	0.02543	0.0106	0.0060

Introduction of the different structure models:

Rhombohedral *R*$\bar{3}$*c* f^2e^2cb-structure model:

The refinement of the f^2e^2cb-structure model was then obtained by setting the occupancy of the Na3-site to zero and refining the data until convergence was reached.

Monoclinic *C*2/*c* f^9e^2a-structure model:

In order to refine the monoclinic structure models we used the subgroup symmetry relationship as depicted in **Figure S1** (of the main supplement) to derive an initial monoclinic structure model from the refined rhombohedral f^3e^2cb-model of the reference data sample. This initial monoclinic structure model $f^{12}e^2a$ was then modified, the Na4, Na5 and Na6 positions were set to zero to get the reduced f^9e^2a-structure model and then stepwise refined as described above.

Monoclinic *C*2/*c* $f^{10}e^2a$-structure model:

The $f^{10}e^2a$-model was then refined by adding the positional and occupancy parameters of Na4 to the refinement.

Monoclinic *C*2/*c* $f^{12}e^2a$ and $f^{11}e^2a$-structure models:

For the $f^{12}e^2a$-model, Na5 and Na6 were added to the previous $f^{10}e^2a$ refinement. The monoclinic $f^{11}e^2a$-model was not tested separately, as it was quickly apparent that it was directly obtained from the $f^{12}e^2a$-model refinements as the Na6 occupancy was refined to zero value for temperatures ≤ 400 K.

1. Rietveld refinement results of six different structure models used for each dataset for $Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$ (NaZr) sample

*isotropic displacement parameter calculated in HighScore according to $F_{hkl} = F_0 \times \exp[-B_{iso} \times (Q/4\pi)^2]$
**Refinements were carried out using only Si^{4+} atom form factors with site occupancy of 1 for the mixed Si/P site. For X-rays Si^{4+} and P^{5+} are nearly identical, but for P^{5+} no atom form factor is reported in literature and thus it would introduce a much larger error to the refinement when mixing the Si^{4+} form factor, with the P^0 form factor function when applying a mixed site occupancy. The mixed site occupancy is calculated only manually from the nominal sample composition. It was not used in the refinements.

Structure model $R\bar{3}c$ - f^2e^2cb

Data-set: NaZr 25 °C (298 K)

Refined crystal data		TCH-U	0.765(29)
Formula sum	$Na_{2.473}Zr_2Si_3O_{12}$	TCH-Y	0.0316(65)
Formula weight	515.56	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2240(1)
Lattice parameters	*a* = 9.09193(56) Å	Coefficient 1	-2887(10)
	c = 22.8276(15) Å	Coefficient 2	1270(1)
		Coefficient 3	-468(8)
Cell volume	1634.19(23) Å^3	Coefficient 4	180(1)
Z	6	Coefficient 5	-95(9)
Density, calculated	3.143 g/cm^3	Coefficient 6	20(1)
Pearson code	hR42	Coefficient 7	-34(9)
Formula type	N2O3P4Q12	Coefficient 8	40(1)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000266(20)

Atom	Wyckoff site	Occupancy	fractional coordinates			B_{iso} [Å^2]*
			x	*y*	*z*	
Na1	6*b*	0.381(20)	0	0	0	0.404(58)
Na2	18*e*	0.6976(90)	0.6342(14)	0	¼	0.404(58)
Zr1	12*c*	1	0	0	0.1487(12)	0.404(58)
Si/P1**	18*e*	0.8/0.2	0.28647(80)	0	¼	0.404(58)
O1	36*f*	1	0.188(11)	0.9809(12)	0.19413(42)	0.404(58)
O2	36*f*	1	0.19047(76)	0.15658(95)	0.08035(50)	0.404(58)

Data-set: NaZr 77 °C (350 K)

Refined crystal data		TCH-U	0.566(19)
Formula sum	$Na_{2.542}Zr_2Si_3O_{12}$	TCH-Y	0.0338(49)
Formula weight	517.14	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2220(1)
Lattice parameters	*a* = 9.0938(4) Å	Coefficient 1	-2720(1)
	c = 22.8499(12) Å	Coefficient 2	968(9)
		Coefficient 3	-349(6)
Cell volume	1636.47(18) Å^3	Coefficient 4	195(8)
Z	6	Coefficient 5	-58(6)
Density, calculated	3.148 g/cm^3	Coefficient 6	43(8)
Pearson code	hR42	Coefficient 7	10(6)
Formula type	N2O3P4Q12	Coefficient 8	18(7)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000271(10)

Atom	Wyckoff site	Occupancy	fractional coordinates			B_{iso} [Å^2]*
			x	*y*	*z*	
Na1	6*b*	0.406(17)	0	0	0	0.538(51)
Na2	18*e*	0.7119(75)	0.6352(11)	0	¼	0.538(51)
Zr1	12*c*	1	0	0	0.1485(11)	0.538(51)
Si/P1**	18*e*	0.8/0.2	0.28599(68)	0	¼	0.538(51)
O1	36*f*	1	0.18781(89)	0.9801(10)	0.19422(36)	0.538(51)
O2	36*f*	1	0.19078(65)	0.15943(81)	0.08192(45)	0.538(51)

Data-set: NaZr 127 °C (400 K)

Refined crystal data		TCH-U	0.2561(67)
Formula sum	$Na_{2.518}Zr_2Si_3O_{12}$	TCH-Y	0.0381(25)
Formula weight	516.58	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2238(7)
Lattice parameters	*a* = 9.09515(22) Å	Coefficient 1	-2598(8)
	c = 22.87139(61) Å	Coefficient 2	1102(7)
		Coefficient 3	-350(6)
Cell volume	1638.49(9) Å^3	Coefficient 4	148(7)
Z	6	Coefficient 5	-74(6)
Density, calculated	3.141 g/cm^3	Coefficient 6	19(7)
Pearson code	hR42	Coefficient 7	-15(6)
Formula type	N2O3P4Q12	Coefficient 8	13(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000276(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*$_{iso}$ [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.365(11)	0	0	0	0.712(35)
Na2	18*e*	0.7175(50)	0.63731(75)	0	¼	0.712(35)
Zr1	12*c*	1	0	0	0.148333(71)	0.712(35)
Si/P1**	18*e*	0.8/0.2	0.28799(46)	0	¼	0.712(35)
O1	36*f*	1	0.18418(57)	0.97606(66)	0.19403(23)	0.712(35)
O2	36*f*	1	0.19044(45)	0.16456(53)	0.08257(29)	0.712(35)

Data-set: NaZr 177 °C (450 K)

Refined crystal data		TCH-U	0.173(46)
Formula sum	$Na_{2.51}Zr_2Si_3O_{12}$	TCH-Y	0.0397(21)
Formula weight	516.4	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2192(6)
Lattice parameters	*a* = 9.09562(18) Å	Coefficient 1	-2547(8)
	c = 22.90463(50) Å	Coefficient 2	1085(7)
		Coefficient 3	-344(6)
Cell volume	1641.04(7) Å^3	Coefficient 4	156(7)
Z	6	Coefficient 5	-80(6)
Density, calculated	3.135 g/cm^3	Coefficient 6	24(6)
Pearson code	hR42	Coefficient 7	-27(6)
Formula type	N2O3P4Q12	Coefficient 8	17(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000281(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*$_{iso}$ [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.3423(98)	0	0	0	0.812(33)
Na2	18*e*	0.7226(46)	0.6377(68)	0	¼	0.812(33)
Zr1	12*c*	1	0	0	0.148253(66)	0.812(33)
Si/P1**	18*e*	0.8/0.2	0.28797(42)	0	¼	0.812(33)
O1	36*f*	1	0.18221(52)	0.97456(60)	0.19428(21)	0.812(33)
O2	36*f*	1	0.19077(41)	0.16696(48)	0.08286(26)	0.812(33)

Data-set: NaZr 217 °C (490 K)

Refined crystal data		TCH-U	0.141(40)
Formula sum	$Na_{2.487}Zr_2Si_3O_{12}$	TCH-Y	0.0406(19)
Formula weight	515.87	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2152(6)
Lattice parameters	*a* = 9.09614(17) Å	Coefficient 1	-2479(8)
	c = 22.92697(47) Å	Coefficient 2	992(7)
		Coefficient 3	-302(6)
Cell volume	1642.83(7) $Å^3$	Coefficient 4	124(7)
Z	6	Coefficient 5	-60(6)
Density, calculated	3.128 g/cm^3	Coefficient 6	12(6)
Pearson code	hR42	Coefficient 7	-20(6)
Formula type	N2O3P4Q12	Coefficient 8	26(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000282(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} **[Å²]***
			x	***y***	***z***	
Na1	6*b*	0.322(95)	0	0	0	0.882(33)
Na2	18*e*	0.7216(45)	0.63763(67)	0	¼	0.882(33)
Zr1	12*c*	1	0	0	0.14834(65)	0.882(33)
Si/P1**	18*e*	0.8/0.2	0.28816(42)	0	¼	0.882(33)
O1	36*f*	1	0.18046(51)	0.9729(59)	0.19413(20)	0.882(33)
O2	36*f*	1	0.19124(41)	0.16827(47)	0.08267(26)	0.882(33)

Data-set: NaZr 267 °C (540 K)

Refined crystal data		TCH-U	0.114136(10)
Formula sum	$Na_{2.459}Zr_2Si_3O_{12}$	TCH-Y	0.04071(13)
Formula weight	515.22	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2181(5)
Lattice parameters	*a* = 9.096817(17) Å	Coefficient 1	-2425(7)
	c = 22.95004(57) Å	Coefficient 2	996(6)
		Coefficient 3	-281(6)
Cell volume	1644.72(1) $Å^3$	Coefficient 4	103(6)
Z	6	Coefficient 5	-56(6)
Density, calculated	3.121 g/cm^3	Coefficient 6	31(6)
Pearson code	hR42	Coefficient 7	-21(6)
Formula type	N2O3P4Q12	Coefficient 8	20(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000283(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} **[Å²]***
			x	***y***	***z***	
Na1	6*b*	0.3098(61)	0	0	0	0.919(14)
Na2	18*e*	0.7163(34)	0.63783(42)	0	¼	0.919(14)
Zr1	12*c*	1	0	0	0.148364(36)	0.919(14)
Si/P1**	18*e*	0.8/0.2	0.28834(24)	0	¼	0.919(14)
O1	36*f*	1	0.18004(33)	0.9727(38)	0.19367(13)	0.919(14)
O2	36*f*	1	0.19146(28)	0.16889(30)	0.08247(15)	0.919(14)

Data-set: NaZr 317 °C (590 K)

Refined crystal data		TCH-U	0.0932(28)
Formula sum	$Na_{2.444}Zr_2Si_3O_{12}$	TCH-Y	0.0411(16)
Formula weight	514.89	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2235(6)
Lattice parameters	*a* = 9.09795(14) Å	Coefficient 1	-2404(8)
	c = 22.9701(41) Å	Coefficient 2	962(7)
		Coefficient 3	-251(6)
Cell volume	1646.57(6) $Å^3$	Coefficient 4	114(6)
Z	6	Coefficient 5	-77(6)
Density, calculated	3.115 g/cm^3	Coefficient 6	43(6)
Pearson code	hR42	Coefficient 7	-26(6)
Formula type	N2O3P4Q12	Coefficient 8	30(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000286(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	6*b*	0.3051(92)	0	0	0	1.024(33)
Na2	18*e*	0.713(44)	0.63806(66)	0	¼	1.024(33)
Zr1	12*c*	1	0	0	0.148367(64)	1.024(33)
Si/P1**	18*e*	0.8/0.2	0.28751(41)	0	¼	1.024(33)
O1	36*f*	1	0.17931(50)	0.97177(57)	0.19387(20)	1.024(33)
O2	36*f*	1	0.19262(40)	0.16981(46)	0.08284(25)	1.024(33)

Data-set: NaZr 367 °C (640 K)

Refined crystal data		TCH-U	0.073525(10)
Formula sum	$Na_{2.463}Zr_2Si_3O_{12}$	TCH-Y	0.0419(15)
Formula weight	515.33	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2238(5)
Lattice parameters	*a* = 9.098589(20) Å	Coefficient 1	-2434(7)
	c = 22.98862(67) Å	Coefficient 2	914(6)
		Coefficient 3	-241(6)
Cell volume	1648.13(1) $Å^3$	Coefficient 4	110(6)
Z	6	Coefficient 5	-78(6)
Density, calculated	3.115 g/cm^3	Coefficient 6	39(6)
Pearson code	hR42	Coefficient 7	-30(6)
Formula type	N2O3P4Q12	Coefficient 8	25(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000284(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	6*b*	0.317(65)	0	0	0	1.035(14)
Na2	18*e*	0.7155(35)	0.63894(45)	0	¼	1.035(14)
Zr1	12*c*	1	0	0	0.14829(40)	1.035(14)
Si/P1**	18*e*	0.8/0.2	0.28748(26)	0	¼	1.035(14)
O1	36*f*	1	0.17859(35)	0.97099(40)	0.1944(14)	1.035(14)
O2	36*f*	1	0.19232(30)	0.16996(32)	0.08377(17)	1.035(14)

Structure model $R\bar{3}c$ – f^3e^2cb

Data-set: NaZr 25 °C (298 K)

Refined crystal data		TCH-U	0.74845(10)
Formula sum	$Na_{2.91}Zr_2Si_3O_{12}$	TCH-Y	0.03292(14)
Formula weight	525.60	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2242(7)
Lattice parameters	*a* = 9.092317(17) Å	Coefficient 1	-2880(1)
	c = 22.82704(55) Å	Coefficient 2	1260(1)
		Coefficient 3	-468(10)
Cell volume	1634.29(1) Å^3	Coefficient 4	174(10)
Z	6	Coefficient 5	-85(10)
Density, calculated	3.204 g/cm^3	Coefficient 6	21(10)
Pearson code	hR54	Coefficient 7	-19(9)
Formula type	N2O3P10Q12	Coefficient 8	34(94)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000273(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*$_{iso}$ [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.4271(80)	0	0	0	0.452(16)
Na2	18*e*	0.416(10)	0.6262(11)	0	¼	0.452(16)
Na3	36*f*	0.206(57)	0.669(18)	0.7004(19)	0.04549(75)	0.452(16)
Zr1	12*c*	1	0.149284(48)	0.7004(19)	0.04549(75)	0.452(16)
Si/P1**	18*e*	0.8/0.2	0.29018(32)	0	¼	0.452(16)
O1	36*f*	1	0.18299(45)	0.97797(51)	0.19442(18)	0.452(16)
O2	36*f*	1	0.1915(37)	0.15652(39)	0.08079(20)	0.452(16)

Data-set: NaZr 77 °C (350 K)

Refined crystal data		TCH-U	0.560742(10)
Formula sum	$Na_{2.981}Zr_2Si_3O_{12}$	TCH-Y	0.03403(14)
Formula weight	527.24	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2224(7)
Lattice parameters	*a* = 9.094105(16) Å	Coefficient 1	-2720(1)
	c = 22.84907(52) Å	Coefficient 2	1120(9)
		Coefficient 3	-422(9)
Cell volume	1636.51(1) Å^3	Coefficient 4	166(8)
Z	6	Coefficient 5	-83(9)
Density, calculated	3.210 g/cm^3	Coefficient 6	-1(9)
Pearson code	hR54	Coefficient 7	-10(8)
Formula type	N2O3P10Q12	Coefficient 8	14.4(83)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000278(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*$_{iso}$ [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.4405(73)	0	0	0	0.597(16)
Na2	18*e*	0.4469(94)	0.62638(99)	0	¼	0.597(16)
Na3	36*f*	0.2000(52)	0.681(17)	0.7075(18)	0.04546(72)	0.597(16)
Zr1	12*c*	1	0.149035(45)	0.7075(18)	0.04546(72)	0.597(16)
Si/P1**	18*e*	0.8/0.2	0.28962(30)	0	¼	0.597(16)
O1	36*f*	1	0.18295(41)	0.97777(47)	0.19476(17)	0.597(16)
O2	36*f*	1	0.19172(34)	0.15919(36)	0.08257(19)	0.597(16)

Data-set: NaZr 127 °C (400 K)

Refined crystal data		TCH-U	0.2548(62)
Formula sum	$Na_{2.962}Zr_2Si_3O_{12}$	TCH-Y	0.0382(24)
Formula weight	526.79	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2239(6)
Lattice parameters	*a* = 9.09533(21) Å	Coefficient 1	-2594(8)
	c = 22.87069(57) Å	Coefficient 2	1097(7)
		Coefficient 3	-354(6)
Cell volume	1638.50(9) $Å^3$	Coefficient 4	148(7)
Z	6	Coefficient 5	-75(6)
Density, calculated	3.203 g/cm^3	Coefficient 6	15(6)
Pearson code	hR54	Coefficient 7	-9(6)
Formula type	N2O3P10Q12	Coefficient 8	4.5(60)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000281(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	6*b*	0.391(10)	0	0	0	0.764(33)
Na2	18*e*	0.458(20)	0.6312(17)	0	¼	0.764(33)
Na3	36*f*	0.1995(97)	0.6971(29)	0.7222(32)	0.0478(14)	0.764(33)
Zr1	12*c*	1	0.148791(72)	0.7222(32)	0.0478(14)	0.764(33)
Si/P1**	18*e*	0.8/0.2	0.29147(47)	0	¼	0.764(33)
O1	36*f*	1	0.18032(55)	0.9747(63)	0.19513(25)	0.764(33)
O2	36*f*	1	0.19136(42)	0.16379(50)	0.08415(31)	0.764(33)

Data-set: NaZr 177 °C (450 K)

Refined crystal data		TCH-U	0.1782(44)
Formula sum	$Na_{3.075}Zr_2Si_3O_{12}$	TCH-Y	0.0383(19)
Formula weight	529.40	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2200(6)
Lattice parameters	*a* = 9.09577(17) Å	Coefficient 1	-2542(7)
	c = 22.90399(47) Å	Coefficient 2	1083(6)
		Coefficient 3	-345(6)
Cell volume	1641.05(7) $Å^3$	Coefficient 4	158(6)
Z	6	Coefficient 5	-78(6)
Density, calculated	3.214 g/cm^3	Coefficient 6	20(6)
Pearson code	hR54	Coefficient 7	-19(5)
Formula type	N2O3P10Q12	Coefficient 8	4.9(56)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000286(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	6*b*	0.3729(90)	0	0	0	0.883(31)
Na2	18*e*	0.509(13)	0.6324(13)	0	¼	0.883(31)
Na3	36*f*	0.1961(72)	0.7145(24)	0.7365(26)	0.0452(11)	0.883(31)
Zr1	12*c*	1	0.148655(66)	0.7365(26)	0.0452(11)	0.883(31)
Si/P1**	18*e*	0.8/0.2	0.29199(43)	0	¼	0.883(31)
O1	36*f*	1	0.17861(50)	0.97389(57)	0.19607(23)	0.883(31)
O2	36*f*	1	0.19186(39)	0.1656(46)	0.08563(29)	0.883(31)

Data-set: NaZr 217 °C (490 K)

Refined crystal data		TCH-U	0.145319(10)
Formula sum	$Na_{3.038}Zr_2Si_3O_{12}$	TCH-Y	0.03955(13)
Formula weight	528.55	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2159(4)
Lattice parameters	*a* = 9.096258(15) Å	Coefficient 1	-2474(7)
	c = 22.9264(50) Å	Coefficient 2	989(6)
		Coefficient 3	-302(6)
Cell volume	1642.83(1) $Å^3$	Coefficient 4	128(6)
Z	6	Coefficient 5	-59(6)
Density, calculated	3.205 g/cm^3	Coefficient 6	9(6)
Pearson code	hR54	Coefficient 7	-13(5)
Formula type	N2O3P10Q12	Coefficient 8	14.9(55)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000287(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	6*b*	0.3543(56)	0	0	0	0.954(13)
Na2	18*e*	0.525(61)	0.63299(64)	0	¼	0.954(13)
Na3	36*f*	0.1849(39)	0.7175(14)	0.7384(14)	0.04495(58)	0.954(13)
Zr1	12*c*	1	0.148698(36)	0.7384(14)	0.04495(58)	0.954(13)
Si/P1**	18*e*	0.8/0.2	0.29192(24)	0	¼	0.954(13)
O1	36*f*	1	0.17732(31)	0.9725(36)	0.19594(13)	0.954(13)
O2	36*f*	1	0.19228(26)	0.16687(28)	0.08555(16)	0.954(13)

Data-set: NaZr 267 °C (540 K)

Refined crystal data		TCH-U	0.1185(31)
Formula sum	$Na_{3.07}Zr_2Si_3O_{12}$	TCH-Y	0.0393(16)
Formula weight	529.28	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2190(5)
Lattice parameters	*a* = 9.09692(14) Å	Coefficient 1	-2418(7)
	c = 22.94951(40) Å	Coefficient 2	994(6)
		Coefficient 3	-281(6)
Cell volume	1644.72(6) $Å^3$	Coefficient 4	107(6)
Z	6	Coefficient 5	-55(6)
Density, calculated	3.206 g/cm^3	Coefficient 6	29(6)
Pearson code	hR54	Coefficient 7	-13(5)
Formula type	N2O3P10Q12	Coefficient 8	8.4(55)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000289(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	6*b*	0.3522(85)	0	0	0	1.006(30)
Na2	18*e*	0.525(11)	0.6336(11)	0	¼	1.006(30)
Na3	36*f*	0.1905(64)	0.7178(23)	0.7409(24)	1.0433(10)	1.006(30)
Zr1	12*c*	1	0.148691(64)	0.7409(24)	1.0433(10)	1.006(30)
Si/P1**	18*e*	0.8/0.2	0.29214(42)	0	¼	1.006(30)
O1	36*f*	1	0.17651(47)	0.97209(54)	0.19564(22)	1.006(30)
O2	36*f*	1	0.19275(38)	0.16757(44)	0.0858(28)	1.006(30)

Data-set: NaZr 317 °C (590 K)

Refined crystal data		TCH-U	0.0943(26)
Formula sum	$Na_{3.041}Zr_2Si_3O_{12}$	TCH-Y	0.0405(15)
Formula weight	528.62	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2244(5)
Lattice parameters	*a* = 9.09806(13) Å	Coefficient 1	-2394(7)
	c = 22.96969(38) Å	Coefficient 2	959(6)
		Coefficient 3	-252(6)
Cell volume	1646.58(5) Å^3	Coefficient 4	119(6)
Z	6	Coefficient 5	-77(6)
Density, calculated	3.198 g/cm^3	Coefficient 6	41(6)
Pearson code	hR54	Coefficient 7	-19(5)
Formula type	N2O3P10Q12	Coefficient 8	18.3(55)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000292(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.3421(84)	0	0	0	1.128(31)
Na2	18*e*	0.513(12)	0.634(12)	0	¼	1.128(31)
Na3	36*f*	0.1935(66)	0.7186(23)	0.7413(24)	1.0446(10)	1.128(31)
Zr1	12*c*	1	0.148693(64)	0.7413(24)	1.0446(10)	1.128(31)
Si/P1**	18*e*	0.8/0.2	0.29142(42)	0	¼	1.128(31)
O1	36*f*	1	0.17606(47)	0.97127(54)	0.19595(22)	1.128(31)
O2	36*f*	1	0.19375(38)	0.16834(44)	0.08613(28)	1.128(31)

Data-set: NaZr 367 °C (640 K)

Refined crystal data		TCH-U	0.0757(21)
Formula sum	$Na_{3.143}Zr_2Si_3O_{12}$	TCH-Y	0.041(14)
Formula weight	530.96	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2248(5)
Lattice parameters	*a* = 9.09867(12) Å	Coefficient 1	-2424(7)
	c = 22.98837(36) Å	Coefficient 2	914(6)
		Coefficient 3	-240(6)
Cell volume	1648.14(5) Å^3	Coefficient 4	117(6)
Z	6	Coefficient 5	-76(6)
Density, calculated	3.210 g/cm^3	Coefficient 6	38(6)
Pearson code	hR54	Coefficient 7	-20(5)
Formula type	N2O3P10Q12	Coefficient 8	10.9(55)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000291(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å^2]***
			x	***y***	***z***	
Na1	6*b*	0.3512(84)	0	0	0	1.159(31)
Na2	18*e*	0.5509(92)	0.6353(10)	0	¼	1.159(31)
Na3	36*f*	0.1899(59)	0.7305(21)	0.7493(23)	1.04094(92)	1.159(31)
Zr1	12*c*	1	0.148581(65)	0.7493(23)	1.04094(92)	1.159(31)
Si/P1**	18*e*	0.8/0.2	0.29139(42)	0	¼	1.159(31)
O1	36*f*	1	0.1749(48)	0.97102(54)	0.1962(22)	1.159(31)
O2	36*f*	1	0.1941(39)	0.16904(45)	0.08745(28)	1.159(31)

Structure model *C2/c* - f^9e^2a

Data-set: NaZr 25 °C (298 K)

Refined crystal data			
Formula sum	$Na_{2.811}Zr_2Si_3O_{12}$	TCH-U	0.1711(55)
Formula weight	523.32	TCH-Y	0.0391(24)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1325(85) Å	Coefficient 0	2244(6)
	b = 9.09752(26) Å	Coefficient 1	-2854(4)
	c = 22.817(12) Å	Coefficient 2	1256(7)
	β = 161.0239(14)°	Coefficient 3	-465(4)
Cell volume	1088.94(82) $Å^3$	Coefficient 4	180(7)
Z	4	Coefficient 5	-101(4)
Density, calculated	3.192 g/cm^3	Coefficient 6	20(6)
Pearson code	mC84	Coefficient 7	-16(4)
Formula type	N2O3P4Q12	Coefficient 8	26(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000606(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.4035(94)	0	0	0	0.512(28)
Na2	4*e*	0.938(17)	0	0.6293(19)	¼	0.512(28)
Na3	8*f*	0.735(10)	0.9325(23)	0.6722(14)	0.8475(16)	0.512(28)
Zr1	8*f*	1	-0.00308(50)	-0.0026(70)	0.14659(34)	0.512(28)
Si/P1**	4*e*	0.8/0.2	0	0.297(16)	¼	0.512(28)
Si/P2**	8*f*	0.8/0.2	0.4411(17)	0.8659(11)	0.5469(11)	0.512(28)
O1	8*f*	1	0.035(20)	0.2158(15)	0.2229(14)	0.512(28)
O2	8*f*	1	0.1779(26)	0.4274(15)	0.9764(18)	0.512(28)
O3	8*f*	1	0.2414(27)	0.8994(15)	0.3548(19)	0.512(28)
O4	8*f*	1	0.3028(27)	0.0535(18)	0.2884(19)	0.512(28)
O5	8*f*	1	0.2685(29)	0.599(15)	0.9306(20)	0.512(28)
O6	8*f*	1	0.4646(31)	0.3072(18)	0.0557(21)	0.512(28)

Data-set: NaZr 77 °C (350 K)

Refined crystal data			
Formula sum	$Na_{2.817}Zr_2Si_3O_{12}$	TCH-U	0.1744(10)
Formula weight	523.46	TCH-Y	0.03534(12)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.14437(74) Å	Coefficient 0	2223(5)
	b = 9.098044(22) Å	Coefficient 1	-2701(8)
	c = 22.8453(10) Å	Coefficient 2	1123(7)
	β = 161.0305(13)°	Coefficient 3	-419(6)
Cell volume	1090.78(7) $Å^3$	Coefficient 4	174(6)
Z	4	Coefficient 5	-90(6)
Density, calculated	3.187 g/cm^3	Coefficient 6	1(6)
Pearson code	mC84	Coefficient 7	-1(5)
Formula type	N2O3P4Q12	Coefficient 8	13(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000614(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.3903(57)	0	0	0	0.612(14)
Na2	4*e*	0.9998(89)	0	0.62407(70)	¼	0.612(14)
Na3	8*f*	0.7135(57)	0.9398(11)	0.66711(63)	0.85286(80)	0.612(14)
Zr1	8*f*	1	-0.00247(21)	-0.00274(25)	0.14701(15)	0.612(14)
Si/P1**	4*e*	0.8/0.2	0	0.29556(58)	¼	0.612(14)
Si/P2**	8*f*	0.8/0.2	0.44211(67)	0.86691(41)	0.54787(47)	0.612(14)
O1	8*f*	1	0.0313(11)	0.21286(75)	0.22019(78)	0.612(14)
O2	8*f*	1	0.1803(12)	0.43262(67)	0.98034(86)	0.612(14)
O3	8*f*	1	0.253(12)	0.89764(70)	0.36134(89)	0.612(14)
O4	8*f*	1	0.3056(13)	0.05416(70)	0.29034(89)	0.612(14)
O5	8*f*	1	0.2719(12)	0.60064(67)	0.9323(88)	0.612(14)
O6	8*f*	1	0.486(13)	0.30795(74)	0.07118(95)	0.612(14)

Data-set: NaZr 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{2.753}Zr_2Si_3O_{12}$	TCH-U	0.1538(50)
Formula weight	522.00	TCH-Y	0.0362(22)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.147(13) Å	Coefficient 0	2228(6)
	b = 9.09743(38) Å	Coefficient 1	-2592(7)
	c = 22.873(19) Å	Coefficient 2	1108(6)
	β = 161.0259(23)°	Coefficient 3	-353(5)
Cell volume	1092.41(127) $Å^3$	Coefficient 4	153(6)
Z	4	Coefficient 5	-72(5)
Density, calculated	3.174 g/cm^3	Coefficient 6	18(6)
Pearson code	mC84	Coefficient 7	-3(5)
Formula type	N2O3P4Q12	Coefficient 8	9(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000622(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.3582(91)	0	0	0	0.688(31)
Na2	4*e*	0.885(25)	0	0.6196(25)	¼	0.688(31)
Na3	8*f*	0.755(14)	0.9449(29)	0.6651(17)	0.8585(19)	0.688(31)
Zr1	8*f*	1	-0.001(79)	-0.00291(78)	0.14804(53)	0.688(31)
Si/P1**	4*e*	0.8/0.2	0	0.2962(25)	¼	0.688(31)
Si/P2**	8*f*	0.8/0.2	0.4398(23)	0.8653(17)	0.5461(16)	0.688(31)
O1	8*f*	1	0.0241(30)	0.2007(28)	0.2132(22)	0.688(31)
O2	8*f*	1	0.1831(37)	0.4358(23)	0.9853(26)	0.688(31)
O3	8*f*	1	0.268(40)	0.884(25)	0.3697(28)	0.688(31)
O4	8*f*	1	0.2916(37)	0.051(24)	0.2821(26)	0.688(31)
O5	8*f*	1	0.2652(43)	0.5964(23)	0.9281(29)	0.688(31)
O6	8*f*	1	0.4873(41)	0.3004(20)	0.0699(28)	0.688(31)

Data-set: NaZr 177 °C (450 K)

Refined crystal data			
Formula sum	$Na_{2.789}Zr_2Si_3O_{12}$	TCH-U	0.1612(48)
Formula weight	522.82	TCH-Y	0.0388(19)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.154(17) Å	Coefficient 0	2179(6)
	b = 9.0957(54) Å	Coefficient 1	-2545(7)
	c = 22.904(24) Å	Coefficient 2	1092(7)
	β = 161.0299(29)°	Coefficient 3	-343(5)
Cell volume	1094.03(162) $Å^3$	Coefficient 4	163(6)
Z	4	Coefficient 5	-75(5)
Density, calculated	3.174 g/cm^3	Coefficient 6	24(6)
Pearson code	mC84	Coefficient 7	-11(5)
Formula type	N2O3P4Q12	Coefficient 8	-4(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000624(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.439(13)	0	0	0	0.713(34)
Na2	4*e*	0.475(36)	0	0.6046(48)	¼	0.713(34)
Na3	8*f*	0.938(17)	0.9479(24)	0.6641(15)	0.8639(16)	0.713(34)
Zr1	8*f*	1	0.0021(15)	0.00063(94)	0.14971(99)	0.713(34)
Si/P1**	4*e*	0.8/0.2	0	0.282(31)	¼	0.713(34)
Si/P2**	8*f*	0.8/0.2	0.4415(32)	0.8553(25)	0.5474(21)	0.713(34)
O1	8*f*	1	0.0334(53)	0.1781(30)	0.2196(37)	0.713(34)
O2	8*f*	1	0.1769(71)	0.4181(34)	0.9822(50)	0.713(34)
O3	8*f*	1	0.2658(51)	0.8641(35)	0.369(36)	0.713(34)
O4	8*f*	1	0.2609(41)	0.0518(28)	0.2616(28)	0.713(34)
O5	8*f*	1	0.2108(42)	0.583(23)	0.9001(31)	0.713(34)
O6	8*f*	1	0.4309(46)	0.3024(27)	0.0336(30)	0.713(34)

Data-set: NaZr 217 °C (490 K)

Refined crystal data			
Formula sum	$Na_{2.743}Zr_2Si_3O_{12}$	TCH-U	0.1404(38)
Formula weight	521.75	TCH-Y	0.0402(18)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.163(17) Å	Coefficient 0	2137(6)
	b = 9.09553(57) Å	Coefficient 1	-2480(6)
	c = 22.927(24) Å	Coefficient 2	999(7)
	β = 161.0385(29)°	Coefficient 3	-298(5)
Cell volume	1095.20(163) $Å^3$	Coefficient 4	133(7)
Z	4	Coefficient 5	-60(5)
Density, calculated	3.164 g/cm^3	Coefficient 6	15(6)
Pearson code	mC84	Coefficient 7	0(5)
Formula type	N2O3P4Q12	Coefficient 8	5(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000618(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.419(14)	0	0	0	0.722(35)
Na2	4*e*	0.368(44)	0	0.5881(59)	¼	0.722(35)
Na3	8*f*	0.978(21)	0.9503(24)	0.665(17)	0.8676(16)	0.722(35)
Zr1	8*f*	1	0.0015(23)	0.00021(81)	0.1493(15)	0.722(35)
Si/P1**	4*e*	0.8/0.2	0	0.2812(29)	¼	0.722(35)
Si/P2**	8*f*	0.8/0.2	0.4415(31)	0.8558(24)	0.5483(20)	0.722(35)
O1	8*f*	1	0.0487(79)	0.1701(28)	0.2248(54)	0.722(35)
O2	8*f*	1	0.1827(88)	0.4136(31)	0.9825(59)	0.722(35)
O3	8*f*	1	0.2757(71)	0.8623(36)	0.3841(50)	0.722(35)
O4	8*f*	1	0.2593(44)	0.0554(31)	0.2576(29)	0.722(35)
O5	8*f*	1	0.2185(55)	0.5914(27)	0.9074(42)	0.722(35)
O6	8*f*	1	0.4365(50)	0.3019(33)	0.0366(35)	0.722(35)

Data-set: NaZr 267 °C (540 K)

Refined crystal data			
Formula sum	$Na_{2.776}Zr_2Si_3O_{12}$	TCH-U	0.1144(31)
Formula weight	522.52	TCH-Y	0.0399(16)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.178(15) Å	Coefficient 0	2169(6)
	b = 9.09619(49) Å	Coefficient 1	-2423(7)
	c = 22.95(22) Å	Coefficient 2	1005(7)
	β = 161.0549(26)°	Coefficient 3	-277(5)
Cell volume	1096.47(147) $Å^3$	Coefficient 4	113(6)
Z	4	Coefficient 5	-51(5)
Density, calculated	3.165 g/cm^3	Coefficient 6	35(6)
Pearson code	mC84	Coefficient 7	1(5)
Formula type	N2O3P4Q12	Coefficient 8	0(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000625(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.428(13)	0	0	0	0.793(33)
Na2	4*e*	0.417(41)	0	0.5861(52)	¼	0.793(33)
Na3	8*f*	0.966(20)	0.9525(22)	0.6657(16)	0.8672(15)	0.793(33)
Zr1	8*f*	1	0.0024(21)	-0.00078(78)	0.15(14)	0.793(33)
Si/P1**	4*e*	0.8/0.2	0	0.2785(26)	¼	0.793(33)
Si/P2**	8*f*	0.8/0.2	0.4461(29)	0.8582(20)	0.5518(18)	0.793(33)
O1	8*f*	1	0.054(79)	0.1728(29)	0.2286(53)	0.793(33)
O2	8*f*	1	0.1924(80)	0.4138(29)	0.9912(53)	0.793(33)
O3	8*f*	1	0.2761(68)	0.8591(34)	0.3803(48)	0.793(33)
O4	8*f*	1	0.2554(43)	0.0536(28)	0.2561(28)	0.793(33)
O5	8*f*	1	0.2153(54)	0.5892(25)	0.9039(40)	0.793(33)
O6	8*f*	1	0.435(48)	0.2973(32)	0.037(32)	0.793(33)

Data-set: NaZr 317 °C (590 K)

Refined crystal data			
Formula sum	$Na_{2.629}Zr_2Si_3O_{12}$	TCH-U	0.08378(10)
Formula weight	519.14	TCH-Y	0.04034(20)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1961(11) Å	Coefficient 0	2213(4)
	b = 9.100658(31) Å	Coefficient 1	-2409(7)
	c = 22.9722(16) Å	Coefficient 2	970(6)
	β = 161.0824(19)°	Coefficient 3	-256(6)
Cell volume	1097.76(11) $Å^3$	Coefficient 4	112(5)
Z	4	Coefficient 5	-79(5)
Density, calculated	3.141 g/cm^3	Coefficient 6	36(5)
Pearson code	mC84	Coefficient 7	-13(5)
Formula type	N2O3P4Q12	Coefficient 8	16(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000639(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.3112(65)	0	0	0	0.848(17)
Na2	4*e*	0.745(18)	0	0.6118(14)	¼	0.848(17)
Na3	8*f*	0.7866(99)	0.9497(15)	0.66774(94)	0.86281(98)	0.848(17)
Zr1	8*f*	1	0.00355(34)	-0.00469(30)	0.15103(23)	0.848(17)
Si/P1**	4*e*	0.8/0.2	0	0.28868(95)	¼	0.848(17)
Si/P2**	8*f*	0.8/0.2	0.4425(10)	0.8631(74)	0.54936(68)	0.848(17)
O1	8*f*	1	0.0345(20)	0.1901(13)	0.2112(13)	0.848(17)
O2	8*f*	1	0.2245(20)	0.4366(12)	1.0115(13)	0.848(17)
O3	8*f*	1	0.3031(20)	0.8665(12)	0.4042(14)	0.848(17)
O4	8*f*	1	0.2521(18)	0.085(12)	0.257(12)	0.848(17)
O5	8*f*	1	0.2714(18)	0.6328(11)	0.9216(13)	0.848(17)
O6	8*f*	1	0.4718(23)	0.3085(12)	0.0689(15)	0.848(17)

Data-set: NaZr 367 °C (640 K)

Refined crystal data			
Formula sum	$Na_{2.639}Zr_2Si_3O_{12}$	TCH-U	0.0705(21)
Formula weight	519.38	TCH-Y	0.0419(13)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.204(15) Å	Coefficient 0	2215(6)
	b = 9.09977(49) Å	Coefficient 1	-2441(7)
	c = 22.989(22) Å	Coefficient 2	921(6)
	β = 161.0864(26)°	Coefficient 3	-245(5)
Cell volume	1098.77(147) $Å^3$	Coefficient 4	113(6)
Z	4	Coefficient 5	-83(6)
Density, calculated	3.139 g/cm^3	Coefficient 6	35(6)
Pearson code	mC84	Coefficient 7	-17(5)
Formula type	N2O3P4Q12	Coefficient 8	8(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000629(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.318(11)	0	0	0	0.834(34)
Na2	4*e*	0.545(46)	0	0.6315(60)	¼	0.834(34)
Na3	8*f*	0.888(25)	0.9398(34)	0.6722(19)	0.8571(23)	0.834(34)
Zr1	8*f*	1	0.0002(18)	-0.00368(74)	0.1487(12)	0.834(34)
Si/P1**	4*e*	0.8/0.2	0	0.2882(34)	¼	0.834(34)
Si/P2**	8*f*	0.8/0.2	0.4399(30)	0.8609(23)	0.547(22)	0.834(34)
O1	8*f*	1	0.0455(56)	0.1903(40)	0.221(40)	0.834(34)
O2	8*f*	1	0.2355(52)	0.4287(27)	1.0168(35)	0.834(34)
O3	8*f*	1	0.2994(48)	0.8593(30)	0.4034(30)	0.834(34)
O4	8*f*	1	0.2446(32)	0.098(24)	0.2532(24)	0.834(34)
O5	8*f*	1	0.2753(39)	0.6298(30)	0.9261(29)	0.834(34)
O6	8*f*	1	0.451(51)	0.3065(28)	0.0564(35)	0.834(34)

Structure model *C2/c* – $f^{10}e^2a$

Data-set: NaZr 25 °C (298 K)

Refined crystal data			
Formula sum	$Na_{3.366}Zr_2Si_3O_{12}$	TCH-U	0.188162(10)
Formula weight	536.09	TCH-Y	0.03512(12)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1351(62) Å	Coefficient 0	2277(4)
	b = 9.097274(18) Å	Coefficient 1	-2828(5)
	c = 22.82162(88) Å	Coefficient 2	1277(5)
	β = 161.0295(11)°	Coefficient 3	-446(4)
Cell volume	1088.98(6) $Å^3$	Coefficient 4	199(4)
Z	4	Coefficient 5	-85(4)
Density, calculated	3.270 g/cm^3	Coefficient 6	41(4)
Pearson code	mC92	Coefficient 7	-14(4)
Formula type	N2O3P6Q12	Coefficient 8	25(4)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000613(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.3852(59)	0	0	0	0.684(14)
Na2	4*e*	1	0	0.6387(63)	¼	0.684(14)
Na3	8*f*	0.6403(55)	0.9408(12)	0.66768(64)	0.8592(90)	0.684(14)
Na4	8*f*	0.3503(64)	0.7431(20)	0.131(12)	0.8135(15)	0.684(14)
Zr1	8*f*	1	-0.00463(19)	-0.00001(25)	0.14506(14)	0.684(14)
Si/P1**	4*e*	0.8/0.2	0	0.30128(52)	¼	0.684(14)
Si/P2**	8*f*	0.8/0.2	0.43393(65)	0.86855(37)	0.5416(46)	0.684(14)
O1	8*f*	1	0.0121(11)	0.2023(76)	0.20631(75)	0.684(14)
O2	8*f*	1	0.1721(11)	0.43336(62)	0.9726(79)	0.684(14)
O3	8*f*	1	0.2489(12)	0.89025(66)	0.36217(84)	0.684(14)
O4	8*f*	1	0.2937(12)	0.05641(66)	0.28862(82)	0.684(14)
O5	8*f*	1	0.2719(11)	0.60046(62)	0.93277(80)	0.684(14)
O6	8*f*	1	0.4702(13)	0.29604(68)	0.06871(90)	0.684(14)

Data-set: NaZr 77 °C (350 K)

Refined crystal data			
Formula sum	$Na_{3.34}Zr_2Si_3O_{12}$	TCH-U	0.182544(10)
Formula weight	535.49	TCH-Y	0.03201(10)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.14671(64) Å	Coefficient 0	2253(4)
	b = 9.097141(17) Å	Coefficient 1	-2676(6)
	c = 22.84906(90) Å	Coefficient 2	1142(5)
	β = 161.0331(11)°	Coefficient 3	-398(5)
Cell volume	1090.86(6) $Å^3$	Coefficient 4	191(5)
Z	4	Coefficient 5	-73(5)
Density, calculated	3.260 g/cm^3	Coefficient 6	21(5)
Pearson code	mC92	Coefficient 7	1(4)
Formula type	N2O3P6Q12	Coefficient 8	11(4)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000622(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.3898(59)	0	0	0	0.762(14)
Na2	4*e*	1	0	0.63931(66)	¼	0.762(14)
Na3	8*f*	0.6441(54)	0.9452(12)	0.66222(66)	0.86244(91)	0.762(14)
Na4	8*f*	0.3312(63)	0.7598(22)	0.1277(13)	0.8277(16)	0.762(14)
Zr1	8*f*	1	-0.00354(20)	-0.00015(26)	0.14568(14)	0.762(14)
Si/P1**	4*e*	0.8/0.2	0	0.30032(53)	¼	0.762(14)
Si/P2**	8*f*	0.8/0.2	0.43412(63)	0.86966(39)	0.54163(44)	0.762(14)
O1	8*f*	1	0.0037(11)	0.19913(79)	0.20091(80)	0.762(14)
O2	8*f*	1	0.1746(12)	0.43598(63)	0.97525(80)	0.762(14)
O3	8*f*	1	0.2618(12)	0.88545(67)	0.37119(88)	0.762(14)
O4	8*f*	1	0.2978(12)	0.05344(67)	0.29191(84)	0.762(14)
O5	8*f*	1	0.2744(11)	0.60198(64)	0.93462(83)	0.762(14)
O6	8*f*	1	0.4912(14)	0.29612(67)	0.08547(98)	0.762(14)

Data-set: NaZr 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{3.196}Zr_2Si_3O_{12}$	TCH-U	0.156405(10)
Formula weight	532.16	TCH-Y	0.03481(13)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.14831(74) Å	Coefficient 0	2245(4)
	b = 9.097216(22) Å	Coefficient 1	-2583(6)
	c = 22.8748(11) Å	Coefficient 2	1121(5)
	β = 161.0286(13)°	Coefficient 3	-341(5)
Cell volume	1092.46(7) $Å^3$	Coefficient 4	162(5)
Z	4	Coefficient 5	-66(5)
Density, calculated	3.235 g/cm^3	Coefficient 6	30(5)
Pearson code	mC92	Coefficient 7	0(5)
Formula type	N2O3P6Q12	Coefficient 8	1(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000623(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	4*a*	0.3368(62)	0	0	0	0.737(16)
Na2	4*e*	0.918(11)	0	0.63791(89)	¼	0.737(16)
Na3	8*f*	0.7024(67)	0.938(13)	0.66061(75)	0.85647(92)	0.737(16)
Na4	8*f*	0.2682(73)	0.7598(32)	0.1271(19)	0.828(23)	0.737(16)
Zr1	8*f*	1	-0.00043(23)	-0.0003(28)	0.14792(16)	0.737(16)
Si/P1**	4*e*	0.8/0.2	0	0.30108(65)	¼	0.737(16)
Si/P2**	8*f*	0.8/0.2	0.43301(73)	0.86614(48)	0.54127(52)	0.737(16)
O1	8*f*	1	0.0028(14)	0.17777(98)	0.19984(94)	0.737(16)
O2	8*f*	1	0.1789(14)	0.44008(81)	0.98111(98)	0.737(16)
O3	8*f*	1	0.2873(14)	0.87124(84)	0.3832(10)	0.737(16)
O4	8*f*	1	0.285(14)	0.05302(82)	0.28203(99)	0.737(16)
O5	8*f*	1	0.2638(14)	0.5989(81)	0.9272(10)	0.737(16)
O6	8*f*	1	0.4868(16)	0.29018(79)	0.08(11)	0.737(16)

Data-set: NaZr 177 °C (450 K)

Refined crystal data			
Formula sum	$Na_{3.189}Zr_2Si_3O_{12}$	TCH-U	0.147567(10)
Formula weight	532.02	TCH-Y	0.03717(17)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.15981(89) Å	Coefficient 0	2194(4)
	b = 9.096863(26) Å	Coefficient 1	-2535(6)
	c = 22.907(13) Å	Coefficient 2	1106(6)
	β = 161.0401(15)°	Coefficient 3	-341(5)
Cell volume	1094.09(9) $Å^3$	Coefficient 4	169(5)
Z	4	Coefficient 5	-72(5)
Density, calculated	3.230 g/cm^3	Coefficient 6	29(5)
Pearson code	mC92	Coefficient 7	-12(5)
Formula type	N2O3P6Q12	Coefficient 8	2(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000636(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	4*a*	0.3074(66)	0	0	0	0.816(17)
Na2	4*e*	0.899(14)	0	0.6442(11)	¼	0.816(17)
Na3	8*f*	0.7246(83)	0.9357(14)	0.66301(85)	0.85373(96)	0.816(17)
Na4	8*f*	0.2666(74)	0.7776(35)	0.1167(22)	0.8415(25)	0.816(17)
Zr1	8*f*	1	-0.00004(25)	-0.00078(33)	0.14809(18)	0.816(17)
Si/P1**	4*e*	0.8/0.2	0	0.29348(80)	¼	0.816(17)
Si/P2**	8*f*	0.8/0.2	0.43658(86)	0.86353(60)	0.54278(61)	0.816(17)
O1	8*f*	1	0.0041(16)	0.1746(11)	0.2015(11)	0.816(17)
O2	8*f*	1	0.1761(17)	0.44107(98)	0.981(12)	0.816(17)
O3	8*f*	1	0.2915(16)	0.8718(10)	0.384(11)	0.816(17)
O4	8*f*	1	0.2868(16)	0.05173(98)	0.2828(11)	0.816(17)
O5	8*f*	1	0.2606(17)	0.5987(10)	0.9254(12)	0.816(17)
O6	8*f*	1	0.488(19)	0.29075(89)	0.0819(13)	0.816(17)

Data-set: NaZr 217 °C (490 K)

Refined crystal data			
Formula sum	$Na_{3.165}Zr_2Si_3O_{12}$	TCH-U	0.134314(10)
Formula weight	531.47	TCH-Y	0.03724(17)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.17075(91) Å	Coefficient 0	2150(4)
	b = 9.098203(26) Å	Coefficient 1	-2476(6)
	c = 22.9292(13) Å	Coefficient 2	1012(6)
	β = 161.0548(15)°	Coefficient 3	-300(5)
Cell volume	1095.24(9) $Å^3$	Coefficient 4	135(5)
Z	4	Coefficient 5	-51(5)
Density, calculated	3.223 g/cm^3	Coefficient 6	15(5)
Pearson code	mC92	Coefficient 7	-6(5)
Formula type	N2O3P6Q12	Coefficient 8	12(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000635(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.2935(67)	0	0	0	0.844(17)
Na2	4*e*	0.885(16)	0	0.6466(12)	¼	0.844(17)
Na3	8*f*	0.7278(92)	0.9349(15)	0.66381(94)	0.8537(10)	0.844(17)
Na4	8*f*	0.2655(75)	0.7769(36)	0.1084(23)	0.8431(25)	0.844(17)
Zr1	8*f*	1	-0.00005(27)	-0.00113(34)	0.14811(19)	0.844(17)
Si/P1**	4*e*	0.8/0.2	0	0.29129(87)	¼	0.844(17)
Si/P2**	8*f*	0.8/0.2	0.4374(90)	0.86323(68)	0.54276(63)	0.844(17)
O1	8*f*	1	0.0045(17)	0.174(11)	0.2013(12)	0.844(17)
O2	8*f*	1	0.1753(17)	0.4431(10)	0.9812(12)	0.844(17)
O3	8*f*	1	0.292(16)	0.8709(11)	0.3836(11)	0.844(17)
O4	8*f*	1	0.2869(18)	0.0535(11)	0.283(12)	0.844(17)
O5	8*f*	1	0.2605(18)	0.5996(11)	0.9253(13)	0.844(17)
O6	8*f*	1	0.4881(20)	0.29027(92)	0.0823(13)	0.844(17)

Data-set: NaZr 267 °C (540 K)

Refined crystal data			
Formula sum	$Na_{3.13}Zr_2Si_3O_{12}$	TCH-U	0.11332(10)
Formula weight	530.66	TCH-Y	0.0373(16)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.18358(94) Å	Coefficient 0	2177(4)
	b = 9.099291(27) Å	Coefficient 1	-2422(6)
	c = 22.9526(13) Å	Coefficient 2	1016(6)
	β = 161.0703(16)°	Coefficient 3	-279(5)
Cell volume	1096.49(9) $Å^3$	Coefficient 4	112(5)
Z	4	Coefficient 5	-46(5)
Density, calculated	3.214 g/cm^3	Coefficient 6	32(5)
Pearson code	mC92	Coefficient 7	-6(5)
Formula type	N2O3P6Q12	Coefficient 8	7(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000639(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.2745(68)	0	0	0	0.865(16)
Na2	4*e*	0.836(17)	0	0.6505(13)	¼	0.865(16)
Na3	8*f*	0.7444(97)	0.9337(15)	0.66703(95)	0.85244(99)	0.865(16)
Na4	8*f*	0.2652(73)	0.7776(37)	0.0973(24)	0.842(26)	0.865(16)
Zr1	8*f*	1	-0.00007(30)	-0.00139(33)	0.14815(21)	0.865(16)
Si/P1**	4*e*	0.8/0.2	0	0.29127(87)	¼	0.865(16)
Si/P2**	8*f*	0.8/0.2	0.4372(92)	0.86334(67)	0.54334(63)	0.865(16)
O1	8*f*	1	0.0052(18)	0.1731(12)	0.2014(12)	0.865(16)
O2	8*f*	1	0.1753(18)	0.4434(11)	0.9817(12)	0.865(16)
O3	8*f*	1	0.2932(17)	0.8683(11)	0.3835(12)	0.865(16)
O4	8*f*	1	0.2855(18)	0.053(11)	0.2832(12)	0.865(16)
O5	8*f*	1	0.2609(19)	0.5993(12)	0.9245(13)	0.865(16)
O6	8*f*	1	0.4894(20)	0.28812(90)	0.0834(14)	0.865(16)

Data-set: NaZr 317 °C (590 K)

Refined crystal data			
Formula sum	$Na_{3.152}Zr_2Si_3O_{12}$	TCH-U	0.0884(27)
Formula weight	531.15	TCH-Y	0.0395(15)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.196(17) Å	Coefficient 0	2233(5)
	b = 9.09925(56) Å	Coefficient 1	-2388(7)
	c = 22.972(24) Å	Coefficient 2	981(6)
	β = 161.0792(29)°	Coefficient 3	-253(5)
Cell volume	1097.74(165) $Å^3$	Coefficient 4	125(6)
Z	4	Coefficient 5	-70(5)
Density, calculated	3.214 g/cm^3	Coefficient 6	41(5)
Pearson code	mC92	Coefficient 7	-8(5)
Formula type	N2O3P6Q12	Coefficient 8	15(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000652(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.264(11)	0	0	0	1.041(34)
Na2	4*e*	0.867(33)	0	0.6612(29)	¼	1.041(34)
Na3	8*f*	0.738(21)	0.9204(31)	0.6709(21)	0.8433(20)	1.041(34)
Na4	8*f*	0.272(12)	0.7718(78)	0.0891(62)	0.8376(56)	1.041(34)
Zr1	8*f*	1	0.0003(12)	-0.00206(66)	0.14842(80)	1.041(34)
Si/P1**	4*e*	0.8/0.2	0	0.2894(32)	¼	1.041(34)
Si/P2**	8*f*	0.8/0.2	0.4361(30)	0.8598(25)	0.5426(22)	1.041(34)
O1	8*f*	1	0.0127(40)	0.1692(31)	0.2076(29)	1.041(34)
O2	8*f*	1	0.1753(47)	0.4425(25)	0.9809(34)	1.041(34)
O3	8*f*	1	0.3018(36)	0.8685(26)	0.3905(26)	1.041(34)
O4	8*f*	1	0.2655(41)	0.0687(38)	0.2712(30)	1.041(34)
O5	8*f*	1	0.268(46)	0.6214(27)	0.9295(34)	1.041(34)
O6	8*f*	1	0.4904(46)	0.2935(22)	0.0835(31)	1.041(34)

Data-set: NaZr 367 °C (640 K)

Refined crystal data			
Formula sum	$Na_{3.166}Zr_2Si_3O_{12}$	TCH-U	0.0723(22)
Formula weight	531.49	TCH-Y	0.0399(13)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.206(15) Å	Coefficient 0	2234(5)
	b = 9.10073(51) Å	Coefficient 1	-2421(7)
	c = 22.99(22) Å	Coefficient 2	934(6)
	β = 161.0925(26)°	Coefficient 3	-245(5)
Cell volume	1098.76(149) $Å^3$	Coefficient 4	120(5)
Z	4	Coefficient 5	-71(5)
Density, calculated	3.213 g/cm^3	Coefficient 6	36(5)
Pearson code	mC92	Coefficient 7	-11(5)
Formula type	N2O3P6Q12	Coefficient 8	9(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000648(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.269(10)	0	0	0	1.043(34)
Na2	4*e*	0.859(35)	0	0.6647(29)	¼	1.043(34)
Na3	8*f*	0.744(21)	0.9207(29)	0.6719(20)	0.8434(19)	1.043(34)
Na4	8*f*	0.275(12)	0.77(75)	0.0906(61)	0.8362(54)	1.043(34)
Zr1	8*f*	1	0.0003(13)	-0.00186(65)	0.14841(84)	1.043(34)
Si/P1**	4*e*	0.8/0.2	0	0.2892(32)	¼	1.043(34)
Si/P2**	8*f*	0.8/0.2	0.4358(31)	0.8589(25)	0.5422(22)	1.043(34)
O1	8*f*	1	0.0126(41)	0.1689(31)	0.2076(29)	1.043(34)
O2	8*f*	1	0.1758(48)	0.4434(24)	0.9808(34)	1.043(34)
O3	8*f*	1	0.3011(36)	0.8686(25)	0.3907(26)	1.043(34)
O4	8*f*	1	0.2652(41)	0.0691(36)	0.2711(31)	1.043(34)
O5	8*f*	1	0.2679(45)	0.6211(26)	0.9296(33)	1.043(34)
O6	8*f*	1	0.4897(46)	0.2937(22)	0.0843(30)	1.043(34)

Structure model *C2/c* – $f^{12}e^2a$

Data-set: NaZr 25 °C (298 K)

Refined crystal data			
Formula sum	$Na_{3.545}Zr_2Si_3O_{12}$	TCH-U	0.1803(55)
Formula weight	540.19	TCH-Y	0.0368(24)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1351(84) Å	Coefficient 0	2276(5)
	b = 9.09662(25) Å	Coefficient 1	-2829(5)
	c = 22.822(12) Å	Coefficient 2	1272(6)
	β = 161.0276(14) °	Coefficient 3	-449(4)
Cell volume	1089.03(81) $Å^3$	Coefficient 4	197(6)
Z	4	Coefficient 5	-92(4)
Density, calculated	3.295 g/cm^3	Coefficient 6	40(5)
Pearson code	mC108	Coefficient 7	-16(4)
Formula type	N2O3P8Q12	Coefficient 8	19(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000614(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.383(11)	0	0	0	0.699(29)
Na2	4*e*	1	0	0.6347(19)	¼	0.699(29)
Na3	8*f*	0.649(11)	0.9488(32)	0.6697(16)	0.8644(22)	0.699(29)
Na4	8*f*	0.122(14)	0.131(13)	0.4562(81)	0.7122(91)	0.699(29)
Na5	8*f*	0.310(14)	0.2642(51)	0.8656(33)	0.1929(38)	0.699(29)
Zr1	8*f*	1	0.99507(53)	0.00134(77)	0.64485(36)	0.699(29)
Si/P1**	4*e*	0.8/0.2	0	0.2974(16)	¼	0.699(29)
Si/P2**	8*f*	0.8/0.2	0.4354(17)	0.8644(13)	0.5416(12)	0.699(29)
O1	8*f*	1	0.2491(28)	0.8942(16)	0.3617(20)	0.699(29)
O2	8*f*	1	0.007(22)	0.206(19)	0.2025(16)	0.699(29)
O3	8*f*	1	0.1803(30)	0.4308(17)	0.98(21)	0.699(29)
O4	8*f*	1	0.3008(27)	0.0503(17)	0.2943(18)	0.699(29)
O5	8*f*	1	0.2608(27)	0.5991(15)	0.9243(20)	0.699(29)
O6	8*f*	1	0.468(32)	0.3051(19)	0.0663(21)	0.699(29)

Data-set: NaZr 77 °C (350 K)

Refined crystal data			
Formula sum	$Na_{3.511}Zr_2Si_3O_{12}$	TCH-U	0.1806(57)
Formula weight	539.40	TCH-Y	0.0332(25)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1469(92) Å	Coefficient 0	2242(5)
	b = 9.09759(26) Å	Coefficient 1	-2688(6)
	c = 22.849(13) Å	Coefficient 2	1127(5)
	β = 161.0334(16)°	Coefficient 3	-409(5)
Cell volume	1090.92(88) $Å^3$	Coefficient 4	183(5)
Z	4	Coefficient 5	-85(5)
Density, calculated	3.284 g/cm^3	Coefficient 6	11(5)
Pearson code	mC108	Coefficient 7	1(4)
Formula type	N2O3P8Q12	Coefficient 8	0(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000619(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.380(12)	0	0	0	0.729(30)
Na2	4*e*	1	0	0.6327(20)	¼	0.729(30)
Na3	8*f*	0.670(11)	0.9512(29)	0.6678(20)	0.8652(20)	0.729(30)
Na4	8*f*	0.180(15)	0.1544(85)	0.5132(77)	0.7265(59)	0.729(30)
Na5	8*f*	0.216(13)	0.235(73)	0.8799(53)	0.1687(54)	0.729(30)
Zr1	8*f*	1	-0.00368(53)	0.00125(66)	0.64562(37)	0.729(30)
Si/P1**	4*e*	0.8/0.2	0	0.2849(19)	¼	0.729(30)
Si/P2**	8*f*	0.8/0.2	0.4411(18)	0.8614(14)	0.546(12)	0.729(30)
O1	8*f*	1	0.2549(30)	0.8898(18)	0.3637(22)	0.729(30)
O2	8*f*	1	-0.0012(22)	0.2077(19)	0.1952(17)	0.729(30)
O3	8*f*	1	0.1895(29)	0.4266(18)	0.9898(21)	0.729(30)
O4	8*f*	1	0.3173(28)	0.0719(21)	0.3061(20)	0.729(30)
O5	8*f*	1	0.2497(31)	0.6173(18)	0.9157(22)	0.729(30)
O6	8*f*	1	0.4775(28)	0.3374(17)	0.0744(19)	0.729(30)

Data-set: NaZr 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{3.659}Zr_2Si_3O_{12}$	TCH-U	0.1569(49)
Formula weight	542.83	TCH-Y	0.0337(21)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.149(11) Å	Coefficient 0	2241(5)
	b = 9.09697(29) Å	Coefficient 1	-2595(6)
	c = 22.874(15) Å	Coefficient 2	1115(6)
	β = 161.0276(18)°	Coefficient 3	-341(5)
Cell volume	1090.50(103) Å^3	Coefficient 4	151(6)
Z	4	Coefficient 5	-70(5)
Density, calculated	3.300 g/cm^3	Coefficient 6	23(6)
Pearson code	mC108	Coefficient 7	2(5)
Formula type	N2O3P8Q12	Coefficient 8	-13(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000618(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å^2]*
			x	***y***	***z***	
Na1	4*a*	0.363(13)	0	0	0	0.687(32)
Na2	4*e*	0.881(24)	0	0.6276(31)	¼	0.687(32)
Na3	8*f*	0.725(14)	0.9403(30)	0.6565(21)	0.8616(21)	0.687(32)
Na4	8*f*	0.206(18)	0.24(10)	0.446(57)	0.8057(72)	0.687(32)
Na5	8*f*	0.276(18)	0.0575(71)	0.7353(53)	0.0702(48)	0.687(32)
Zr1	8*f*	1	-0.00286(75)	0.0027(68)	0.64645(51)	0.687(32)
Si/P1**	4*e*	0.8/0.2	0	0.2914(22)	¼	0.687(32)
Si/P2**	8*f*	0.8/0.2	0.4376(21)	0.8676(17)	0.5459(14)	0.687(32)
O1	8*f*	1	0.2412(38)	0.8792(26)	0.3543(27)	0.687(32)
O2	8*f*	1	0.0031(28)	0.2109(22)	0.1946(21)	0.687(32)
O3	8*f*	1	0.2072(35)	0.429(25)	1.0038(24)	0.687(32)
O4	8*f*	1	0.2863(40)	0.0988(20)	0.2843(28)	0.687(32)
O5	8*f*	1	0.2692(36)	0.6414(17)	0.9263(25)	0.687(32)
O6	8*f*	1	0.4575(37)	0.3455(16)	0.0655(25)	0.687(32)

Data-set: NaZr 177 °C (450 K)

Refined crystal data			
Formula sum	$Na_{3.67}Zr_2Si_3O_{12}$	TCH-U	0.142007(10)
Formula weight	543.06	TCH-Y	0.03639(14)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1611(79) Å	Coefficient 0	2189(5)
	b = 9.095915(25) Å	Coefficient 1	-2550(8)
	c = 22.9062(11) Å	Coefficient 2	1098(7)
	β = 161.0381(13)°	Coefficient 3	-340(7)
Cell volume	1094.14(8) Å^3	Coefficient 4	158(7)
Z	4	Coefficient 5	-78(6)
Density, calculated	3.297 g/cm^3	Coefficient 6	24(6)
Pearson code	mC108	Coefficient 7	-11(5)
Formula type	N2O3P10Q12	Coefficient 8	-12(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.00063(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å^2]*
			x	***y***	***z***	
Na1	4*a*	0.318(13)	0	0	0	0.750(16)
Na2	4*e*	0.889(13)	0	0.6282(11)	¼	0.750(16)
Na3	8*f*	0.7105(81)	0.9474(14)	0.6592(83)	0.8658(10)	0.750(16)
Na4	8*f*	0.1583(86)	0.2275(62)	0.4588(35)	0.7988(44)	0.750(16)
Na5	8*f*	0.2995(96)	0.0512(35)	0.7433(20)	0.066(24)	0.750(16)
Na6	8*f*	0.0630(92)	0.426(19)	0.5751(97)	0.929(13)	0.750(16)
Zr1	8*f*	1	-0.00195(24)	0.00335(27)	0.64698(17)	0.750(16)
Si/P1**	4*e*	0.8/0.2	0	0.2885(73)	¼	0.750(16)
Si/P2**	8*f*	0.8/0.2	0.44101(83)	0.86713(55)	0.5475(58)	0.750(16)
O1	8*f*	1	0.245(16)	0.87714(99)	0.356(11)	0.750(16)
O2	8*f*	1	0.0048(15)	0.20811(99)	0.1953(10)	0.750(16)
O3	8*f*	1	0.2057(15)	0.43238(98)	1.0053(10)	0.750(16)
O4	8*f*	1	0.2838(17)	0.10102(91)	0.2808(12)	0.750(16)
O5	8*f*	1	0.2691(17)	0.6452(85)	0.9282(12)	0.750(16)
O6	8*f*	1	0.4619(17)	0.34428(76)	0.0704(12)	0.750(16)

Data-set: NaZr 217 °C (490 K)

Refined crystal data			
Formula sum	$Na_{3.690}Zr_2Si_3O_{12}$	TCH-U	0.1253(39)
Formula weight	543.52	TCH-Y	0.0377(17)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.172(12) Å	Coefficient 0	2147(5)
	b = 9.09727(38) Å	Coefficient 1	-2481(7)
	c = 22.928(17) Å	Coefficient 2	1004(6)
	β = 161.0525(21) °	Coefficient 3	-302(5)
Cell volume	1095.30(117) $Å^3$	Coefficient 4	130(6)
Z	4	Coefficient 5	-60(5)
Density, calculated	3.296 g/cm^3	Coefficient 6	13(6)
Pearson code	mC108	Coefficient 7	-4(5)
Formula type	N2O3P10Q12	Coefficient 8	-1(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000634(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.248(42)	0	0	0	0.833(34)
Na2	4*e*	0.905(29)	0	0.6313(34)	¼	0.833(34)
Na3	8*f*	0.700(17)	0.9516(41)	0.6631(27)	0.8682(29)	0.833(34)
Na4	8*f*	0.152(18)	0.243(18)	0.5437(85)	0.788(12)	0.833(34)
Na5	8*f*	0.311(20)	0.0391(75)	0.7481(46)	0.0588(50)	0.833(34)
Na6	8*f*	0.105(21)	0.458(38)	0.585(17)	0.965(25)	0.833(34)
Zr1	8*f*	1	-0.0019(12)	0.00399(63)	0.64719(83)	0.833(34)
Si/P1**	4*e*	0.8/0.2	0	0.2863(27)	¼	0.833(34)
Si/P2**	8*f*	0.8/0.2	0.4427(26)	0.8669(19)	0.5484(18)	0.833(34)
O1	8*f*	1	0.2458(50)	0.8755(28)	0.3549(34)	0.833(34)
O2	8*f*	1	0.0076(38)	0.2054(24)	0.1989(26)	0.833(34)
O3	8*f*	1	0.2038(41)	0.4324(29)	0.0047(28)	0.833(34)
O4	8*f*	1	0.2832(46)	0.1024(23)	0.2804(31)	0.833(34)
O5	8*f*	1	0.2689(44)	0.6442(19)	0.9294(30)	0.833(34)
O6	8*f*	1	0.4687(46)	0.3412(19)	0.0735(31)	0.833(34)

Data-set: NaZr 267 °C (540 K)

Refined crystal data			
Formula sum	$Na_{3.735}Zr_2Si_3O_{12}$	TCH-U	0.1077(33)
Formula weight	544.56	TCH-Y	0.0372(16)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.185(11) Å	Coefficient 0	2178(5)
	b = 9.09843(37) Å	Coefficient 1	-2427(7)
	c = 22.951(16) Å	Coefficient 2	1008(6)
	β = 161.0681(19)°	Coefficient 3	-279(5)
Cell volume	1096.54(110) $Å^3$	Coefficient 4	109(6)
Z	4	Coefficient 5	-54(5)
Density, calculated	3.298 g/cm^3	Coefficient 6	34(6)
Pearson code	mC108	Coefficient 7	-3(5)
Formula type	N2O3P10Q12	Coefficient 8	-10(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000637(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	4*a*	0.243(34)	0	0	0	0.876(32)
Na2	4*e*	0.877(31)	0	0.6333(38)	¼	0.876(32)
Na3	8*f*	0.697(19)	0.9504(44)	0.6667(27)	0.8683(31)	0.876(32)
Na4	8*f*	0.161(19)	0.237(17)	0.5642(80)	0.785(12)	0.876(32)
Na5	8*f*	0.333(19)	0.0385(69)	0.7372(42)	0.0591(47)	0.876(32)
Na6	8*f*	0.116(19)	0.478(29)	0.592(14)	0.973(19)	0.876(32)
Zr1	8*f*	1	-0.0017(13)	0.00274(72)	0.6474(89)	0.876(32)
Si/P1**	4*e*	0.8/0.2	0	0.2902(26)	¼	0.876(32)
Si/P2**	8*f*	0.8/0.2	0.4363(26)	0.8669(19)	0.5457(18)	0.876(32)
O1	8*f*	1	0.2463(53)	0.8734(28)	0.3548(37)	0.876(32)
O2	8*f*	1	0.0136(40)	0.2059(24)	0.2032(28)	0.876(32)
O3	8*f*	1	0.2095(42)	0.4322(30)	0.0073(28)	0.876(32)
O4	8*f*	1	0.2843(43)	0.1046(22)	0.2795(29)	0.876(32)
O5	8*f*	1	0.2736(43)	0.6442(19)	0.9325(30)	0.876(32)
O6	8*f*	1	0.4688(46)	0.3409(18)	0.0748(31)	0.876(32)

Data-set: NaZr 317 °C (590 K)

Refined crystal data			
Formula sum	$Na_{3.995}Zr_2Si_3O_{12}$	TCH-U	0.0823(25)
Formula weight	550.53	TCH-Y	0.0391(14)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.1978(97) Å	Coefficient 0	2230(5)
	b = 9.09988(30) Å	Coefficient 1	-2409(6)
	c = 22.972(14) Å	Coefficient 2	973(6)
	β = 161.0827(16)°	Coefficient 3	-254(5)
Cell volume	1097.76(94) $Å^3$	Coefficient 4	119(5)
Z	4	Coefficient 5	-82(5)
Density, calculated	3.331 g/cm^3	Coefficient 6	45(5)
Pearson code	mC108	Coefficient 7	-13(5)
Formula type	N2O3P10Q12	Coefficient 8	5(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000641(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	4*a*	0.155(29)	0	0	0	0.965(33)
Na2	4*e*	0.854(31)	0	0.6292(31)	¼	0.965(33)
Na3	8*f*	0.725(19)	0.9733(39)	0.6651(23)	0.8799(25)	0.965(33)
Na4	8*f*	0.180(21)	0.241(16)	0.5642(71)	0.746(11)	0.965(33)
Na5	8*f*	0.356(20)	0.0528(59)	0.769(34)	0.0639(38)	0.965(33)
Na6	8*f*	0.232(14)	0.659(12)	0.5347(73)	1.0923(78)	0.965(33)
Zr1	8*f*	1	0(13)	0.00532(53)	0.64841(88)	0.965(33)
Si/P1**	4*e*	0.8/0.2	0	0.2791(26)	¼	0.965(33)
Si/P2**	8*f*	0.8/0.2	0.4474(24)	0.8642(19)	0.5508(16)	0.965(33)
O1	8*f*	1	0.2567(51)	0.8687(28)	0.3649(35)	0.965(33)
O2	8*f*	1	0.0221(38)	0.1987(25)	0.2047(25)	0.965(33)
O3	8*f*	1	0.2152(41)	0.4351(28)	0.0133(26)	0.965(33)
O4	8*f*	1	0.2858(43)	0.1042(27)	0.2791(28)	0.965(33)
O5	8*f*	1	0.2322(47)	0.6463(18)	0.9082(31)	0.965(33)
O6	8*f*	1	0.4532(38)	0.3474(18)	0.068(26)	0.965(33)

Data-set: NaZr 367 °C (640 K)

Refined crystal data			
Formula sum	$Na_{4.059}Zr_2Si_3O_{12}$	TCH-U	0.0670(21)
Formula weight	552.01	TCH-Y	0.0395(13)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C2/c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.2086(91) Å	Coefficient 0	2232(5)
	b = 9.10097(28) Å	Coefficient 1	-2442(7)
	c = 22.991(13) Å	Coefficient 2	925(6)
	β = 161.096(15)°	Coefficient 3	-244(5)
Cell volume	1098.77(88) $Å^3$	Coefficient 4	114(5)
Z	4	Coefficient 5	-83(5)
Density, calculated	3.337 g/cm^3	Coefficient 6	39(5)
Pearson code	mC108	Coefficient 7	-15(5)
Formula type	N2O3P10Q12	Coefficient 8	-2(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000636(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	4*a*	0.172(26)	0	0	0	0.965(33)
Na2	4*e*	0.827(34)	0	0.6311(33)	¼	0.965(33)
Na3	8*f*	0.737(19)	0.9727(38)	0.6662(23)	0.8804(25)	0.965(33)
Na4	8*f*	0.195(22)	0.242(14)	0.5617(61)	0.7532(92)	0.965(33)
Na5	8*f*	0.367(20)	0.0496(57)	0.7672(34)	0.0624(38)	0.965(33)
Na6	8*f*	0.231(14)	0.661(11)	0.5375(68)	0.0908(76)	0.965(33)
Zr1	8*f*	1	0(14)	0.00484(57)	0.64838(91)	0.965(33)
Si/P1**	4*e*	0.8/0.2	0	0.2797(26)	¼	0.965(33)
Si/P2**	8*f*	0.8/0.2	0.4455(24)	0.8637(20)	0.5496(16)	0.965(33)
O1	8*f*	1	0.2557(51)	0.8668(28)	0.3652(35)	0.965(33)
O2	8*f*	1	0.0211(40)	0.1978(25)	0.2047(26)	0.965(33)
O3	8*f*	1	0.216(42)	0.4343(29)	0.0128(27)	0.965(33)
O4	8*f*	1	0.2845(42)	0.104(27)	0.2787(28)	0.965(33)
O5	8*f*	1	0.2319(49)	0.6466(18)	0.9089(32)	0.965(33)
O6	8*f*	1	0.4512(38)	0.3471(17)	0.0688(26)	0.965(33)

2. Rietveld refinement results of six different structure models used for each dataset for $Na_{3.4}Sc_{0.4}Zr_{1.6}Si_2PO_{12}$ (NaSc) sample

*isotropic displacement parameter calculated in HighScore according to $F_{hkl} = F_0 \times \exp[-B_{iso} \times (Q/4\pi)^2]$
**Refinements were carried out using only Si^{4+} atom form factors with site occupancy of 1 for the mixed Si/P site. For X-rays Si^{4+} and P^{5+} are nearly identical, but for P^{5+} no atom form factor is reported in literature and thus it would introduce a much larger error to the refinement when mixing the Si^{4+} form factor, with the P^0 form factor function when applying a mixed site occupancy. The mixed site occupancy is calculated manually from the nominal sample composition. It was not used in the refinements.

Structure model $R\bar{3}c$ - f^2e^2cb

Data-set: NaSc 25 °C (298 K)

Refined crystal data		TCH-U	0.341(12)
Formula sum	$Na_{2.585}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0394(39)
Formula weight	501.46	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2222(8)
Lattice parameters	*a* = 9.07297(34) Å	Coefficient 1	-2290(1)
	c = 22.71875(91) Å	Coefficient 2	910(1)
		Coefficient 3	-140(1)
		Coefficient 4	-150(1)
Cell volume	1619.62(14) $Å^3$	Coefficient 5	196(10)
Z	6	Coefficient 6	-189(10)
Density, calculated	3.085 g/cm^3	Coefficient 7	100(1)
Pearson code	hR42	Coefficient 8	-33(9)
Formula type	N2O3P4Q12	Coefficient 9	-18(9)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000261(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*iso [Å²]***
			x	***y***	***z***	
Na1	6*b*	0.494(16)	0	0	0	0.573(48)
Na2	18*e*	0.6968(63)	0.6399(10)	0	¼	0.573(48)
Zr1	12*c*	0.82	0	0	0.14824(10)	0.573(48)
Sc1	12*c*	0.18	0	0	0.14824(10)	0.573(48)
Si/P1**	18*e*	0.8/0.2	0.2889(59)	0	¼	0.573(48)
O1	36*f*	1	0.18808(78)	0.97753(91)	0.19354(31)	0.573(48)
O2	36*f*	1	0.1909(60)	0.16626(71)	0.08402(43)	0.573(48)

Data-set: NaSc 77 °C (350 K)

Refined crystal data		TCH-U	0.1432(43)
Formula sum	$Na_{2.635}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0422(21)
Formula weight	502.63	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2134(6)
Lattice parameters	*a* = 9.07329(18) Å	Coefficient 1	-2110(10)
	c = 22.73119(49) Å	Coefficient 2	787(8)
		Coefficient 3	-75(8)
		Coefficient 4	-149(8)
Cell volume	1620.62(7) $Å^3$	Coefficient 5	178(8)
Z	6	Coefficient 6	-167(7)
Density, calculated	3.090 g/cm^3	Coefficient 7	79(8)
Pearson code	hR42	Coefficient 8	-48(6)
Formula type	N2O3P4Q12	Coefficient 9	-33(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000265(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*iso [Å²]***
			x	***y***	***z***	
Na1	6*b*	0.494(11)	0	0	0	0.659(33)
Na2	18*e*	0.7136(43)	0.64123(68)	0	¼	0.659(33)
Zr1	12*c*	0.82	0	0	0.148027(71)	0.659(33)
Sc1	12*c*	0.18	0	0	0.148027(71)	0.659(33)
Si/P1**	18*e*	0.8/0.2	0.29005(41)	0	¼	0.659(33)
O1	36*f*	1	0.18495(52)	0.9749(62)	0.19419(21)	0.659(33)
O2	36*f*	1	0.1915(42)	0.16897(49)	0.0856(29)	0.659(33)

Data-set: NaSc 127 °C (400 K)

Refined crystal data		TCH-U	0.0945(31)
Formula sum	$Na_{2.612}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0432(18)
Formula weight	502.09	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2149(6)
Lattice parameters	*a* = 9.07255(15) Å	Coefficient 1	-1974(9)
	c = 22.75715(42) Å	Coefficient 2	722(8)
		Coefficient 3	-50(8)
		Coefficient 4	-151(8)
Cell volume	1622.21(6) $Å^3$	Coefficient 5	154(7)
Z	6	Coefficient 6	-160(7)
Density, calculated	3.084 g/cm^3	Coefficient 7	76(8)
Pearson code	hR42	Coefficient 8	-20(6)
Formula type	N2O3P4Q12	Coefficient 9	-36(6)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000268(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	6*b*	0.4671(99)	0	0	0	0.738(33)
Na2	18*e*	0.715(42)	0.64175(65)	0	¼	0.738(33)
Zr1	12*c*	0.82	0	0	0.148011(68)	0.738(33)
Sc1	12*c*	0.18	0	0	0.148011(68)	0.738(33)
Si/P1**	18*e*	0.8/0.2	0.29013(39)	0	¼	0.738(33)
O1	36*f*	1	0.1825(50)	0.97263(59)	0.19411(20)	0.738(33)
O2	36*f*	1	0.19186(40)	0.17122(47)	0.08542(27)	0.738(33)

Structure model $R\bar{3}c$ – f^3e^2cb

Data-set: NaSc 25 °C (298 K)

Refined crystal data		TCH-U	0.335(11)
Formula sum	$Na_{2.956}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0398(37)
Formula weight	510.00	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2222(8)
Lattice parameters	*a* = 9.07331(32) Å	Coefficient 1	-2300(1)
	c = 22.718(87) Å	Coefficient 2	910(1)
		Coefficient 3	-158(10)
		Coefficient 4	-160(10)
Cell volume	1619.69(13) $Å^3$	Coefficient 5	201(10)
Z	6	Coefficient 6	-202(9)
Density, calculated	3.137 g/cm^3	Coefficient 7	113(10)
Pearson code	hR54	Coefficient 8	-42(8)
Formula type	N2O3P10Q12	Coefficient 9	-15(8)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000268(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	6*b*	0.511(15)	0	0	0	0.578(46)
Na2	18*e*	0.409(26)	0.6325(24)	0	¼	0.578(46)
Na3	36*f*	0.203(13)	0.6608(40)	0.6923(43)	0.0462(17)	0.578(46)
Zr1	12*c*	0.82	0	0	0.14894(10)	0.578(46)
Sc1	12*c*	0.18	0	0	0.14894(10)	0.578(46)
Si/P1**	18*e*	0.8/0.2	0.29198(58)	0	¼	0.578(46)
O1	36*f*	1	0.18258(74)	0.97427(87)	0.19335(32)	0.578(46)
O2	36*f*	1	0.19176(57)	0.16675(66)	0.08316(43)	0.578(46)

Data-set: NaSc 77 °C (350 K)

Refined crystal data		TCH-U	0.1455(40)
Formula sum	$Na_{3.029}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0414(20)
Formula weight	511.67	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2147(5)
Lattice parameters	*a* = 9.07344(16) Å	Coefficient 1	-2131(9)
	c = 22.73067(45) Å	Coefficient 2	801(7)
		Coefficient 3	-89(7)
		Coefficient 4	-150(7)
Cell volume	1620.64(7) $Å^3$	Coefficient 5	186(7)
Z	6	Coefficient 6	-185(7)
Density, calculated	3.145 g/cm^3	Coefficient 7	99(7)
Pearson code	hR54	Coefficient 8	-66(6)
Formula type	N2O3P10Q12	Coefficient 9	-20(6)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000271(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*iso [Å²]***
			x	***y***	***z***	
Na1	6*b*	0.4966(96)	0	0	0	0.690(31)
Na2	18*e*	0.440(19)	0.6337(16)	0	¼	0.690(31)
Na3	36*f*	0.2022(93)	0.6929(25)	0.716(28)	0.0489(13)	0.690(31)
Zr1	12*c*	0.82	0	0	0.148619(71)	0.690(31)
Sc1	12*c*	0.18	0	0	0.148619(71)	0.690(31)
Si/P1**	18*e*	0.8/0.2	0.29356(41)	0	¼	0.690(31)
O1	36*f*	1	0.18062(49)	0.97327(58)	0.19503(22)	0.690(31)
O2	36*f*	1	0.19217(39)	0.16835(45)	0.08614(28)	0.690(31)

Data-set: NaSc 127 °C (400 K)

Refined crystal data		TCH-U	0.0971(29)
Formula sum	$Na_{2.995}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0424(17)
Formula weight	510.90	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	2159(5)
Lattice parameters	*a* = 9.07267(13) Å	Coefficient 1	-1984(9)
	c = 22.75667(39) Å	Coefficient 2	730(7)
		Coefficient 3	-58(7)
		Coefficient 4	-151(7)
Cell volume	1622.22(5) $Å^3$	Coefficient 5	161(7)
Z	6	Coefficient 6	-174(7)
Density, calculated	3.138 g/cm^3	Coefficient 7	95(7)
Pearson code	hR54	Coefficient 8	-36(6)
Formula type	N2O3P10Q12	Coefficient 9	-23(6)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000274(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			***B*iso [Å²]***
			x	***y***	***z***	
Na1	6*b*	0.4696(89)	0	0	0	0.780(30)
Na2	18*e*	0.425(21)	0.6383(17)	0	¼	0.780(30)
Na3	36*f*	0.2085(98)	0.6934(24)	0.7206(26)	0.0507(13)	0.780(30)
Zr1	12*c*	0.82	0	0	0.148584(68)	0.780(30)
Sc1	12*c*	0.18	0	0	0.148584(68)	0.780(30)
Si/P1**	18*e*	0.8/0.2	0.29343(40)	0	¼	0.780(30)
O1	36*f*	1	0.17879(46)	0.97118(54)	0.19504(21)	0.780(30)
O2	36*f*	1	0.19235(37)	0.17045(43)	0.08612(27)	0.780(30)

Structure model *C*2/*c* - f^9e^2a

Data-set: NaSc 25 °C (298 K)

Refined crystal data			
Formula sum	$Na_{2.802}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-U	0.1029(37)
Formula weight	506.45	TCH-Y	0.0362(22)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.0559(73) Å	Coefficient 0	2234(5)
	b = 9.07466(22) Å	Coefficient 1	-2308(8)
	c = 22.718(10) Å	Coefficient 2	922(6)
	β = 160.9562(12)°	Coefficient 3	-153(6)
		Coefficient 4	-149(6)
Cell volume	1080.01(69) $Å^3$	Coefficient 5	204(6)
Z	4	Coefficient 6	-204(6)
Density, calculated	3.115 g/cm^3	Coefficient 7	129(6)
Pearson code	mC84	Coefficient 8	-53(5)
Formula type	N2O3P4Q12	Coefficient 9	3(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000581(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [$Å^2$]*
			x	***y***	***z***	
Na1	4*a*	0.545(10)	0	0	0	0.567(30)
Na2	4*e*	0.824(19)	0	0.6477(21)	¼	0.567(30)
Na3	8*f*	0.716(11)	0.9374(24)	0.6755(16)	0.8571(18)	0.567(30)
Zr1	8*f*	0.82	-0.00499(57)	0.00129(75)	0.64477(39)	0.567(30)
Sc1	8*f*	0.18	-0.00499(57)	0.00129(75)	0.64477(39)	0.567(30)
Si/P1**	4*e*	0.8/0.2	0	0.2816(17)	¼	0.567(30)
Si/P2**	8*f*	0.8/0.2	0.4486(17)	0.8588(13)	0.5516(12)	0.567(30)
O1	8*f*	1	0.2328(26)	0.8796(20)	0.349(19)	0.567(30)
O2	8*f*	1	0.0318(22)	0.2211(16)	0.22(16)	0.567(30)
O3	8*f*	1	0.1898(29)	0.417(17)	0.9853(20)	0.567(30)
O4	8*f*	1	0.3025(35)	0.0872(19)	0.2955(25)	0.567(30)
O5	8*f*	1	0.2503(33)	0.6192(18)	0.917(22)	0.567(30)
O6	8*f*	1	0.4612(29)	0.3378(16)	0.0585(20)	0.567(30)

Data-set: NaSc 77 °C (350 K)

Refined crystal data			
Formula sum	$Na_{2.814}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-U	0.0932(34)
Formula weight	506.73	TCH-Y	0.0385(19)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.05(1) Å	Coefficient 0	2136(5)
	b = 9.07412(31) Å	Coefficient 1	-2145(8)
	c = 22.732(15) Å	Coefficient 2	813(7)
	β = 160.9504(18)°	Coefficient 3	-87(7)
		Coefficient 4	-144(6)
Cell volume	1080.55(98) $Å^3$	Coefficient 5	193(7)
Z	4	Coefficient 6	-184(6)
Density, calculated	3.155 g/cm^3	Coefficient 7	116(7)
Pearson code	mC84	Coefficient 8	-71(6)
Formula type	N2O3P4Q12	Coefficient 9	-8(5)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000589(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [$Å^2$]*
			x	***y***	***z***	
Na1	4*a*	0.515(10)	0	0	0	0.522(32)
Na2	4*e*	0.829(24)	0	0.6445(27)	¼	0.522(32)
Na3	8*f*	0.735(14)	0.9334(28)	0.6669(19)	0.8536(20)	0.522(32)
Zr1	8*f*	0.82	-0.00493(81)	0.00164(75)	0.64473(55)	0.522(32)
Sc1	8*f*	0.18	-0.00493(81)	0.00164(75)	0.64473(55)	0.522(32)
Si/P1**	4*e*	0.8/0.2	0	0.2799(21)	¼	0.522(32)
Si/P2**	8*f*	0.8/0.2	0.446(22)	0.851(19)	0.5479(15)	0.522(32)
O1	8*f*	1	0.2442(34)	0.8802(24)	0.3542(24)	0.522(32)
O2	8*f*	1	0.0342(32)	0.2166(21)	0.2205(23)	0.522(32)
O3	8*f*	1	0.1959(36)	0.4189(21)	0.9946(25)	0.522(32)
O4	8*f*	1	0.2788(43)	0.1008(20)	0.2805(29)	0.522(32)
O5	8*f*	1	0.2466(37)	0.6318(18)	0.9145(25)	0.522(32)
O6	8*f*	1	0.4586(37)	0.3401(17)	0.0577(26)	0.522(32)

Data-set: NaSc 127 °C (400 K)

Refined crystal data		TCH-U	0.072(27)
Formula sum	$Na_{2.758}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0404(16)
Formula weight	505.44	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2142(5)
Lattice parameters	*a* = 16.061(10) Å	Coefficient 1	-1993(9)
	b = 9.07522(33) Å	Coefficient 2	739(7)
	c = 22.759(14) Å	Coefficient 3	-54(7)
	β = 160.9722(17)°	Coefficient 4	-151(7)
Cell volume	1081.54(97) Å^3	Coefficient 5	163(7)
Z	4	Coefficient 6	-175(6)
Density, calculated	3.104 g/cm^3	Coefficient 7	105(7)
Pearson code	mC84	Coefficient 8	-42(6)
Formula type	N2O3P4Q12	Coefficient 9	-17(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000595(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å^2]*
			x	***y***	***z***	
Na1	4*a*	0.4538(97)	0	0	0	0.582(32)
Na2	4*e*	0.578(28)	0	0.6414(50)	¼	0.582(32)
Na3	8*f*	0.863(15)	0.937(29)	0.6701(19)	0.8574(20)	0.582(32)
Zr1	8*f*	0.82	0.99503(97)	0.00174(91)	0.64473(66)	0.582(32)
Sc1	8*f*	0.18	0.99503(97)	0.00174(91)	0.64473(66)	0.582(32)
Si/P1**	4*e*	0.8/0.2	0	0.2815(24)	¼	0.582(32)
Si/P2**	8*f*	0.8/0.2	0.4462(24)	0.8524(20)	0.5494(16)	0.582(32)
O1	8*f*	1	0.2821(46)	0.8561(21)	0.3863(30)	0.582(32)
O2	8*f*	1	0.0364(38)	0.1979(30)	0.2162(26)	0.582(32)
O3	8*f*	1	0.2277(38)	0.4209(21)	0.014(25)	0.582(32)
O4	8*f*	1	0.2672(42)	0.0991(22)	0.2716(28)	0.582(32)
O5	8*f*	1	0.2364(39)	0.6319(20)	0.9038(25)	0.582(32)
O6	8*f*	1	0.4607(40)	0.3311(25)	0.0602(27)	0.582(32)

Structure model *C*2/*c* – $f^{10}e^2a$

Data-set: NaSc 25 °C (298 K)

Refined crystal data		TCH-U	0.0988(35)
Formula sum	$Na_{3.112}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0363(21)
Formula weight	513.59	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2244(5)
Lattice parameters	*a* = 16.0559(73) Å	Coefficient 1	-2290(7)
	b = 9.07434(22) Å	Coefficient 2	930(6)
	c = 22.718(10) Å	Coefficient 3	-146(6)
	β = 160.9571(12)°	Coefficient 4	-142(6)
Cell volume	1079.95(69) Å^3	Coefficient 5	210(6)
Z	4	Coefficient 6	-198(6)
Density, calculated	3.159 g/cm^3	Coefficient 7	133(6)
Pearson code	mC92	Coefficient 8	-55(5)
Formula type	N2O3P6Q12	Coefficient 9	5(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000591(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å^2]*
			x	***y***	***z***	
Na1	4*a*	0.451(14)	0	0	0	0.678(30)
Na2	4*e*	0.935(18)	0	0.6503(18)	¼	0.678(30)
Na3	8*f*	0.663(11)	0.9394(27)	0.6758(17)	0.8588(19)	0.678(30)
Na4	8*f*	0.2(11)	0.2398(90)	0.545(45)	0.804(64)	0.678(30)
Zr1	8*f*	1	-0.00496(55)	0.0014(74)	0.64474(38)	0.678(30)
Sc1	8*f*	1	-0.00496(55)	0.0014(74)	0.64474(38)	0.678(30)
Si/P1**	4*e*	0.8/0.2	0	0.285(17)	¼	0.678(30)
Si/P2**	8*f*	0.8/0.2	0.4438(17)	0.8599(13)	0.5484(12)	0.678(30)
O1	8*f*	1	0.248(27)	0.8815(21)	0.3583(20)	0.678(30)
O2	8*f*	1	0.0158(22)	0.2144(18)	0.2066(17)	0.678(30)
O3	8*f*	1	0.186(30)	0.4205(18)	0.9857(21)	0.678(30)
O4	8*f*	1	0.3018(33)	0.0843(20)	0.297(23)	0.678(30)
O5	8*f*	1	0.2375(30)	0.6164(18)	0.9065(21)	0.678(30)
O6	8*f*	1	0.4606(27)	0.3391(15)	0.0617(19)	0.678(30)

Data-set: NaSc 77 °C (350 K)

Refined crystal data		TCH-U	0.0871(31)
Formula sum	$Na_{3.051}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0377(18)
Formula weight	512.19	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2139(5)
Lattice parameters	*a* = 16.052(10) Å	Coefficient 1	-2158(8)
	b = 9.07323(28) Å	Coefficient 2	809(7)
	c = 22.733(14) Å	Coefficient 3	-89(6)
	β = 160.9515(18)°	Coefficient 4	-147(6)
Cell volume	1080.56(98) $Å^3$	Coefficient 5	193(6)
Z	4	Coefficient 6	-193(6)
Density, calculated	3.148 g/cm^3	Coefficient 7	121(6)
Pearson code	mC92	Coefficient 8	-85(5)
Formula type	N2O3P6Q12	Coefficient 9	-6(5)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000577(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.407(15)	0	0	0	0.469(30)
Na2	4*e*	0.948(24)	0	0.6396(26)	¼	0.469(30)
Na3	8*f*	0.659(14)	0.932(32)	0.6648(21)	0.8532(22)	0.469(30)
Na4	8*f*	0.189(11)	0.257(94)	0.5193(74)	0.8216(64)	0.469(30)
Zr1	8*f*	1	0.99504(73)	0.00173(90)	0.64473(50)	0.469(30)
Sc1	8*f*	1	0.99504(73)	0.00173(90)	0.64473(50)	0.469(30)
Si/P1**	4*e*	0.8/0.2	0	0.2859(23)	¼	0.469(30)
Si/P2**	8*f*	0.8/0.2	0.4476(19)	0.8618(17)	0.5503(13)	0.469(30)
O1	8*f*	1	0.2596(39)	0.8761(28)	0.3649(28)	0.469(30)
O2	8*f*	1	0.019(31)	0.2093(25)	0.2057(23)	0.469(30)
O3	8*f*	1	0.1953(38)	0.4241(25)	0.9949(26)	0.469(30)
O4	8*f*	1	0.2859(43)	0.089(25)	0.2889(30)	0.469(30)
O5	8*f*	1	0.2503(38)	0.6238(20)	0.9147(26)	0.469(30)
O6	8*f*	1	0.4674(36)	0.3378(20)	0.0674(25)	0.469(30)

Data-set: NaSc 127 °C (400 K)

Refined crystal data		TCH-U	0.0724(26)
Formula sum	$Na_{3.12}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0387(16)
Formula weight	513.76	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2151(5)
Lattice parameters	*a* = 16.063(10) Å	Coefficient 1	-1986(8)
	b = 9.07418(32) Å	Coefficient 2	745(7)
	c = 22.759(14) Å	Coefficient 3	-50(7)
	β = 160.9723(18)°	Coefficient 4	-147(7)
Cell volume	1081.52(98) $Å^3$	Coefficient 5	174(6)
Z	4	Coefficient 6	-175(6)
Density, calculated	3.155 g/cm^3	Coefficient 7	111(7)
Pearson code	mC92	Coefficient 8	-45(6)
Formula type	N2O3P6Q12	Coefficient 9	-17(6)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000603(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.358(14)	0	0	0	0.673(31)
Na2	4*e*	0.778(25)	0	0.6498(32)	¼	0.673(31)
Na3	8*f*	0.778(15)	0.9331(28)	0.6673(20)	0.8542(19)	0.673(31)
Na4	8*f*	0.213(11)	0.2837(82)	0.5332(54)	0.8327(58)	0.673(31)
Zr1	8*f*	1	-0.00497(88)	0.00174(88)	0.64473(60)	0.673(31)
Sc1	8*f*	1	-0.00497(88)	0.00174(88)	0.64473(60)	0.673(31)
Si/P1**	4*e*	0.8/0.2	0	0.2841(25)	¼	0.673(31)
Si/P2**	8*f*	0.8/0.2	0.4447(23)	0.8557(23)	0.548(16)	0.673(31)
O1	8*f*	1	0.2775(42)	0.8655(23)	0.378(29)	0.673(31)
O2	8*f*	1	0.0237(35)	0.1985(28)	0.2088(24)	0.673(31)
O3	8*f*	1	0.2099(39)	0.4226(23)	1.0062(26)	0.673(31)
O4	8*f*	1	0.2755(44)	0.0945(24)	0.2796(30)	0.673(31)
O5	8*f*	1	0.2339(37)	0.6333(17)	0.9033(25)	0.673(31)
O6	8*f*	1	0.4705(41)	0.3347(22)	0.0708(27)	0.673(31)

Structure model *C*2/*c* – $f^{12}e^2a$

Data-set: NaSc 25 °C (298 K)

Refined crystal data		TCH-U	0.0986(35)
Formula sum	$Na_{3.333}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.036(21)
Formula weight	518.67	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2242(5)
Lattice parameters	*a* = 16.0563(71) Å	Coefficient 1	-2291(7)
	b = 9.07449(21) Å	Coefficient 2	932(6)
	c = 22.719(10) Å	Coefficient 3	-143(6)
	β = 160.9575(12)°	Coefficient 4	-139(6)
Cell volume	1080.02(68) $Å^3$	Coefficient 5	214(6)
Z	4	Coefficient 6	-195(5)
Density, calculated	3.190 g/cm^3	Coefficient 7	139(6)
Pearson code	mC108	Coefficient 8	-55(5)
Formula type	N2O3P8Q12	Coefficient 9	8(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000591(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.458(14)	0	0	0	0.658(30)
Na2	4*e*	0.928(18)	0	0.6473(19)	¼	0.658(30)
Na3	8*f*	0.657(12)	0.9515(30)	0.6778(19)	0.8662(21)	0.658(30)
Na4	8*f*	0.171(15)	0.1645(91)	0.5431(56)	0.7251(64)	0.658(30)
Na5	8*f*	0.145(13)	0.192(11)	0.9098(72)	0.117(75)	0.658(30)
Zr1	8*f*	1	-0.00497(58)	0.00167(66)	0.64473(40)	0.658(30)
Sc1	8*f*	1	-0.00497(58)	0.00167(66)	0.64473(40)	0.658(30)
Si/P1**	4*e*	0.8/0.2	0	0.2801(16)	¼	0.658(30)
Si/P2**	8*f*	0.8/0.2	0.4468(17)	0.8578(13)	0.55(12)	0.658(30)
O1	8*f*	1	0.2446(27)	0.8797(20)	0.3571(20)	0.658(30)
O2	8*f*	1	0.0113(23)	0.2153(17)	0.2023(17)	0.658(30)
O3	8*f*	1	0.1899(29)	0.4163(18)	0.9892(21)	0.658(30)
O4	8*f*	1	0.3042(34)	0.0851(21)	0.2996(24)	0.658(30)
O5	8*f*	1	0.2323(29)	0.6182(20)	0.9058(21)	0.658(30)
O6	8*f*	1	0.4616(25)	0.3436(13)	0.0616(17)	0.658(30)

Data-set: NaSc 77 °C (350 K)

Refined crystal data		TCH-U	0.0901(32)
Formula sum	$Na_{3.287}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0368(18)
Formula weight	517.60	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2148(5)
Lattice parameters	*a* = 16.0514(99) Å	Coefficient 1	-2134(8)
	b = 9.07344(27) Å	Coefficient 2	822(7)
	c = 22.733(14) Å	Coefficient 3	-78(6)
	β = 160.9519(17)°	Coefficient 4	-140(6)
Cell volume	1080.52(95) $Å^3$	Coefficient 5	202(6)
Z	4	Coefficient 6	-182(6)
Density, calculated	3.182 g/cm^3	Coefficient 7	125(6)
Pearson code	mC108	Coefficient 8	-73(5)
Formula type	N2O3P8Q12	Coefficient 9	-6(5)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.000595(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.412(14)	0	0	0	0.606(30)
Na2	4*e*	0.907(24)	0	0.6458(25)	¼	0.606(30)
Na3	8*f*	0.699(14)	0.939(32)	0.6639(21)	0.8579(22)	0.606(30)
Na4	8*f*	0.106(15)	0.237(16)	0.518(12)	0.778(12)	0.606(30)
Na5	8*f*	0.179(15)	0.2463(99)	1.0422(60)	0.1636(71)	0.606(30)
Zr1	8*f*	1	-0.00491(73)	0.0017(81)	0.64472(50)	0.606(30)
Sc1	8*f*	1	-0.00491(73)	0.0017(81)	0.64472(50)	0.606(30)
Si/P1**	4*e*	0.8/0.2	0	0.287(24)	¼	0.606(30)
Si/P2**	8*f*	0.8/0.2	0.4438(21)	0.8593(19)	0.5467(15)	0.606(30)
O1	8*f*	1	0.2564(35)	0.8759(26)	0.3638(25)	0.606(30)
O2	8*f*	1	0.0186(29)	0.2119(22)	0.2063(21)	0.606(30)
O3	8*f*	1	0.2033(38)	0.4202(22)	1.0006(26)	0.606(30)
O4	8*f*	1	0.2882(40)	0.0973(23)	0.2902(28)	0.606(30)
O5	8*f*	1	0.2348(36)	0.6294(20)	0.9061(25)	0.606(30)
O6	8*f*	1	0.4606(32)	0.3429(16)	0.0645(22)	0.606(30)

Data-set: NaSc 127 °C (400 K)

Refined crystal data		TCH-U	0.0729(26)
Formula sum	$Na_{3.981}Zr_{1.64}Sc_{0.36}Si_3O_{12}$	TCH-Y	0.0384(16)
Formula weight	533.56	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	2150(5)
Lattice parameters	*a* = 16.063(10) Å	Coefficient 1	-2003(8)
	b = 9.07471(31) Å	Coefficient 2	744(7)
	c = 22.76(14) Å	Coefficient 3	-57(7)
	β = 160.9743(17)°	Coefficient 4	-157(6)
Cell volume	1081.58(97) $Å^3$	Coefficient 5	172(6)
Z	4	Coefficient 6	-174(6)
Density, calculated	3.276 g/cm^3	Coefficient 7	111(7)
Pearson code	mC108	Coefficient 8	-59(6)
Formula type	N2O3P10Q12	Coefficient 9	-10(6)
Wyckoff sequence	$f^{12}e^2a$	Scale Factor	0.0006(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [$Å^2$]*
			x	***y***	***z***	
Na1	4*a*	0.384(14)	0	0	0	0.646(31)
Na2	4*e*	0.806(30)	0	0.6523(31)	¼	0.646(31)
Na3	8*f*	0.802(16)	0.9317(29)	0.6649(18)	0.8573(20)	0.646(31)
Na4	8*f*	0.228(18)	0.503(11)	0.8873(55)	0.8688(78)	0.646(31)
Na5	8*f*	0.193(13)	0.1991(91)	0.9641(64)	0.1646(65)	0.646(31)
Na6	8*f*	0.173(19)	0.381(12)	0.7415(67)	0.8879(80)	0.646(31)
Zr1	8*f*	1	-0.00498(89)	0.00173(94)	0.64473(61)	0.646(31)
Sc1	8*f*	1	-0.00498(89)	0.00173(94)	0.64473(61)	0.646(31)
Si/P1**	4*e*	0.8/0.2	0	0.2803(27)	¼	0.646(31)
Si/P2**	8*f*	0.8/0.2	0.4414(23)	0.8571(23)	0.5458(15)	0.646(31)
O1	8*f*	1	0.2613(45)	0.8706(26)	0.3642(31)	0.646(31)
O2	8*f*	1	0.019(35)	0.1985(33)	0.2066(24)	0.646(31)
O3	8*f*	1	0.2236(40)	0.4274(26)	0.0147(27)	0.646(31)
O4	8*f*	1	0.2726(43)	0.0983(24)	0.28(30)	0.646(31)
O5	8*f*	1	0.2498(41)	0.6286(20)	0.9124(27)	0.646(31)
O6	8*f*	1	0.4671(43)	0.3307(25)	0.0687(29)	0.646(31)

3. Rietveld refinement results of six different structure models used for each dataset for $Na_{3.4}Al_{0.2}Y_{0.2}Zr_{1.6}Si_2PO_{12}$ (NaAlY) sample

*isotropic displacement parameter calculated in HighScore according to $F_{hkl} = F_0 \times \exp[-B_{iso} \times (Q/4\pi)^2]$
**Refinements were carried out using only Si^{4+} atom form factors with site occupancy of 1 for the mixed Si/P site. For X-rays Si^{4+} and P^{5+} are nearly identical, but for P^{5+} no atom form factor is reported in literature and thus it would introduce a much larger error to the refinement when mixing the Si^{4+} form factor, with the P^0 form factor function when applying a mixed site occupancy. The mixed site occupancy is calculated manually from the nominal sample composition. It was not used in the refinements.

Structure model $R\bar{3}c$ - f^2e^2cb

Data-set: NaAlY 25 °C (298 K)

Refined crystal data		TCH-U	0.832(39)
Formula sum	$Na_{2.742}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-Y	0.0883(76)
Formula weight	508.41	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	1865(10)
Lattice parameters	*a* = 9.09096(74) Å	Coefficient 1	-1710(1)
	c = 22.8737(20) Å	Coefficient 2	950(1)
		Coefficient 3	-290(1)
		Coefficient 4	100(1)
Cell volume	1637.14(30) $Å^3$	Coefficient 5	-25(10)
Z	6	Coefficient 6	-5(10)
Density, calculated	3.094 g/cm^3	Coefficient 7	-60(1)
Pearson code	hR42	Coefficient 8	62(9)
Formula type	N2O3P4Q12	Coefficient 9	-86(9)
Wyckoff sequence	f^2e^2cb	Scale Factor	0.000203(10)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [$Å^2$]***
			x	***y***	***z***	
Na1	6*b*	0.475(22)	0	0	0	0.622(79)
Na2	18*e*	0.755(10)	0.618(14)	0	¼	0.622(79)
Zr1	12*c*	0.8	0	0	0.14987(14)	0.622(79)
Y1	12*c*	0.1	0	0	0.14987(14)	0.622(79)
Al1	12*c*	0.1	0	0	0.14987(14)	0.622(79)
Si/P1**	18*e*	0.8/0.2	0.28063(86)	0	¼	0.622(79)
O1	36*f*	1	0.2084(11)	0.993(13)	0.19809(46)	0.622(79)
O2	36*f*	1	0.18662(77)	0.1375(11)	0.08051(52)	0.622(79)

ZrO_2 impurity (7.5%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001182(48)
Lattice parameters:	
a [Å]	5.1488(31)
b [Å]	5.2362(35)
c [Å]	5.3111(35)
β [°]	99.0324(95)
TCH Y Left	0.247(15)

Data-set: NaAlY 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{2.837}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.484(23)
Formula weight	510.61	TCH-Y	0.0924(56)
Crystal system	trigonal	FCJ-S/L	0.027861
Space group	*R* -3 c (no. 167)	FCJ-D/L	0.027861
Lattice parameters	*a* = 9.09661(60) Å	Coefficient 0	1818(8)
	c = 22.9091(16) Å	Coefficient 1	-1460(1)
Cell volume	1641.71(25) $Å^3$	Coefficient 2	818(10)
Z	6	Coefficient 3	-193(10)
Density, calculated	3.099 g/cm^3	Coefficient 4	81(8)
Pearson code	hR42	Coefficient 5	-10(8)
Formula type	N2O3P4Q12	Scale Factor	0.000206(10)
Wyckoff sequence	f^2e^2cb		

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [$Å^2$]*
			x	***y***	***z***	
Na1	6*b*	0.551(20)	0	0	0	0.663(69)
Na2	18*e*	0.7622(89)	0.6234(12)	0	¼	0.663(69)
Zr1	12*c*	0.8	0	0	0.14941(13)	0.663(69)
Y1	12*c*	0.1	0	0	0.14941(13)	0.663(69)
Al1	12*c*	0.1	0	0	0.14941(13)	0.663(69)
Si/P1**	18*e*	0.8/0.2	0.28257(79)	0	¼	0.663(69)
O1	36*f*	1	0.2065(10)	0.9899(12)	0.19858(43)	0.663(69)
O2	36*f*	1	0.19065(71)	0.14176(98)	0.08356(52)	0.663(69)

ZrO_2 impurity (8.4%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001369(51)
Lattice parameters:	
a [Å]	5.1591(35)
b [Å]	5.2104(36)
c [Å]	5.3253(38)
β [°]	99.015(10)
TCH Y Left	0.294(16)

Structure model $R\bar{3}c$ – f^3e^2cb

Data-set: NaAlY 25 °C (298 K)

Refined crystal data		TCH-U	0.800(33)
Formula sum	$Na_{5.507}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-Y	0.087(67)
Formula weight	571.99	FCJ-S/L	0.027861
Crystal system	trigonal	FCJ-D/L	0.027861
Space group	*R* -3 c (no. 167)	Coefficient 0	1906(8)
Lattice parameters	*a* = 9.09244(62) Å	Coefficient 1	-1700(1)
	c = 22.8623(19) Å	Coefficient 2	975(10)
		Coefficient 3	-301(9)
		Coefficient 4	113(9)
Cell volume	1636.86(26) $Å^3$	Coefficient 5	-4(9)
Z	6	Coefficient 6	-18(9)
Density, calculated	3.481 g/cm^3	Coefficient 7	-42(9)
Pearson code	hR54	Coefficient 8	51(8)
Formula type	N2O3P10Q12	Coefficient 9	-71(8)
Wyckoff sequence	f^3e^2cb	Scale Factor	0.000200(20)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			**B_{iso} [Å²]***
			x	***y***	***z***	
Na1	6*b*	0.788(25)	0	0	0	1.045(75)
Na2	18*e*	0.850(11)	0.6228(12)	0	¼	1.045(75)
Na3	36*f*	0.362(12)	0.5663(26)	0.6594(33)	0.9903(11)	1.045(75)
Zr1	12*c*	0.8	0	0	0.14914(15)	1.045(75)
Y1	12*c*	0.1	0	0	0.14914(15)	1.045(75)
Al1	12*c*	0.1	0	0	0.14914(15)	1.045(75)
Si/P1**	18*e*	0.8/0.2	0.28763(92)	0	¼	1.045(75)
O1	36*f*	1	0.1869(13)	0.9685(16)	0.20314(66)	1.045(75)
O2	36*f*	1	0.17429(93)	0.1428(10)	0.08338(63)	1.045(75)

ZrO_2 impurity (7.3%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001266(47)
Lattice parameters:	
a [Å]	5.1483(33)
b [Å]	5.237(37)
c [Å]	5.314(38)
β [°]	98.9934(100)
TCH Y Left	0.291(16)

Data-set: NaAlY 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{4.797}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.485(21)
Formula weight	555.66	TCH-Y	0.0908(52)
Crystal system	trigonal	FCJ-S/L	0.027861
Space group	*R* -3 c (no. 167)	FCJ-D/L	0.027861
Lattice parameters	*a* = 9.09782(53) Å	Coefficient 0	1832(8)
	c = 22.9029(15) Å	Coefficient 1	-1440(1)
Cell volume	1641.70(22) $Å^3$	Coefficient 2	831(9)
Z	6	Coefficient 3	-208(9)
Density, calculated	3.372 g/cm^3	Coefficient 4	93(8)
Pearson code	hR54	Coefficient 5	-2(7)
Formula type	N2O3P10Q12	Scale Factor	0.000206(20)
Wyckoff sequence	f^3e^2cb		

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	6*b*	0.781(23)	0	0	0	0.954(69)
Na2	18*e*	0.810(10)	0.6271(12)	0	¼	0.954(69)
Na3	36*f*	0.264(11)	0.5655(31)	0.655(38)	0.9962(14)	0.954(69)
Zr1	12*c*	0.8	0	0	0.14887(14)	0.954(69)
Y1	12*c*	0.1	0	0	0.14887(14)	0.954(69)
Al1	12*c*	0.1	0	0	0.14887(14)	0.954(69)
Si/P1**	18*e*	0.8/0.2	0.28818(86)	0	¼	0.954(69)
O1	36*f*	1	0.192(12)	0.9728(15)	0.20303(59)	0.954(69)
O2	36*f*	1	0.18323(87)	0.14505(98)	0.08536(60)	0.954(69)

ZrO_2 impurity (8.7%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001546(55)
Lattice parameters:	
a [Å]	5.1577(43)
b [Å]	5.1994(46)
c [Å]	5.3522(46)
β [°]	98.942(13)
TCH Y Left	0.383(19)

Structure model *C*2/*c* - f^9e^2a

Data-set: NaAlY 25 °C (298 K)

Refined crystal data			
Formula sum	$Na_{2.639}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.333(18)
Formula weight	506.05	TCH-Y	0.0902(51)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.17(22) Å	Coefficient 0	1852(7)
	b = 9.10285(56) Å	Coefficient 1	-1770(1)
	c = 22.881(32) Å	Coefficient 2	978(8)
	β = 161.089(38)°	Coefficient 3	-285(7)
		Coefficient 4	115(7)
Cell volume	1091.49(214) $Å^3$	Coefficient 5	-19(7)
Z	4	Coefficient 6	-10(7)
Density, calculated	3.079 g/cm^3	Coefficient 7	-2(8)
Pearson code	mC84	Coefficient 8	9(7)
Formula type	N2O3P4Q12	Coefficient 9	-63(6)
Wyckoff sequence	f^9e^2a	Scale Factor	0.000436(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.621(19)	0	0	0	0.124(61)
Na2	4*e*	1.000(33)	0	0.6158(29)	¼	0.124(61)
Na3	8*f*	0.509(20)	0.9473(61)	0.6746(42)	0.884(41)	0.124(61)
Zr1	8*f*	0.8	0.0031(10)	0.01122(53)	0.65147(71)	0.124(61)
Y1	8*f*	0.1	0.0031(10)	0.01122(53)	0.65147(71)	0.124(61)
Al1	8*f*	0.1	0.0031(10)	0.01122(53)	0.65147(71)	0.124(61)
Si/P1**	4*e*	0.8/0.2	0	0.2813(23)	¼	0.124(61)
Si/P2**	8*f*	0.8/0.2	0.4503(28)	0.8661(16)	0.5596(19)	0.124(61)
O1	8*f*	1	0.284(53)	0.9024(25)	0.392(41)	0.124(61)
O2	8*f*	1	0.0044(40)	0.2384(28)	0.1965(29)	0.124(61)
O3	8*f*	1	0.1792(48)	0.4191(29)	0.9826(32)	0.124(61)
O4	8*f*	1	0.3007(46)	0.0866(28)	0.2928(33)	0.124(61)
O5	8*f*	1	0.283(54)	0.6763(19)	0.934(37)	0.124(61)
O6	8*f*	1	0.4722(52)	0.3794(16)	0.0676(36)	0.124(61)

ZrO_2 impurity (7.6%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001141(34)
Lattice parameters:	
a [Å]	5.1605(20)
b [Å]	5.1841(21)
c [Å]	5.3561(23)
β [°]	99.1773(64)
TCH Y Left	0.229(11)

Data-set: NaAlY 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{2.812}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.308(17)
Formula weight	510.03	TCH-Y	0.0926(45)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.176(27) Å	Coefficient 0	1769(8)
	b = 9.11148(67) Å	Coefficient 1	-1490(1)
	c = 22.919(38) Å	Coefficient 2	798(8)
	β = 161.0939(46)°	Coefficient 3	-188(8)
Cell volume	1094.51(261) $Å^3$	Coefficient 4	71(8)
Z	4	Coefficient 5	-21(7)
Density, calculated	3.095 g/cm^3	Coefficient 6	1(6)
Pearson code	mC84	Scale Factor	0.000456(30)
Formula type	N2O3P4Q12		
Wyckoff sequence	f^9e^2a		

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.621(19)	0	0	0	0.209(60)
Na2	4*e*	1.000(35)	0	0.6158(29)	¼	0.209(60)
Na3	8*f*	0.509(20)	0.9473(61)	0.6746(42)	0.884(41)	0.209(60)
Zr1	8*f*	0.8	0.0031(10)	0.01122(53)	0.65147(71)	0.209(60)
Y1	8*f*	0.1	0.0031(10)	0.01122(53)	0.65147(71)	0.209(60)
Al1	8*f*	0.1	0.0031(10)	0.01122(53)	0.65147(71)	0.209(60)
Si/P1**	4*e*	0.8/0.2	0	0.2813(23)	¼	0.209(60)
Si/P2**	8*f*	0.8/0.2	0.4503(28)	0.8661(16)	0.5596(19)	0.209(60)
O1	8*f*	1	0.284(53)	0.9024(25)	0.392(41)	0.209(60)
O2	8*f*	1	0.0044(40)	0.2384(28)	0.1965(29)	0.209(60)
O3	8*f*	1	0.1792(48)	0.4191(29)	0.9826(32)	0.209(60)
O4	8*f*	1	0.3007(46)	0.0866(28)	0.2928(33)	0.209(60)
O5	8*f*	1	0.283(54)	0.6763(19)	0.934(37)	0.209(60)
O6	8*f*	1	0.4722(52)	0.3794(16)	0.0676(36)	0.209(60)

ZrO_2 impurity (7.7%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.00121(39)
Lattice parameters:	
a [Å]	5.165(27)
b [Å]	5.1891(28)
c [Å]	5.3489(31)
β [°]	99.1239(83)
TCH Y Left	0.268(13)

Structure model *C*2/*c* – $f^{10}e^2a$

Data-set: NaAlY 25 °C (298 K)

Refined crystal data		TCH-U	0.374(18)
Formula sum	$Na_{4.081}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-Y	0.0853(51)
Formula weight	539.22	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	1860(7)
Lattice parameters	*a* = 16.174(24) Å	Coefficient 1	-1765(10)
	b = 9.10395(58) Å	Coefficient 2	978(7)
	c = 22.888(34) Å	Coefficient 3	-291(7)
	β = 161.0944(40)°	Coefficient 4	106(7)
Cell volume	1091.92(230) $Å^3$	Coefficient 5	-3(7)
Z	4	Coefficient 6	-17(7)
Density, calculated	3.280 g/cm^3	Coefficient 7	-11(7)
Pearson code	mC92	Coefficient 8	25(6)
Formula type	N2O3P6Q12	Coefficient 9	-58(6)
Wyckoff sequence	$f^{10}e^2a$	Scale Factor	0.000437(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.753(23)	0	0	0	0.271(60)
Na2	4*e*	1.000(36)	0	0.6251(28)	¼	0.271(60)
Na3	8*f*	0.608(25)	0.9281(51)	0.6652(30)	0.8789(35)	0.271(60)
Na4	8*f*	0.556(26)	0.6326(67)	0.8867(37)	0.9254(46)	0.271(60)
Zr1	8*f*	0.8	0.00381(100)	0.01088(61)	0.65165(69)	0.271(60)
Y1	8*f*	0.1	0.00381(100)	0.01088(61)	0.65165(69)	0.271(60)
Al1	8*f*	0.1	0.00381(100)	0.01088(61)	0.65165(69)	0.271(60)
Si/P1**	4*e*	0.8/0.2	0	0.2904(26)	¼	0.271(60)
Si/P2**	8*f*	0.8/0.2	0.4472(27)	0.8659(17)	0.5554(19)	0.271(60)
O1	8*f*	1	0.2886(52)	0.8943(23)	0.3943(40)	0.271(60)
O2	8*f*	1	0.0273(43)	0.2286(30)	0.2188(30)	0.271(60)
O3	8*f*	1	0.1719(44)	0.4384(30)	0.9849(29)	0.271(60)
O4	8*f*	1	0.2772(51)	0.11(34)	0.2876(35)	0.271(60)
O5	8*f*	1	0.2987(52)	0.6622(22)	0.9514(35)	0.271(60)
O6	8*f*	1	0.4703(52)	0.383(18)	0.0589(36)	0.271(60)

ZrO_2 impurity (6.9%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001097(33)
Lattice parameters:	
a [Å]	5.1609(20)
b [Å]	5.1838(21)
c [Å]	5.353(23)
β [°]	99.2111(64)
TCH Y Left	0.229(11)

Data-set: NaAlY 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{3.718}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.320(16)
Formula weight	530.85	TCH-Y	0.0878(44)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.176(26) Å	Coefficient 0	1778(7)
	b = 9.11344(65) Å	Coefficient 1	-1500(1)
	c = 22.919(37) Å	Coefficient 2	816(8)
	β = 161.096(44)°	Coefficient 3	-204(8)
Cell volume	1094.63(253) $Å^3$	Coefficient 4	75(7)
Z	4	Coefficient 5	-17(6)
Density, calculated	3.221 g/cm^3	Coefficient 6	-10(6)
Pearson code	mC92	Scale Factor	0.000463(30)
Formula type	N2O3P6Q12		
Wyckoff sequence	$f^{10}e^2a$		

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.598(20)	0	0	0	0.292(58)
Na2	4*e*	1.000(36)	0	0.6073(30)	¼	0.292(58)
Na3	8*f*	0.664(20)	0.0046(60)	0.7008(26)	0.905(41)	0.292(58)
Na4	8*f*	0.396(25)	0.6627(77)	0.8617(37)	0.9318(57)	0.292(58)
Zr1	8*f*	0.8	0.0097(12)	0.01075(60)	0.65604(82)	0.292(58)
Y1	8*f*	0.1	0.0097(12)	0.01075(60)	0.65604(82)	0.292(58)
Al1	8*f*	0.1	0.0097(12)	0.01075(60)	0.65604(82)	0.292(58)
Si/P1**	4*e*	0.8/0.2	0	0.2759(26)	¼	0.292(58)
Si/P2**	8*f*	0.8/0.2	0.46(30)	0.8607(18)	0.5626(20)	0.292(58)
O1	8*f*	1	0.2856(58)	0.8914(29)	0.3836(41)	0.292(58)
O2	8*f*	1	0.0146(53)	0.2216(34)	0.208(36)	0.292(58)
O3	8*f*	1	0.1629(49)	0.4342(30)	0.9792(33)	0.292(58)
O4	8*f*	1	0.28(47)	0.0793(31)	0.2808(35)	0.292(58)
O5	8*f*	1	0.2379(55)	0.6526(22)	0.9029(38)	0.292(58)
O6	8*f*	1	0.4511(49)	0.39(19)	0.0392(34)	0.292(58)

ZrO_2 impurity (7.2%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001193(37)
Lattice parameters:	
a [Å]	5.1654(25)
b [Å]	5.1878(27)
c [Å]	5.3499(29)
β [°]	99.1728(79)
TCH Y Left	0.264(12)

Structure model *C*2/*c* – $f^{12}e^{2}a$

Data-set: NaAlY 25 °C (298 K)

Refined crystal data		TCH-U	0.418(17)
Formula sum	$Na_{5.538}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-Y	0.077(47)
Formula weight	572.71	FCJ-S/L	0.027861
Crystal system	monoclinic	FCJ-D/L	0.027861
Space group	*C*2/*c* (no. 15)	Coefficient 0	1873(7)
Lattice parameters	*a* = 16.173(21) Å	Coefficient 1	-1763(9)
	b = 9.10483(53) Å	Coefficient 2	995(7)
	c = 22.886(29) Å	Coefficient 3	-271(7)
	β = 161.091(35)°	Coefficient 4	99(6)
Cell volume	1092.13(199) $Å^3$	Coefficient 5	11(6)
Z	4	Coefficient 6	-9(6)
Density, calculated	3.483 g/cm^3	Coefficient 7	0(7)
Pearson code	mC108	Coefficient 8	13(6)
Formula type	N2O3P10Q12	Coefficient 9	-40(6)
Wyckoff sequence	$f^{12}e^{2}a$	Scale Factor	0.000443(30)

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å²]*
			x	***y***	***z***	
Na1	4*a*	0.718(24)	0	0	0	0.302(61)
Na2	4*e*	1.000(37)	0	0.6196(27)	¼	0.302(61)
Na3	8*f*	0.633(21)	0.9688(53)	0.6828(32)	0.9072(34)	0.302(61)
Na4	8*f*	0.572(26)	0.6155(58)	0.8969(30)	0.9069(42)	0.302(61)
Na5	8*f*	0.235(16)	0.0845(84)	0.011(11)	0.1306(62)	0.302(61)
Na6	8*f*	0.469(23)	0.3826(52)	0.6959(39)	0.9064(35)	0.302(61)
Zr1	8*f*	0.8	0.00675(89)	0.01053(60)	0.65461(63)	0.302(61)
Y1	8*f*	0.1	0.00675(89)	0.01053(60)	0.65461(63)	0.302(61)
Al1	8*f*	0.1	0.00675(89)	0.01053(60)	0.65461(63)	0.302(61)
Si/P1**	4*e*	0.8/0.2	0	0.2891(22)	¼	0.302(61)
Si/P2**	8*f*	0.8/0.2	0.4361(27)	0.8705(19)	0.5509(19)	0.302(61)
O1	8*f*	1	0.2773(48)	0.8852(23)	0.3875(40)	0.302(61)
O2	8*f*	1	0.9983(40)	0.224(32)	0.1949(30)	0.302(61)
O3	8*f*	1	0.1947(37)	0.4538(26)	0.0003(25)	0.302(61)
O4	8*f*	1	0.3196(47)	0.1239(29)	0.3173(35)	0.302(61)
O5	8*f*	1	0.3086(45)	0.6568(21)	0.9596(31)	0.302(61)
O6	8*f*	1	0.4681(53)	0.3555(20)	0.0755(38)	0.302(61)

ZrO_2 impurity (6.2%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.001044(31)
Lattice parameters:	
a [Å]	5.1606(20)
b [Å]	5.1829(21)
c [Å]	5.351(23)
β [°]	99.2101(63)
TCH Y Left	0.234(10)

Data-set: NaAlY 127 °C (400 K)

Refined crystal data			
Formula sum	$Na_{5.928}Zr_{1.6}Y_{0.2}Al_{0.2}Si_3O_{12}$	TCH-U	0.337(15)
Formula weight	581.67	TCH-Y	0.0807(42)
Crystal system	monoclinic	FCJ-S/L	0.027861
Space group	*C*2/*c* (no. 15)	FCJ-D/L	0.027861
Lattice parameters	*a* = 16.176(23) Å	Coefficient 0	1802(7)
	b = 9.11488(58) Å	Coefficient 1	-1485(10)
	c = 22.914(33) Å	Coefficient 2	828(7)
	β = 161.0906(40)°	Coefficient 3	-180(7)
Cell volume	1094.87(226) $Å^3$	Coefficient 4	62(6)
Z	4	Coefficient 5	9(6)
Density, calculated	3.529 g/cm^3	Scale Factor	0.000465(30)
Pearson code	mC108		
Formula type	N2O3P10Q12		
Wyckoff sequence	$f^{12}e^2a$		

Atom	**Wyckoff site**	**Occupancy**	**fractional coordinates**			B_{iso} [Å^2]*
			x	***y***	***z***	
Na1	4*a*	0.750(23)	0	0	0	0.434(60)
Na2	4*e*	0.950(41)	0	0.6249(30)	¼	0.434(60)
Na3	8*f*	0.739(24)	0.966(51)	0.683(26)	0.9089(32)	0.434(60)
Na4	8*f*	0.548(28)	0.6368(62)	0.8976(33)	0.9188(44)	0.434(60)
Na5	8*f*	0.315(17)	0.1048(65)	0.9978(87)	0.1441(48)	0.434(60)
Na6	8*f*	0.512(26)	0.3775(51)	0.7075(40)	0.9027(35)	0.434(60)
Zr1	8*f*	0.8	0.0081(100)	0.01159(58)	0.65506(69)	0.434(60)
Y1	8*f*	0.1	0.0081(100)	0.01159(58)	0.65506(69)	0.434(60)
Al1	8*f*	0.1	0.0081(100)	0.01159(58)	0.65506(69)	0.434(60)
Si/P1**	4*e*	0.8/0.2	0	0.2839(24)	¼	0.434(60)
Si/P2**	8*f*	0.8/0.2	0.4451(28)	0.8722(20)	0.5524(19)	0.434(60)
O1	8*f*	1	0.277(54)	0.8865(27)	0.3836(44)	0.434(60)
O2	8*f*	1	0.0014(48)	0.2192(34)	0.201(33)	0.434(60)
O3	8*f*	1	0.1916(43)	0.4519(26)	0.0006(29)	0.434(60)
O4	8*f*	1	0.3169(53)	0.1223(33)	0.3182(38)	0.434(60)
O5	8*f*	1	0.3085(52)	0.6554(22)	0.9625(34)	0.434(60)
O6	8*f*	1	0.4636(61)	0.3403(24)	0.0675(42)	0.434(60)

ZrO_2 impurity (6.0%)	
Crystal system	monoclinic
Space group	P21/c (No. 14)
Scale Factor	0.00108(33)
Lattice parameters:	
a [Å]	5.163(24)
b [Å]	5.1893(25)
c [Å]	5.3469(28)
β [°]	99.1688(74)
TCH Y Left	0.249(12)

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