Table M22-001. $Na_3Sc_2(PO_4)_3$. Unit cell parameters of α-, β-, and γ-type crystals in trigonal description [86Col].

Rhombohedral parameters (trigonal description)	Crystal (fusion) α type	Crystal (1470 °C) β type	Crystal (flux) γ type
a [Å]	8.900(4)	8.928(1)	8.949(2)
b [Å]	8.900(4)	8.927(1)	8.950(2)
c [Å]	22.769(11)	22.276(3)	22.230(4)
α [°]	90.70(3)	90.00(2)	90.00(2)
β [°]	89.30(3)	90.01(2)	89.99(2)
γ [°]	119.86(2)	119.99(2)	120.01(2)

Table M22-002. $Na_3Sc_2(PO_4)_3$ (α-type). Fractional coordinates and isotropic temperature parameters at RT [86Col]. *B* is defined by Eq. (e) in Introduction. For Na(1)', Na(2)' and Na(3)', see Fig. M22-002. Each of atomic pairs denoted by *A* and *B* are nearly at the B2/b positions.

4*a* positions of *Bb*	*x*	*y*	*z*	*B* [10^{-4} Å^2]
Na(1)′	0.1944(5)	0.5577(10)	0.1513(6)	504(35)
Na(2)′	–0.0021(6)	0.2415(12)	0.3907(3)	353(30)
Na(3)′	0.3286(5)	0.3090(10)	0.4251(4)	331(30)
P(1) *A*	0.3596(4)	0.2622(8)	0.1084(2)	103(5)
P(1) *B*	0.6444(4)	0.7422(8)	0.8916(2)	103(5)
P(2)	–0.0016(4)	0.2506(8)	0.0453(1)	104(10)
Sc	0.1019(4)	0.0556(8)	0.2462(1)	82(3)
Sc	0.9030(4)	0.9529(8)	0.7477(1)	82(3)
O(1) *A*	0.1472(6)	0.2198(11)	0.4372(6)	136(13)
O(1) *B*	0.8538(6)	0.7828(11)	0.5612(6)	136(15)
O(2) *A*	0.4370(6)	0.0863(11)	0.4496(6)	141(15)
O(2) *B*	0.5332(6)	0.9166(11)	0.5510(6)	141(15)
O(3) *A*	0.2565(6)	0.2083(11)	0.1815(6)	180(15)
O(3) *B*	0.7481(6)	0.7899(11)	0.8231(6)	180(15)
O(4) *A*	0.3845(7)	0.1241(12)	0.1286(7)	245(18)
O(4) *B*	0.6244(7)	0.8863(12)	0.8669(7)	245(18)
O(5) *A*	0.4467(6)	0.4370(12)	0.1814(6)	149(17)
O(5) *B*	0.5591(6)	0.5676(11)	0.8208(6)	149(17)
O(6) *A*	0.0758(6)	0.2418(11)	0.1495(6)	169(15)
O(6) *B*	0.9201(6)	0.7626(11)	0.8581(7)	169(15)

Table M22-003. $Na_3Sc_2(PO_4)_3$ (α-type). Interatomic distances [Å] at T = RT [86Col]. See also the caption of Table M22-002.

Na(1)′	O(1) *B*	2.31	} octahedron face
	O(3) *B*	2.36	
	O(6) *A*	2.41	
	O(2) *B*	2.47	} vacant Na(3)′ polyhedron
	O(5) *B*	2.62	
Na(3)′	O(3) *A*	2.38	
	O(2) *A*	2.40	
	O(1) *A*	2.44	
	O(3) *B*	2.52	
	O(6) *B*	2.56	
	O(5) *A*	2.65	
Na(2)′	O(1) *A*	2.45	
	O(6) *A*	2.46	
	O(1) *B*	2.48	
	O(5) *B*	2.51	
	O(6) *B*	2.58	
	O(4) *A*	2.58	
	O(5) *B*	2.64	
	O(4) *B*	2.72	
Tetrahedra		Average distances	
⟨P 1 *A*–O⟩		1.53	
⟨P 1 *B*–O⟩		1.53	
⟨P 2–O⟩		1.53	
Octahedra			
⟨Sc *A*–O⟩		2.09	
⟨Sc *B*–O⟩		2.09	

Table M22-004. $Na_3Sc_2(PO_4)_3$. Occupancy factors *S*, isotropic temperature parameters *B* and interatomic distances *d* for Na sites [88Col]. *B* is defined by Eq. (e) in Introduction.

T [K]	Na(1)		Na(2)		mid-Na		*d* [Å]	
	S	*B* [Å^2]	*S*	*B* [Å^2]	*S*	*B* [Å^2]	$\langle d_{Na(1)-O} \rangle$	$\langle d_{Na(2)-O} \rangle$
α-type crystal								
298 [a])	0.00	–	2	2.6	1.00	4.0	2.681	2.550
325	0.69	11	2	3.7	0.31	6.5	2.567	2.642
420	0.55	13	2	4.8	0.45	9.0	2.608	2.646
473	0.43	13	2	5.9	0.57	14	2.639	2.647
600	0.34	20	2	6.9	0.66	33	2.667	2.651
β-type crystal								
220	1.00	6	2	2.0	0.00	–	2.501	2.638
298	0.70	8	2	3.3	0.30	9.0	2.559	2.643
473	0.40	9	2	5.8	0.60	18	2.636	2.645
γ-type crystal								
298	0.66	6	2	3.3	0.34	19	2.551	2.648
373	0.58	7	2	4.3	0.42	18	2.580	2.649
473	0.47	8	2	5.7	0.53	13	2.623	2.654
600	0.44	11	2	6.5	0.56	22	2.647	2.655

[a]) Monoclinic modification.