Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Crystal structure, phase transition and thermal expansion property of $NaZr_2(PO_4)_3$-$SrZr_4(PO_4)_6$ solid solutions

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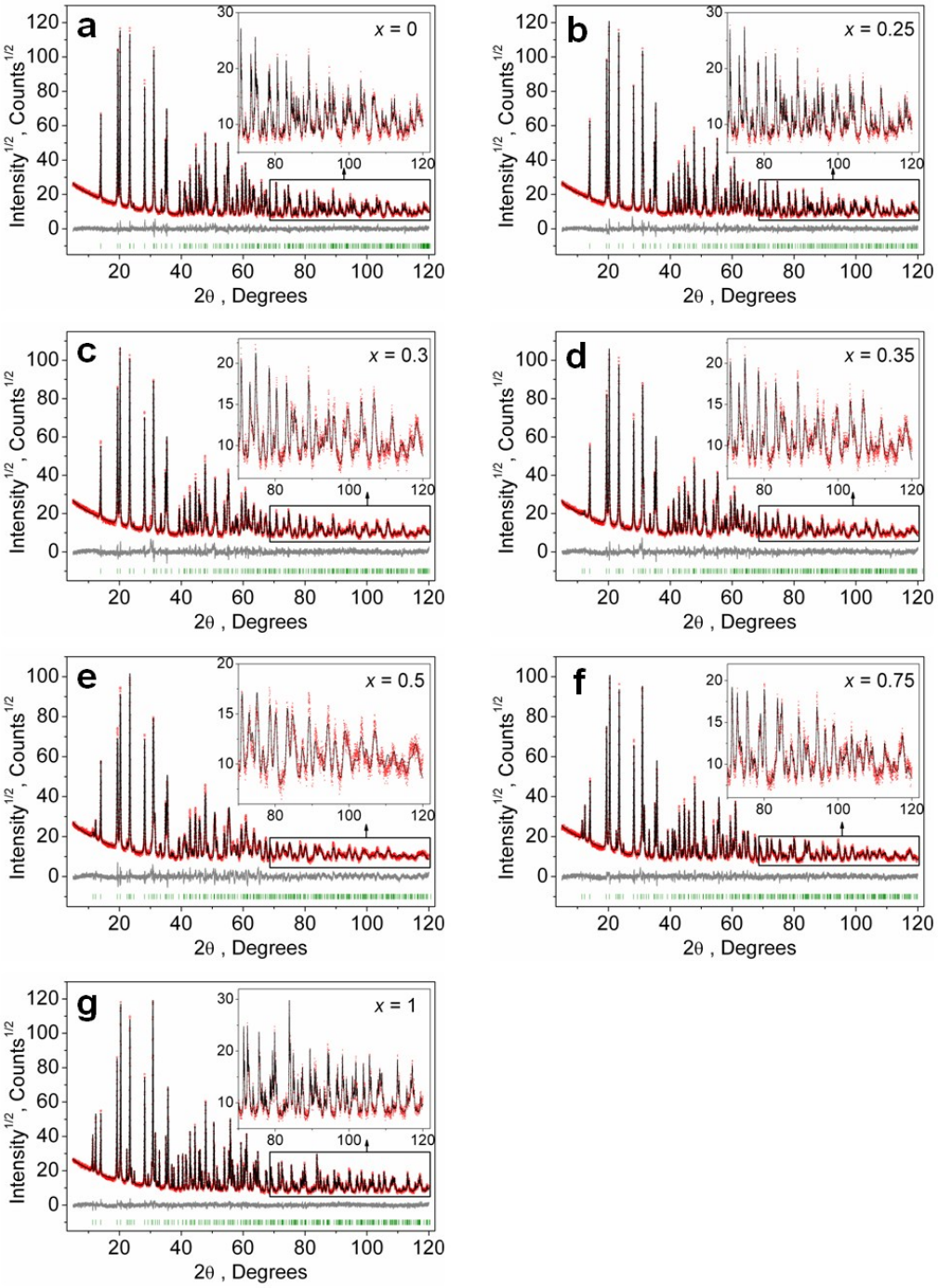

Figure S1. Difference Rietveld plot of $Na_{(2-2x)}Sr_x[\ ]_xZr_4(PO_4)_6$, **a.** $x = 0$, **b.** $x = 0.25$, **c.** $x = 0.3$, **d.** $x = 0.35$, **e.** $x = 0.5$, **f.** $x = 0.75$, **g.** $x = 1$.

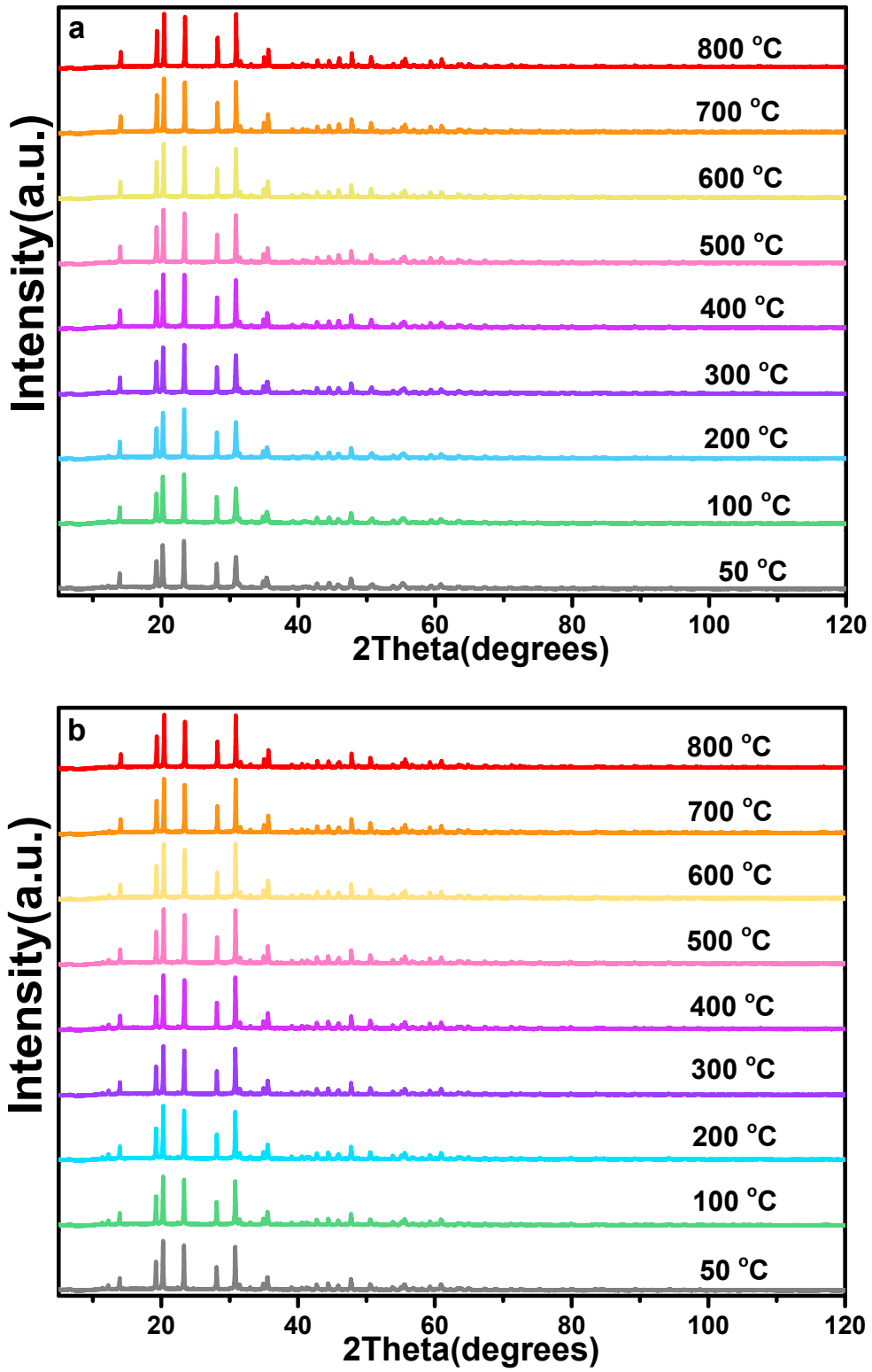

Figure S2. Temperature dependent XRD patterns of $Na_{(2-2x)}Sr_x[\ ]_xZr_4(PO_4)_6$, **a.** $x = 0.5$, **b.** $x = 0.75$.

Table 1S. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $Na_{(2-2x)}Sr_x[\ ]_xZr_4(PO_4)_6$

	x	*y*	*z*	B_{iso}	Occ.
			x = 0		
Na	0	0	0	3.2 (1)	1
Zr	0	0	0.14566 (3)	0.69 (3)	1
P1	0.2918 (2)	0	0.25	0.92 (5)	1
O1	0.1830 (3)	-0.0199 (4)	0.1956 (1)	0.98 (5)	1
O2	0.1937 (3)	0.1692 (3)	0.0875 (1)	0.98 (5)	1
			x = 0.25		
Na	0	0	0	2.9 (2)	0.87 (2)
Sr	0	0	0	2.9 (2)	0.065 (8)
Zr	0	0	0.14592 (3)	0.53 (4)	1
P1	0.2908 (2)	0	0.25	0.90 (6)	1
O1	0.1815 (4)	-0.0218 (4)	0.1952 (1)	1.03 (6)	1
O2	0.1946 (3)	0.1697 (3)	0.0880 (1)	1.03 (6)	1
			x = 0.3		
Na	0	0	0	2.8 (2)	0.85 (2)
Sr	0	0	0	2.8 (2)	0.075 (1)
Zr	0	0	0.14619 (4)	0.66 (5)	1
P1	0.2913 (3)	0	0.25	1.00 (7)	1
O1	0.1793 (5)	-0.0221 (5)	0.1955 (2)	1.06 (8)	1
O2	0.1947 (4)	0.1700 (4)	0.0885 (2)	1.06 (8)	1
			x = 0.35		
Sr1	0	0	0	1.2 (5)	0.14 (1)
Na1	0	0	0	1.2 (5)	0.86 (1)
Na2	0	0	0.5	4 (1)	0.86 (1)
Zr1	0	0	0.1468 (2)	0.6 (1)	1
Zr2	0	0	0.6456 (2)	0.8 (1)	1
P1	0.2927 (7)	0.0018 (14)	0.2529 (5)	0.92 (8)	1
O1	0.1853 (17)	-0.0030 (14)	0.1961 (6)	0.84 (9)	1
O2	0.0420 (14)	-0.1728 (17)	0.6952 (5)	0.84 (9)	1
O3	0.198 (2)	0.166 (2)	0.0893 (7)	0.84 (9)	1

O4	-0.176 (2)	-0.1921 (19)	0.5889 (7)	0.84 (9)	1
			$x = 0.5$		
Sr1	0	0	0	1.3 (3)	0.30 (1)
Na1	0	0	0	1.3 (3)	0.70 (1)
Na2	0	0	0.5	5.9 (15)	0.70 (1)
Zr1	0	0	0.1483 (2)	0.7 (1)	1
Zr2	0	0	0.6450 (2)	1.5 (1)	1
P1	0.2956 (7)	0.008 (1)	0.2534 (4)	1.3 (1)	1
O1	0.178 (2)	0.000 (2)	0.1962 (6)	0.7 (1)	1
O2	0.051 (15)	-0.175 (2)	0.6962 (5)	0.7 (1)	1
O3	0.186 (2)	0.166 (2)	0.0843 (5)	0.7 (1)	1
O4	-0.172 (2)	-0.204 (2)	0.5972 (6)	0.7 (1)	1
			$x = 0.75$		
Sr1	0	0	0	3.0 (2)	0.645 (8)
Na1	0	0	0	3.0 (2)	0.355 (8)
Na2	0	0	0.5	4 (2)	0.355 (7)
Zr1	0	0	0.14906 (9)	0.56 (7)	1
Zr2	0	0	0.6447 (1)	1.13 (7)	1
P1	0.2926 (5)	0.0071 (7)	0.2522 (2)	1.11 (7)	1
O1	0.185 (1)	-0.003 (1)	0.1973 (4)	0.87 (9)	1
O2	0.054 (1)	-0.164 (1)	0.6975 (3)	0.87 (9)	1
O3	0.1791 (9)	0.1718 (9)	0.0869 (3)	0.87 (9)	1
O4	-0.169 (1)	-0.2155 (9)	0.5961 (4)	0.87 (9)	1
			$x = 1$		
Sr1	0	0	0	3.16 (6)	1
Zr1	0	0	0.14949 (5)	0.57 (4)	1
Zr2	0	0	0.64503 (5)	0.58 (4)	1
P1	0.2909 (3)	0.0071 (4)	0.2514 (2)	0.87 (5)	1
O1	0.1914 (6)	-0.0089 (6)	0.1963 (3)	0.94 (6)	1
O2	0.0563 (7)	-0.1530 (6)	0.6982 (2)	0.94 (6)	1
O3	0.1816 (6)	0.1785 (6)	0.0884 (2)	0.94 (6)	1
O4	-0.1600 (7)	-0.2133 (6)	0.5967 (2)	0.94 (6)	1

Table 2S. Main bond lengths (Å) of $Na_{(2-2x)}Sr_x[\ ]_xZr_4(PO_4)_6$

		$x = 0$	
Na—O2	2.561 (3)	P1—O1	1.522 (3)
Zr—O1	2.050 (3)	P1—O2^{i}	1.529 (2)
Zr—O2	2.084 (3)		
		$x = 0.25$	
(Na/Sr)—O2	2.578 (3)	P1—O1	1.532 (3)
Zr—O1	2.041 (3)	P1—O2^{i}	1.528 (3)
Zr—O2	2.088 (3)		
		$x = 0.3$	
(Na/Sr)—O2	2.592 (4)	P1—O1	1.541 (4)
Zr—O1	2.027 (4)	P1—O2^{i}	1.523 (3)
Zr—O2	2.086 (4)		
		$x = 0.35$	
(Na1/Sr1)—O3	2.610 (15)	Zr2—O4	2.077 (15)
Na2—O4	2.605 (15)	P1—O1	1.595 (15)
Zr1—O1	1.994 (12)	P1—O2^{i}	1.50 (2)
Zr1—O3	2.090 (15)	P1—O3^{ii}	1.52 (2)
Zr2—O2	2.074 (13)	P1—O4^{iii}	1.52 (2)
		$x = 0.5$	
(Na2/Sr1)—O3	2.49 (1)	Zr2—O4	2.00 (1)
Na2—O4	2.79 (1)	P1—O1	1.65 (1)
Zr1—O1	1.91 (1)	P1—O2^{i}	1.45 (2)
Zr1—O3	2.14 (1)	P1—O3^{ii}	1.53 (1)
Zr2—O2	2.15 (1)	P1—O4^{iii}	1.53 (1)
		$x = 0.75$	
(Na1/Sr1)—O3	2.535 (7)	Zr2—O4	2.053 (7)
Na2—O4	2.815 (8)	P1—O1	1.559 (9)
Zr1—O1	1.980 (8)	P1—O2^{i}	1.49 (1)
Zr1—O3	2.106 (7)	P1—O3^{ii}	1.564 (7)
Zr2—O2	2.108 (8)	P1—O4^{iii}	1.495 (8)
		$x = 1$	
Sr1—O3	2.592 (5)	P1—O1	1.518 (6)
Zr1—O1	2.026 (5)	P1—O2^{i}	1.542 (6)

Zr1—O3	2.119 (5)	P1—O3^{ii}	1.536 (4)
Zr2—O2	2.052 (5)	P1—O4^{iii}	1.552 (5)
Zr2—O4	2.019 (5)		

Symmetry code for x = 0, 0.25, 0.3: (i) -x+2/3, -y+1/3, -z+1/3.

Symmetry code for x = 0.35, 0.5, 0.75, 1: (i) x-y, x, -z+1; (ii) -x+2/3, -y+1/3, -z+1/3; (iii) -x+y+1/3, -x-1/3, z-1/3.