Crystal structure of tetrasodium octastrontium *catena*-[octaphosphido(3-)]-[diphosphido(4-)]tetraaluminate(III) [diphosphide(4-)], Na₄Sr₈[Al₄P₈(P₂)][P₂]

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Source of material: Na₄Sr₈Al₄P₁₂ was prepared from a mixture of Na₃P, SrP and AlP (ratio 1 : 2 : 1) in a sealed niobium ampoule at 1473 K. The slight excess of sodium was used in order to suppress the formation of Sr₃[AlP₂]₂ (see ref. 1).

The structure of Na₄Sr₈Al₄P₁₂ contains two different anions, namely infinite chains of *catena*-[Al₄P₈(P₂)]¹⁶⁻ ($d(\text{Al-P}) = 2.38 \text{ \AA} - 2.80 \text{ \AA}$) with bridging (P-P)^b ligands ($d(\text{P-P})^b = 2.26 \text{ \AA}$) as well as isolated [P-P]⁴⁻ dumbbells with $d(\text{P-P}) = 2.34 \text{ \AA}$. The cations (Na, Sr) form a framework of condensed trigonal prisms resulting in linear chains of rhombic prisms (black) and zig-zag chains of prisms (shaded) with pentagonal channels. This framework is very similar to that of Na₄EugAl₄P₁₂ (see ref. 2). The Al₂P₂ fragments of the chains are in the channels and the P³⁻ endoligands center the trigonal prisms, whereas the two types of P₂ dumbbells center the rhombic prisms alternating along [010].

Al₄Na₄P₁₂Sr₈, monoclinic, C2/m (No. 12), $a = 13.529(1) \text{ \AA}$, $b = 8.998(1) \text{ \AA}$, $c = 11.473(1) \text{ \AA}$, $\beta = 106.035(4)^\circ$, $V = 1342.3 \text{ \AA}^3$, $Z = 2$, $R(F) = 0.072$, $R_w(F) = 0.073$.

Table 1. Parameters used for the X-ray data collection

Crystal:	black prism, size 0.10 x 0.15 x 0.25 mm
Wavelength:	Mo K α radiation (0.71073 \AA)
μ :	161.9 cm ⁻¹
Diffractometer:	Siemens R3m/V
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	1638
Criterion for F_o :	$F_o > 2 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	81
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in \AA²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	4g	0	0.302(1)	0	0.030(4)	0.027(4)	0.037(4)	0	0.013(3)	0
Na(2)	4i	0.637(1)	0	0.237(1)	0.074(8)	0.025(5)	0.055(7)	0	0.007(6)	0
Sr(1)	8j	0.0282(1)	0.2550(6)	0.6836(1)	0.0279(7)	0.076(1)	0.0221(6)	0.010(2)	0.0068(4)	-0.000(2)
Sr(2)	4e	1/4	1/4	0	0.0199(7)	0.0254(8)	0.0232(7)	0.003(2)	0.0060(5)	-0.007(2)
Sr(3)	4f	1/4	1/4	1/2	0.0237(7)	0.0335(9)	0.0246(7)	0.002(2)	0.0060(5)	-0.001(2)
Al(1)	4i	0.3004(5)	0	0.2607(5)	0.021(2)	0.018(3)	0.022(2)	0	0.005(2)	0
Al(2)	4i	0.0889(5)	0	0.1160(5)	0.025(3)	0.021(3)	0.023(3)	0	0.009(2)	0
P(1)	8j	0.1807(3)	0.2032(4)	0.2285(3)	0.023(2)	0.022(1)	0.023(1)	0.001(1)	0.006(1)	-0.001(1)

Table 2. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
P(2)	4 <i>i</i>	0.095(1)	0	0.874(1)	0.030(4)	0.031(5)	0.064(7)	0	0.009(4)	0
P(3)	4 <i>i</i>	0.4103(7)	0	0.104(1)	0.015(3)	0.015(3)	0.038(4)	0	−0.007(3)	0
P(4)	4 <i>i</i>	0.5833(8)	0	0.498(1)	0.015(3)	0.019(3)	0.054(6)	0	−0.000(3)	0
P(5)	4 <i>i</i>	0.0899(9)	0	0.526(1)	0.023(3)	0.031(4)	0.044(5)	0	0.005(3)	0

References

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