

Sodium scandium diphosphate, NaScP₂O₇, isotypic with α -NaTi(III)P₂O₇

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Sc}-\text{O}) = 0.002$ Å; R factor = 0.025; wR factor = 0.082; data-to-parameter ratio = 10.1.

Crystals of the title compound, NaScP₂O₇, were grown by a flux method. The crystal structure is isotypic with those of α -NaTiP₂O₇, NaYbP₂O₇ and NaLuP₂O₇, and is closely related to that of NaYP₂O₇. The structural set-up consists of a three-dimensional framework of P₂O₇ units that are corner-shared by ScO₆ octahedra, forming tunnels running parallel to [010]. The Na atoms are situated in the tunnels and are surrounded by nine O atoms in a distorted environment.

Related literature

Previous X-ray powder data of NaScP₂O₇ were reported by Vitins *et al.* (2000). NaScP₂O₇ is isotypic with α -NaTiP₂O₇ (Leclaire *et al.*, 1988), NaYbP₂O₇ (Férid *et al.*, 2004) and NaLuP₂O₇ (Yuan *et al.*, 2007) and shows similar structural features as NaYP₂O₇ (Hamady & Jouini, 1996). Both structure types are topologically related to β -cristobalite (Leclaire *et al.*, 1988). For a detailed review on the structures of $A^I M^{III} P_2 O_7$ -type diphosphates, see: Li *et al.* (2005); Schwendtner & Kolitsch (2004). For possible applications as scintillators or phosphor materials based on $A^I M^{III} P_2 O_7$ -type diphosphates, see: Hizhnyi *et al.* (2007, 2008). For background to structural parameters, see: Brese & O'Keeffe (1991); Robinson *et al.* (1971).

Experimental

Crystal data

NaScP ₂ O ₇	$V = 576.1$ (2) Å ³
$M_r = 241.89$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.9044$ (18) Å	$\mu = 1.89$ mm ⁻¹
$b = 5.3300$ (11) Å	$T = 293$ K
$c = 12.516$ (3) Å	$0.40 \times 0.15 \times 0.05$ mm
$\beta = 104.11$ (3)°	

Data collection

Kuma KM-4-CCD diffractometer	5082 measured reflections
Absorption correction: multi-scan (<i>CrysAlis CCD</i> ; Oxford Diffraction, 2003)	1018 independent reflections
$T_{\min} = 0.067$, $T_{\max} = 0.093$	932 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$	101 parameters
$wR(F^2) = 0.082$	$\Delta\rho_{\max} = 0.46$ e Å ⁻³
$S = 1.18$	$\Delta\rho_{\min} = -0.46$ e Å ⁻³
1018 reflections	

Table 1

Selected geometric parameters (Å, °).

Sc—O3	2.0217 (19)	P1—O7	1.5254 (17)
Sc—O6 ⁱ	2.0770 (17)	P1—O4	1.5313 (18)
Sc—O7 ⁱⁱ	2.1112 (17)	P1—O5 ⁱⁱⁱ	1.6114 (17)
Sc—O1	2.1220 (16)	P2—O3	1.5013 (19)
Sc—O2	2.1220 (16)	P2—O1 ^{iv}	1.5278 (16)
Sc—O4	2.1506 (18)	P2—O2 ^v	1.5332 (16)
P1—O6	1.5088 (17)	P2—O5	1.6151 (17)

P1^{vi}—O5—P2 125.47 (10)

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x, -y, -z + 1$; (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (iv) $-x + 1, -y + 1, -z + 1$; (v) $-x + 1, -y, -z + 1$; (vi) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2003); software used to prepare material for publication: *SHELXL97*.

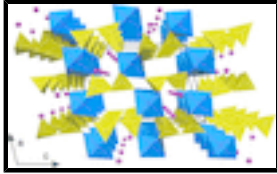
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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2274).

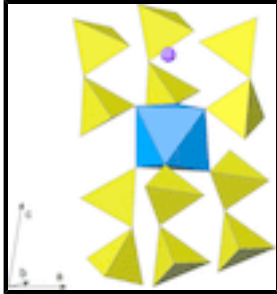
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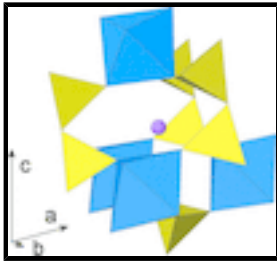
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