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$SrNi_3(P_2O_7)_2$

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(P–O) = 0.001 Å
R factor = 0.021
wR factor = 0.054
Data-to-parameter ratio = 20.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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The title compound, strontium trinickel bis(diphosphate), $SrNi_3(P_2O_7)_2$, is isostructural with all other mixed metal pyrophosphates having the same stoichiometry. The Sr and one of the Ni ions are located on a crystallographic centre of inversion.

Comment

Pyrophosphates are of interest because of their complex network architecture and several structures have been previously determined. The title compound, $SrNi_3(P_2O_7)_2$ (Fig. 1), has already been investigated by powder diffraction (El-Bali, 1993), but since its single-crystal structure has not been determined yet, it is presented here.

The Sr and one of the Ni ions are located on a crystallographic centre of inversion. All other atoms occupy general positions. The structure consists of infinite zigzag chains of NiO_6 octahedra sharing either *trans* or skew edges. These chains are connected by P_2O_7 moieties to form a three-dimensional network into which the Sr ions are incorporated *via* connections to eight O atoms (Table 1). The structure of $SrNi_3(P_2O_7)_2$ is isostructural with all other metal pyrophosphates having the same stoichiometry: $Ni_3Pb(P_2O_7)_2$ (Krasnikov *et al.*, 1985), $CaNi_3(P_2O_7)_2$, $CaCo_3(P_2O_7)_2$ and $SrFe_3(P_2O_7)_2$ (Lii *et al.*, 1993), and $PbCo_3(P_2O_7)_2$ and $PbFe_3(P_2O_7)_2$ (Elmarzouki *et al.*, 1995).

Experimental

A mixture of $(NH_4)_2HPO_4$, $Sr(OH)_2$ and $NiCl_2$ was ground together and heated to approximately 800 K. The molten mass was maintained at this temperature for two days and then cooled down to room temperature (El-Bali, 1993).

Crystal data

$SrNi_3(P_2O_7)_2$
M_r = 611.63
Monoclinic, $P2_1/c$
a = 7.4116 (4) Å
b = 7.6542 (3) Å
c = 9.4486 (6) Å
β = 112.194 (5)°
V = 496.30 (5) Å^3
Z = 2
D_x = 4.093 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 39700 reflections
θ = 3.8–37.3°
μ = 11.69 mm^{-1}
T = 173 (2) K
Block, yellow
0.24 × 0.18 × 0.16 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: empirical (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.101, T_{max} = 0.156
26 742 measured reflections
2076 independent reflections
2027 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 34.3°
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 10$
$l = -14 \rightarrow 14$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.054$
$S = 1.13$
2076 reflections
104 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.4865P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.78$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.096 (2)

Table 1
Selected bond lengths (Å).

Sr1—O7	2.5453 (12)	Ni1—O2^{vi}	2.0841 (12)
Sr1—O2^{i}	2.6234 (13)	Ni1—O1	2.0901 (13)
Sr1—O3^{ii}	2.6541 (13)	Ni1—O3^{ii}	2.1961 (12)
Sr1—O1^{iii}	2.7169 (13)	Ni2—O6^{ii}	2.0458 (12)
Ni1—O6^{iv}	2.0415 (12)	Ni2—O7^{vii}	2.0552 (12)
Ni1—O5^{v}	2.0606 (12)	Ni2—O3^{ii}	2.1163 (12)

Symmetry codes: (i) $x, 1+y, z$; (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (iv) $x-1, \frac{3}{2}-y, z-\frac{1}{2}$; (v) $x-1, y, z$; (vi) $1-x, 1-y, -z$; (vii) $1-x, 2-y, -z$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

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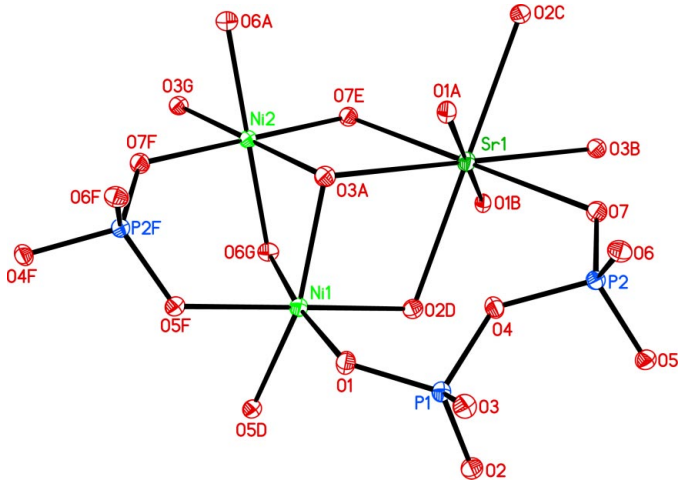

Figure 1
A perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level. Symmetry operators: (*A*) $1-x, y+\frac{1}{2}, \frac{1}{2}-z$; (*B*) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (*C*) $x, y+1, z$; (*D*) $1-x, 1-y, z$; (*E*) $1-x, 2-y, -z$; (*F*) $x-1, y, z$; (*G*) $x-1, \frac{3}{2}-y, \frac{1}{2}-z$.

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