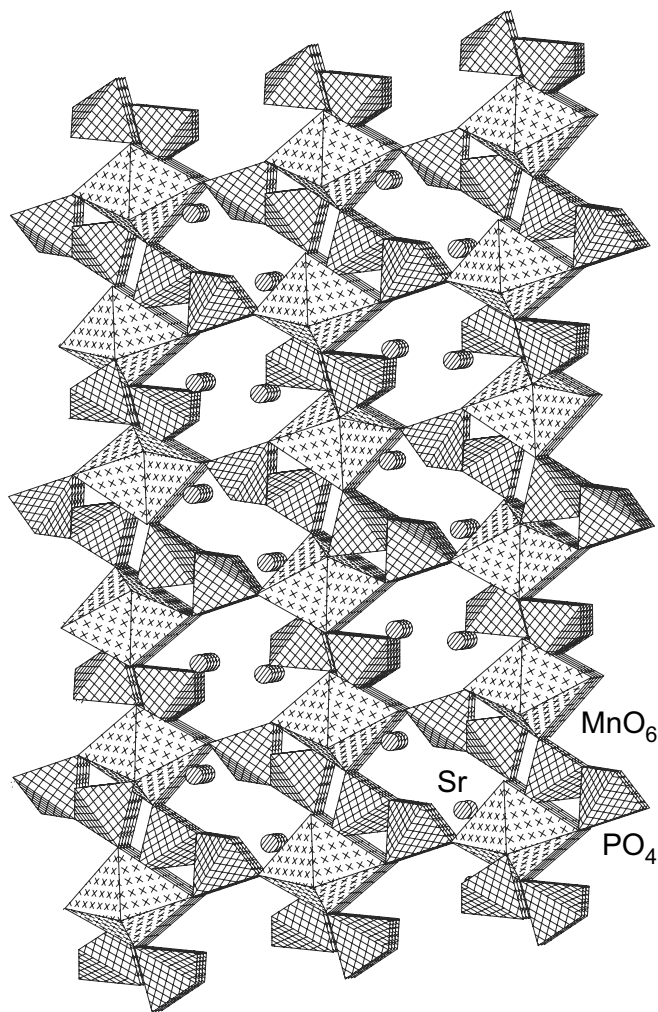


# Crystal structure of distrontium manganese(III) tetraoxophosphate heptaoxodiphosphate, $\text{Sr}_2\text{Mn}[\text{PO}_4][\text{P}_2\text{O}_7]$

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Received March 5, 2007, accepted and available on-line July 18, 2007; CSD no. 409913



(59 mg, 0.4 mmol),  $\text{Mn}_2\text{O}_3$  (63 mg, 0.4 mmol) and 0.2 ml of 85 %  $\text{H}_3\text{PO}_4$ . A reaction mixture was loaded into quartz tubes and filled with 0.5 ml water. The autoclave was heated at 375 °C for 3 days and then cooled to room temperature. The solid products were recovered by suction filtration and washed with distilled water. Very few red block-like crystals of the title compound were obtained. However, reproduction of the crystal preparation was not successful.

## Discussion

The hydrothermal method has been used successfully to synthesize a large variety of novel phosphates, phosphanates and oxides with a number of transition metal ions [1–4]. Open framework phosphates containing transition metals are of particular interest because they show high chemical activity which results from the ability of metals to possess more than one oxidation state and they have high thermal stability [5]. The literature includes extensive work on open framework titanium, cobalt, iron, vanadium and zinc phosphates [6]. However, there have not been many reports of open framework manganese phosphates systems [7].

In the present work we were able to synthesize the manganese-containing phosphate of the formula  $\text{Sr}_2\text{Mn}[\text{PO}_4][\text{P}_2\text{O}_7]$ . The crystal structure is composed of  $\text{MnO}_6$  octahedra and  $\text{PO}_4$  tetrahedra and  $\text{P}_2\text{O}_7$  groups. There is no direct connection between  $\text{MnO}_6$  octahedra in the structure, they are all surrounded with phosphate groups. The manganese atom is connected to two  $\text{PO}_4$  tetrahedra and three  $\text{P}_2\text{O}_7$  groups, one of which is coordinated as a bidentate ligand. Its environment is a distorted octahedron formed by oxygen atoms, and  $\text{Mn—O}$  bonds range from 1.937(5) Å to 2.301(5) Å. Each  $\text{PO}_4$  group shares corners with two  $\text{MnO}_6$  octahedra and has two bonds to each strontium atom. The  $\text{P—O}$  distances range from 1.502(5) Å to 1.634(5) Å. One of the  $\text{P}_2\text{O}_7$  groups is bonded to a Mn atom as a chelate and two of the  $\text{P}_2\text{O}_7$  groups are bonded to two Mn atoms as monodentate ligands. The crystal structure of  $\text{Sr}_2\text{Mn}[\text{PO}_4][\text{P}_2\text{O}_7]$  contains channels where  $\text{Sr}^{2+}$  cations reside. The Sr atom has nine interactions with oxygen atoms ranging from 2.397(5) Å to 3.180(5) Å.

## Abstract

$\text{MnO}_{11}\text{P}_3\text{Sr}_2$ , monoclinic,  $P12_1/c1$  (no. 14),  $a = 6.641(1)$  Å,  $b = 6.834(1)$  Å,  $c = 19.554(4)$  Å,  $\beta = 99.22(3)^\circ$ ,  $V = 876.0$  Å<sup>3</sup>,  $Z = 4$ ,  $R_{\text{gt}}(F) = 0.051$ ,  $wR_{\text{ref}}(F^2) = 0.090$ ,  $T = 298$  K.

## Source of material

The following reagents were used as obtained:  $\text{SrCO}_3$  (Sigma-Aldrich, 98 %),  $\text{Mn}_2\text{O}_3$  (Aldrich, 98 %) and  $\text{H}_3\text{PO}_4$  (Merck, 99 %).  $\text{Sr}_2\text{Mn}(\text{PO}_4)(\text{P}_2\text{O}_7)$  was obtained from the reaction of  $\text{SrCO}_3$

**Table 1.** Data collection and handling.

Crystal:	red column, size 0.034 × 0.055 × 0.420 mm
Wavelength:	Mo $K_{\alpha}$ radiation (0.71073 Å)
$\mu$ :	141.59 cm <sup>-1</sup>
Diffractometer, scan mode:	Bruker SMART 1000 CCD, $\omega$
$2\theta_{\text{max}}$ :	50°
$N(hkl)_{\text{measured}}$ , $N(hkl)_{\text{unique}}$ :	6776, 1491
Criterion for $I_{\text{obs}}$ , $N(hkl)_{\text{gt}}$ :	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$ , 1478
$N(\text{param})_{\text{refined}}$ :	154
Programs:	SHELXS-97 [8], SHELXL-97 [9]

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**Table 2.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	x	y	z	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Sr(1)	4e	0.3120(1)	0.6396(1)	0.42803(3)	0.0125(3)	0.0199(4)	0.0129(3)	0.0030(3)	-0.0017(2)	-0.0029(3)
Sr(2)	4e	0.33686(9)	0.95977(9)	0.23060(3)	0.0107(3)	0.0120(3)	0.0196(3)	-0.0002(2)	0.0033(2)	-0.0025(2)
Mn(1)	4e	0.0410(2)	1.1307(1)	0.37642(5)	0.0103(5)	0.0107(5)	0.0088(5)	-0.0012(4)	0.0003(4)	0.0003(4)
P(1)	4e	-0.4429(2)	1.1359(2)	0.40822(8)	0.0072(8)	0.0112(8)	0.0094(7)	-0.0004(6)	-0.0004(6)	0.0013(6)
P(2)	4e	-0.1761(2)	0.9583(3)	0.22873(8)	0.0072(8)	0.0117(8)	0.0088(7)	0.0000(6)	-0.0003(6)	-0.0010(6)
P(3)	4e	0.1780(3)	1.1913(2)	0.54339(8)	0.0082(8)	0.0127(8)	0.0091(7)	-0.0007(6)	0.0000(6)	0.0011(6)
O(1)	4e	0.3683(7)	1.0214(7)	0.3754(2)	0.009(2)	0.015(2)	0.016(2)	-0.000(2)	-0.001(2)	-0.002(2)
O(2)	4e	-0.2959(7)	1.1782(7)	0.3567(2)	0.012(2)	0.015(2)	0.014(2)	0.000(2)	0.002(2)	0.004(2)
O(3)	4e	0.3141(7)	1.0052(7)	0.5313(2)	0.011(2)	0.020(3)	0.009(2)	0.003(2)	-0.000(2)	0.002(2)
O(4)	4e	0.4920(7)	0.6873(7)	0.5508(2)	0.010(2)	0.013(2)	0.018(2)	-0.001(2)	0.000(2)	-0.000(2)
O(5)	4e	0.0754(7)	1.3849(7)	0.3360(2)	0.011(2)	0.017(2)	0.012(2)	-0.001(2)	0.002(2)	0.002(2)
O(6)	4e	0.3053(7)	0.6352(7)	0.2977(2)	0.015(2)	0.014(2)	0.013(2)	-0.003(2)	0.001(2)	0.000(2)
O(7)	4e	0.0104(7)	1.0146(7)	0.2847(2)	0.008(2)	0.018(2)	0.015(2)	-0.001(2)	-0.002(2)	-0.004(2)
O(8)	4e	0.3102(7)	1.3066(7)	0.2452(2)	0.012(2)	0.012(2)	0.021(2)	0.002(2)	0.003(2)	0.002(2)
O(9)	4e	-0.0010(7)	0.8811(7)	0.4199(2)	0.011(2)	0.016(3)	0.016(2)	-0.001(2)	0.003(2)	0.004(2)
O(10)	4e	0.3072(7)	1.3411(7)	0.5859(2)	0.015(3)	0.020(3)	0.018(2)	-0.005(2)	-0.001(2)	-0.001(2)
O(11)	4e	0.0873(7)	1.2597(7)	0.4676(2)	0.014(2)	0.017(2)	0.007(2)	0.003(2)	-0.001(2)	0.001(2)

*Acknowledgments.* We are indebted to the Scientific and Technological Research Council of Turkey (grant no. TBAG-2160(102T052)) and the L'Oreal Türkýye for support of this work.

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