Crystal structure of potassium diaquamanganese(II) borophosphate monohydrate, $K[Mn(H_2O)_2(BP_2O_8)] \cdot H_2O$

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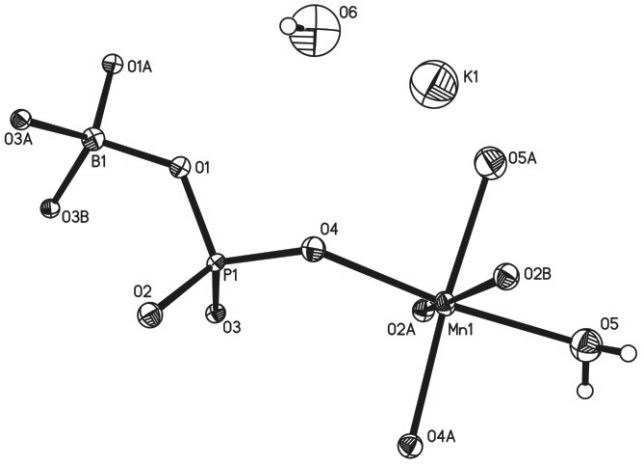

Abstract

$BH_6KMnO_{11}P_2$, hexagonal, $P6_522$ (no. 179), a = 9.683(4) Å, c = 16.139(6) Å, V = 1310.5 Å^3, Z = 6, $R_{gt}(F)$ = 0.057, $wR_{ref}(F^2)$ = 0.182, T = 293 K.

Source of material

All regents were of analytic grade and were used without further purification. A mixture of 1.5285 g $K_2B_4O_7 \cdot 4H_2O$, 0.0371 g Ga_2O_3, 0.4366 g MnO_2, 0.5743 g $MnCO_3$, and 3 mL H_3PO_4 was sealed in a 25 mL Teflon-lined stainless-steel vessel and heated at 448 K for about 20 days under autogenous pressure, then cooled to room temperature. The resulting columnar colorless crystals were collected and dried in air at ambient temperature. IR data are available in the CIF file.

Experimental details

The water H atoms were located in a difference Fourier map and were placed in calculated positions. The contents of the channels described in the discussion are probably more disordered than the reported structure suggests, which leads to the slightly high R values.

Discussion

Open-framework transition metal borophosphates attract much attention because of their rich structural varieties and potential applications as magnetic, optical and ion-exchanging materials [1]. Within a study on the synthesis of such compounds, the crystals of $K[Mn(H_2O)_2(BP_2O_8)] \cdot H_2O$ have been obtained. In the literature, only the unit cell of this compound has been reported [2].

The title crystal structure is composed of $(BP_2O_8)^{3-}$ anions and $[Mn(H_2O)_2]^{2+}$ and K^+ cations. The polyanion $(BP_2O_8)^{3-}$ consists of vertices condensed BO_4 and PO_4 tetrahedra. The polyanions are interlinked by $[Mn(H_2O)_2]^{2+}$ cations to form a three-dimensional framework containing channels, in which the K^+ cations and lattice water molecules reside. In addition, there exists hydrogen bonding not only among H_2O molecules but also between the H_2O molecules and the polyanion framework.

Table 1. Data collection and handling.

Crystal:	colorless column, size 0.15 × 0.19 × 0.24 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	24.07 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ/ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6595, 767
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 726
$N(param)_{refined}$:	88
Programs:	SHELXS-97, SHELXL-97, SHELXTL [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	12c	0.55(2)	0.87(1)	0.095(6)	0.06(4)
H(2)	12c	0.566(4)	0.847(5)	0.022(2)	–0.03(1)
H(3)	12c	0.04(1)	0.090(5)	0.207(5)	0.06(4)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K(1)	6b	0.1841(3)	2x	¼	0.076(2)	0.075(1)	0.074(2)	0.0377(7)	0.001(1)	0
Mn(1)	6b	0.4497(1)	1–x	½	0.0196(6)	U_{11}	0.0237(8)	0.0111(6)	–0.0036(5)	U_{13}
P(1)	12c	0.3837(2)	0.1656(2)	0.0839(1)	0.0120(8)	0.0110(8)	0.0128(8)	0.0044(6)	–0.0001(6)	0.0007(6)
B(1)	6b	0.1495(8)	–x	½	0.021(2)	U_{11}	0.021(2)	0.010(1)	0.0000(7)	U_{13}
O(1)	12c	0.2131(7)	0.0205(7)	0.0977(3)	0.018(2)	0.017(2)	0.018(2)	0.009(1)	0.0000(9)	0.0004(9)
O(2)	12c	0.5100(7)	0.1352(7)	0.1211(3)	0.021(2)	0.022(2)	0.022(2)	0.011(1)	–0.0015(9)	0.0014(9)
O(3)	12c	0.4124(6)	0.1815(6)	–0.0131(3)	0.016(1)	0.016(1)	0.015(1)	0.008(1)	–0.0009(9)	0.0011(9)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(4)	12*c*	0.3798(7)	0.3091(7)	0.1183(3)	0.023(2)	0.022(2)	0.023(2)	0.011(1)	–0.0004(9)	–0.001(1)
O(5)	12*c*	0.504(1)	0.804(1)	0.0584(5)	0.042(2)	0.042(2)	0.042(2)	0.022(1)	–0.002(1)	–0.000(1)
O(6)	6*a*	0	0.116(3)	¼	0.104(2)	U_{11}	U_{11}	$U_{11}/2$	0.0003(9)	$U_{13}/2$

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