SHORT COMMUNICATIONS

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Structure of $K_2Mn(SeO_3)_2$, a further buetschliite-type selenite.

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Abstract

Dipotassium manganese diselenite, $K_2Mn(SeO_3)_2$, M_r = 387.05, trigonal, $R\bar{3}m$, a = 5.615 (1), c = 18.667 (3) Å, V = 509.6 (2) Å^3, Z = 3, D_x = 3.784 Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, μ = 13.45 mm^{-1}, $F(000)$ = 537, T = 295 K. R = 0.033, wR = 0.035 for 421 independent reflections with $F_o > 3\sigma(F_o)$ and 16 refined parameters. $K_2Mn(SeO_3)_2$ is isotypic with the compound $K_2Co(SeO_3)_2$, which was recently described [Wildner (1992). *Acta Cryst.* **C48**, 410–412], as well as with buetschliite-type carbonates.

Crystals of $K_2Mn(SeO_3)_2$ were prepared in analogy to $K_2Co(SeO_3)_2$ (Wildner, 1992). X-ray intensities of a single crystal [diameter ≃ 0.14 mm, crystallographic forms $\{10\bar{1}1\}$ and $\{0001\}$] were measured on a Stoe AED2 four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation: $2\theta/\omega$ scan mode with a minimum of 30 steps per reflection (0.5 to 1.5 s and 0.03° per step), five steps each side for background measurements; three standard reflections every 120 min (maximum drift ± 2.2%), 2265 measured reflections up to $2\theta = 80°$ (h: $-10 \rightarrow 10$, k: $0 \rightarrow 10$, l: $-34 \rightarrow 34$), 435 unique reflections ($R_{\rm int}$ = 0.065); spherical absorption correction (transmission factors: 0.13 to 0.17) and corrections for Lorentz and polarization effects were applied. Complex neutral atomic scattering curves were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The refinement of 16 variables, using 421 reflections with $F_o > 3\sigma(F_o)$, was started with the atomic coordinates of $K_2Co(SeO_3)_2$ and gave R = 0.033, wR = 0.035 $\{w = [\sigma(F_o)]^{-2}\}$, S = 3.50; extinction factor (Zachariasen, 1967) g = 1.5 (1) × 10^{-5}; $(\Delta/\sigma)_{\rm max} < 10^{-3}$; electron densities in final difference Fourier synthesis: $(\Delta\rho)_{\rm max}$ = 1.87, $(\Delta\rho)_{\rm min}$ = −2.27 e Å^{-3}. Lattice parameters were refined from 35 accurate 2θ values in the range $38 < 2\theta < 42°$. All calculations were performed with the program system *STRUCSY* (Stoe & Cie, 1984). Table 1* lists atomic coordinates and isotropic displacement parameters, Table 2 relevant interatomic distances and bond angles.

Table 1. *Atomic coordinates and equivalent isotropic displacement parameters* (Å^2 × 10^4) *for* $K_2Mn(SeO_3)_2$ *with e.s.d.'s in parentheses*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
K	0	0	0.19504 (6)	267 (4)
Mn	0	0	0	165 (2)
Se	0	0	0.62803 (2)	157 (2)
O	0.15808 (20)	−0.15808 (20)	0.59039 (12)	230 (7)

Table 2. *Selected interatomic bond lengths* (Å) *and angles* (°) *in* $K_2Mn(SeO_3)_2$ *with e.s.d.'s in parentheses*

K—O	3.038 (1) (6 ×)			O—O	2.663 (2) (3 ×)
	2.796 (2) (3 ×)				2.952 (2) (6 ×)
					3.708 (4) (6 ×)
Mn—O	2.221 (1) (6 ×)	O—Mn—O	83.30 (9)	O—O	2.952 (2) (6 ×)
			96.70 (9)		3.319 (4) (6 ×)
Se—O	1.690 (1) (3 ×)	O—Se—O	103.93 (9)	O—O	2.663 (2) (3 ×)

The structural features found in $K_2Mn(SeO_3)_2$ are essentially the same as in the isotypic compound $K_2Co(SeO_3)_2$ (Wildner, 1992). As pointed out in the paper on the Co compound, the stereochemical activity of Se$^{\rm IV}$ atoms causes significant modifications of the selenites as compared to the isotypic carbonates $K_2Ca(CO_3)_2$ (buetschliite: Pabst, 1974; Knobloch, Pertlik & Zemann, 1980; Effenberger & Langhof, 1984) and $K_2Mg(CO_3)_2$ (Hesse & Simons, 1982).

References

EFFENBERGER, H. & LANGHOF, H. (1984). *Acta Cryst.* **C40**, 1299–1300.

HESSE, K.-F. & SIMONS, B. (1982). *Z. Kristallogr.* **161**, 289–292.

KNOBLOCH, D., PERTLIK, F. & ZEMANN, J. (1980). *Neues Jahrb. Mineral. Monatsh.* pp. 230–236.

PABST, A. (1974). *Am. Mineral.* **59**, 353–358.

Stoe & Cie (1984). *STRUCSY Structure System Program Package.* Stoe & Cie, Darmstadt, Germany.

WILDNER, M. (1992). *Acta Cryst.* **C48**, 410–412.

ZACHARIASEN, W. H. (1967). *Acta Cryst.* **23**, 558–564.

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* Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54653 (5 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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