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Magnesium selenite dihydrate, $MgSeO_3·2H_2O$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Mg–O) = 0.0014 Å
R factor = 0.023
wR factor = 0.061
Data-to-parameter ratio = 19.1

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

Hydrothermally prepared $MgSeO_3·2H_2O$ consists of pairs of edge-sharing MgO_6 (4O, $2H_2O$) octahedra [d_{av}(Mg—O) = 2.095 (2) Å]. These are linked by pyramidal SeO_3 units [d_{av}(Se—O) = 1.697 (2) Å] and hydrogen bonds forming a three-dimensional network.

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Comment

$MgSeO_3·2H_2O$ is isostructural with the mineral cobaltomenite (Leider & Gattow, 1967) and the synthetic compounds $CoSeO_3.2H_2O$ and $NiSeO_3·2H_2O$ (Wildner, 1990).

The magnesium cation adopts a slightly distorted octahedral coordination with Mg—O distances typical of other magnesium selenites (Mueller *et al.*, 1996; Kohn *et al.*, 1976). The bond valence sum (BVS; Brown, 1996) for Mg of 2.04 is close to the expected value of 2.00. O4 and O5 belong to water molecules and have a significant role in hydrogen bonding.

The SeO_3 unit adopts its usual pyramidal coordination (Hawthorne *et al.*, 1987; Harrison, 1999) with BVS for Se = 4.09 (expected 4.00).

The MgO_6 octahedra form edge-sharing, $Mg_2O_{10}H_8$ pairs (Fig. 1), with each pair connected to six SeO_3 pyramids. Each SeO_3 unit links three octahedral pairs. When viewed down [001] (Fig. 2), the octahedral pairs are situated at the unit-cell corners (UCC) and body centre (BC). This also shows the twisting of the BC $Mg_2O_{10}H_8$ pair relative to the UCC pairs.

Hydrogen bonding, which has been described in detail elsewhere (Wildner, 1990), completes the three-dimensional framework. All four H atoms are involved (Table 2). O4 is a donor, whilst O5 both donates and accepts hydrogen bonds.

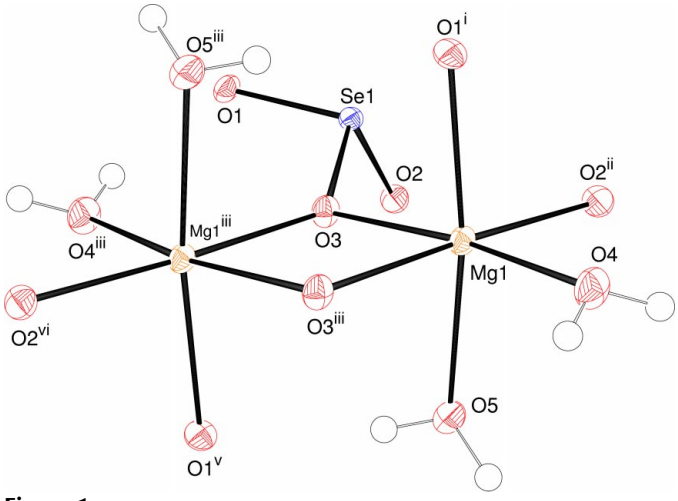

Figure 1
Fragment of the $MgSeO_3.2H_2O$ structure (50% displacement ellipsoids). H atoms are shown as white spheres. Symmetry codes as in Table 1, with the addition of (v) $\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z$ and (vi) $1+x, y, z$.

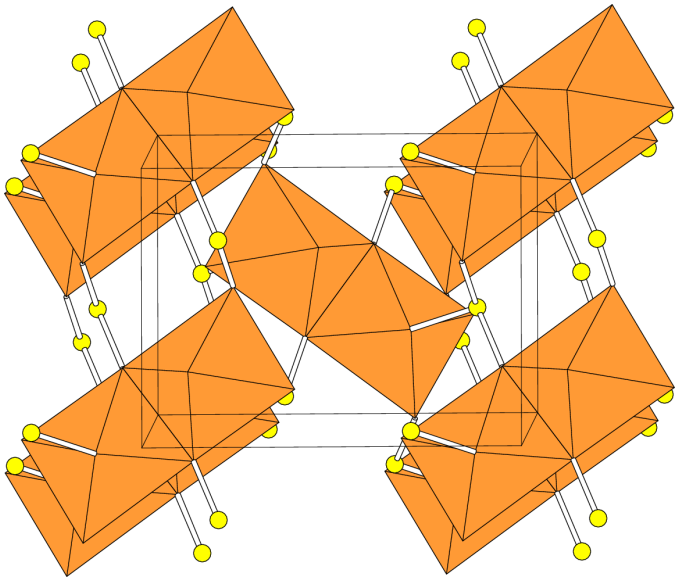

Figure 2
Slice of $MgSeO_3.2H_2O$ viewed down [001], with MgO_6 groups represented as orange octahedra and Se (yellow) atoms represented by spheres of arbitrary radii.

Experimental

Direct reaction of $MgCO_3$ (0.759 g, 9 mmol), SeO_2 (1.333 g, 12 mmol) and 15 ml of water; the reactants were placed in a 23-ml-capacity sealed teflon-lined steel bomb in an oven at 413 K. The bomb was removed after 26 d and cooled over 3 h. Upon opening, the bomb was seen to contain a clear solution and very large (*ca* 1.5 × 0.5 × 0.5 mm maximum) colourless single crystals. The crystals were recovered by suction filtration and washing with water.

Crystal data

$MgSeO_3·2H_2O$
M_r = 187.30
Monoclinic, $P2_1/n$
a = 6.4818 (3) Å
b = 8.7975 (5) Å
c = 7.6367 (4) Å
β = 98.753 (1)°
V = 430.40 (4) Å^3
Z = 4
D_x = 2.891 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3192 reflections
θ = 3.6–32.5°
μ = 8.77 mm^{-1}
T = 293 K
Chunk, colourless
0.52 × 0.18 × 0.15 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.118, T_{max} = 0.268
4223 measured reflections
1545 independent reflections
1426 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 32.5°
$h = -9 \rightarrow 7$
$k = -13 \rightarrow 12$
$l = -10 \rightarrow 11$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.02
1545 reflections
81 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.92 (4)

Table 1
Selected geometric parameters (Å, °).

Se1—O1	1.6996 (13)	Mg1—O3	2.0739 (13)
Se1—O2	1.6864 (13)	Mg1—O3^{iii}	2.1054 (14)
Se1—O3	1.7042 (12)	Mg1—O4	2.0144 (14)
Mg1—O1^{i}	2.1383 (15)	Mg1—O5	2.1822 (16)
Mg1—O2^{ii}	2.0559 (14)		
Se1—O1—Mg1^{iv}	119.11 (7)	Se1—O3—Mg1^{iii}	137.18 (7)
Se1—O2—Mg1^{ii}	123.73 (7)	Mg1—O3—Mg1^{iii}	97.98 (5)
Se1—O3—Mg1	116.10 (7)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···O1^{i}	0.67 (6)	2.09 (6)	2.743 (2)	165 (5)
O4—H2···O5^{ii}	0.80 (4)	2.18 (4)	2.965 (2)	171 (4)
O5—H3···O1^{iii}	0.77 (3)	2.11 (3)	2.8734 (19)	171 (3)
O5—H4···O2^{ii}	0.90 (3)	1.85 (3)	2.741 (2)	167 (3)

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

The highest difference peak is 0.71 Å from Se1 and the deepest difference hole is 0.71 Å from Se1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *ATOMS* (Shape Software, 1999); software used to prepare material for publication: *SHELXL*97.

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