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Magnesium selenate hexahydrate, $MgSeO_4 \cdot 6H_2O$

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$MgSeO_4 \cdot 6H_2O$ is isostructural with its sulfate analogue and the corresponding cobalt(II) salt. The structure is based on alternating layers of $Mg(H_2O)_6$ octahedra and SeO_4 tetrahedra parallel to (001), connected *via* hydrogen bonds. All atoms are on general positions except Mg1 and Mg2 (site symmetries 2 and $\bar{1}$, respectively). The average Mg—O and Se—O bond lengths are 2.066 and 1.639 Å, respectively.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Se–O) = 0.001 Å
R factor = 0.019
wR factor = 0.055
Data-to-parameter ratio = 18.3

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

Comment

Magnesium selenate(VI) hexahydrate, $MgSeO_4 \cdot 6H_2O$, crystallizes in the monoclinic structure type of its sulfate analogue $MgSO_4 \cdot 6H_2O$ (*C*2/*c*; Zalkin *et al.*, 1964), known in nature as the mineral hexahydrite. It is also isostructural with the selenates $Co^{II}SeO_4 \cdot 6H_2O$ (Ojkova *et al.*, 1992) and $Fe^{II}SeO_4 \cdot 6H_2O$ (ICDD-PDF 51-1819). In contrast, both $Ni^{II}SeO_4 \cdot 6H_2O$ (Snyman & Pistorius, 1964; Fuess, 1970; Ptasiewicz-Bak *et al.*, 1993) and $ZnSeO_4 \cdot 6H_2O$ (Hajek & Cepelak, 1965; Stadnicka *et al.*, 1988; Koleva & Stoilova, 1995) are tetragonal with space group $P4_12_12$. Interestingly, the substitution of only about 4%

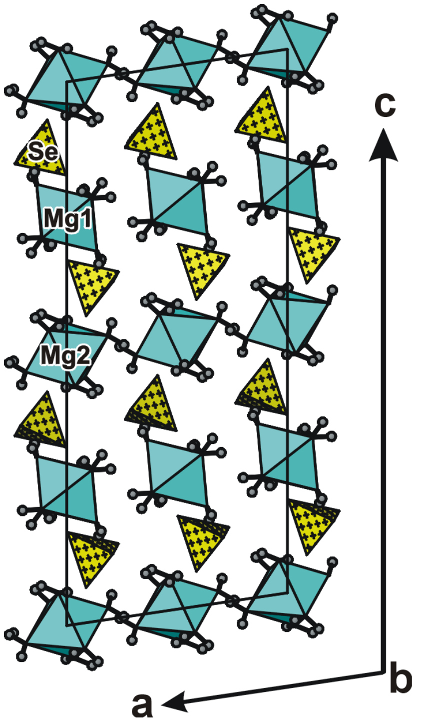

Figure 1
Polyhedral view of $MgSeO_4 \cdot 6H_2O$ along [010]. Layers of $Mg(H_2O)_6$ octahedra (turquoise) parallel to (001) alternate with layers of SeO_4 tetrahedra (yellow and marked with crosses). The unit cell is outlined.

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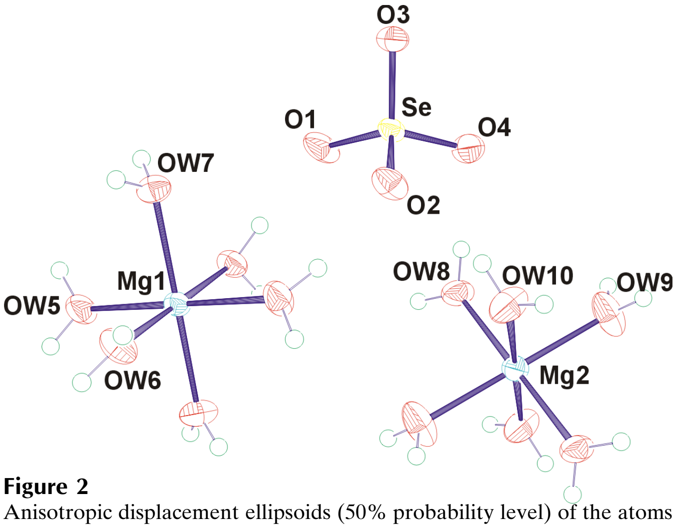

Figure 2
Anisotropic displacement ellipsoids (50% probability level) of the atoms in the two $Mg(H_2O)_6$ octahedra and the SeO_4 tetrahedron.

Ni^{II} for Mg in $MgSeO_4{\cdot}6H_2O$ causes the structure to become tetragonal (Stoilova *et al.*, 1995). No data are available on hypothetical $M^{II}SeO_4{\cdot}6H_2O$ compounds where M = V, Cr, Mn, Cu, Ca, Ru or Cd.

The occurrence of both monoclinic and tetragonal modifications has also been reported for the M^{II}–sulfate hexahydrates (*e.g.* Kutoglu, 1973; Angel & Finger, 1988; Gerkin & Reppart, 1988). In nature, monoclinic and tetragonal $Ni^{II}SO_4{\cdot}6H_2O$ are known as the minerals nickel hexahydrite and retgersite, respectively (Mandarino, 1999). The monoclinic structure type is apparently also found for the fluoroberyllate hexahydrates $M^{II}BeF_4{\cdot}6H_2O$ where M = Co, Ni, Zn (Crouzet & Aleonard, 1969; Tedenac *et al.*, 1969).

The unit-cell volume of the title compound is about 5.2% larger than that of its sulfate analogue (Zalkin *et al.*, 1964). This percentage compares favourably with the volume difference of 5.1% between the isostructural oxysalt pentahydrates $CuSeO_4{\cdot}5H_2O$ and $CuSO_4{\cdot}5H_2O$ (Kolitsch, 2001).

The polyhedral arrangement in the structure of $MgSeO_4{\cdot}6H_2O$ is characterized by alternating layers of $Mg(H_2O)_6$ octahedra and SeO_4 tetrahedra oriented parallel to the (001) plane (Figs. 1 and 2). The average Mg—O and Se—O bond lengths of 2.066 and 1.639 Å, respectively, are close to expected values. The connection between adjacent polyhedra is achieved *via* medium–strong to weak hydrogen bonds accepted by the oxygen ligands of the SeO_4 group (Table 2). Atom H62, which is involved in the longest hydrogen bond [$OW6\cdots OW7^{ii}$ = 3.0671 (19) Å], shows the largest displacement parameter (if freely refined) of all H atoms, and it is also the only H atom which donates a hydrogen bond to a water molecule. A determination of the single-crystal unit-cell parameters at 120 K indicated no structural change in the title compound.

The dehydration of $MgSeO_4{\cdot}6H_2O$ has been studied by Stoilova & Koleva (1995*a*,*b*), who observed the penta-, tetra-, di- and monohydrate, as well as anhydrous magnesium selenate, and found that all compounds are isostructural with their sulfate analogues.

Experimental

The title compound was prepared by controlled evaporation at room temperature of an aqueous solution containing selenic acid and magnesium carbonate. Colourless crude columnar crystals up to several cm in length formed. A single large crystal of the selenite $MgSeO_3{\cdot}6H_2O$ (Andersen & Lindqvist, 1984) accompanied these crystals.

Crystal data

$MgSeO_4{\cdot}6H_2O$
$M_r = 275.37$
Monoclinic, $C2/c$
$a = 10.224$ (1) Å
$b = 7.370$ (1) Å
$c = 24.866$ (2) Å
$\beta = 98.41$ (1)°
$V = 1853.5$ (3) Å^3
$Z = 8$

$D_x = 1.974$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2899 reflections
$\theta = 2.0$–30.0°
$\mu = 4.15$ mm^{-1}
$T = 293$ (2) K
Fragment, colourless
0.15 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*HKL SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.575$, $T_{max} = 0.733$
5214 measured reflections

2705 independent reflections
2510 reflections with $I > 2\sigma(I)$
$R_{int} = 0.010$
$\theta_{max} = 30.0°$
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 10$
$l = -35 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.055$
$S = 1.06$
2705 reflections
148 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 1.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0023 (2)

Table 1
Selected geometric parameters (Å, °).

Se—O1	1.6274 (13)	Mg1—OW6	2.0632 (13)
Se—O2	1.6401 (11)	Mg1—OW7	2.0899 (12)
Se—O3	1.6439 (11)	Mg2—OW8^{ii}	2.0471 (12)
Se—O4	1.6449 (12)	Mg2—OW9^{ii}	2.0493 (13)
Mg1—OW5^{i}	2.0582 (13)	Mg2—OW10	2.0870 (14)
O1—Se—O2	110.95 (6)	OW6—Mg1—OW7	90.65 (5)
O1—Se—O3	110.02 (7)	OW6^{i}—Mg1—OW7	178.56 (5)
O2—Se—O3	110.06 (6)	OW7—Mg1—OW7^{i}	88.35 (7)
O1—Se—O4	110.22 (8)	OW8^{ii}—Mg2—OW8	180.00 (6)
O2—Se—O4	107.50 (7)	OW8^{ii}—Mg2—OW9^{ii}	87.97 (6)
O3—Se—O4	108.01 (6)	OW8—Mg2—OW9^{ii}	92.03 (6)
OW5^{i}—Mg1—OW5	179.96 (8)	OW8^{ii}—Mg2—OW10	92.45 (5)
OW5^{i}—Mg1—OW6	87.12 (6)	OW8—Mg2—OW10	87.55 (5)
OW5—Mg1—OW6	92.91 (6)	OW9^{ii}—Mg2—OW10	91.15 (7)
OW6—Mg1—OW6^{i}	90.37 (8)	OW9—Mg2—OW10	88.85 (7)
OW5^{i}—Mg1—OW7	88.16 (6)	OW8—Mg2—OW10^{ii}	92.45 (5)
OW5—Mg1—OW7	91.81 (5)		

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

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

$D—\mathrm{H}\cdots A$	$D—\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D—\mathrm{H}\cdots A$
O*W*5—H51···O3$^{\mathrm{i}}$	0.855 (17)	1.953 (18)	2.7997 (17)	170 (3)
O*W*5—H52···O2	0.876 (17)	1.922 (18)	2.7783 (17)	165 (3)
O*W*6—H61···O1$^{\mathrm{i}}$	0.855 (17)	1.890 (18)	2.7339 (18)	169 (3)
O*W*6—H62···O*W*7$^{\mathrm{ii}}$	0.832 (17)	2.307 (19)	3.0671 (19)	152 (2)
O*W*7—H71···O1	0.872 (17)	1.828 (17)	2.6962 (17)	174 (3)
O*W*7—H72···O3$^{\mathrm{iii}}$	0.870 (17)	1.929 (18)	2.7784 (17)	165 (3)
O*W*8—H81···O3$^{\mathrm{iv}}$	0.836 (16)	1.951 (17)	2.7763 (17)	169 (3)
O*W*8—H82···O4$^{\mathrm{v}}$	0.835 (17)	1.946 (17)	2.7737 (18)	171 (3)
O*W*9—H91···O4$^{\mathrm{i}}$	0.862 (17)	1.873 (17)	2.7346 (19)	178 (3)
O*W*9—H92···O2$^{\mathrm{iii}}$	0.840 (17)	1.963 (17)	2.8008 (18)	175 (3)
O*W*10—H101···O2	0.839 (17)	2.103 (18)	2.9190 (19)	164 (3)
O*W*10—H102···O4$^{\mathrm{iv}}$	0.859 (18)	2.09 (2)	2.924 (2)	164 (3)

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

All O*W*—H distances were restrained to a length of 0.90 (2) Å, and H atoms were constrained to have a fixed U_{iso} of 0.06 Å^2. (Note: freely refined O—H distances ranged between 0.68 and 0.85 Å; the largest isotropic displacement parameters were shown by the H atoms bonded to O*W*6.)

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Shape Software, 1999) and *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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