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Propane-1,2-diaminium selenite monohydrate

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The title compound, $C_3H_{12}N_2^{2+}\cdot SeO_3^{2-}\cdot H_2O$, contains a network of propane-1,2-diaminium ($C_3H_{12}N_2^{2+}$) cations, selenite (SeO_3^{2-}) anions and water molecules. The crystal packing involves N—H⋯O [average H⋯O = 1.89 Å, N—H⋯O = 165° and N⋯O = 2.777 (3) Å] and O—H⋯O hydrogen bonds, resulting in a layered structure.

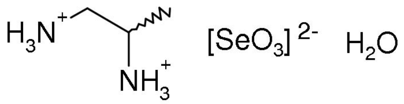
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.068
Data-to-parameter ratio = 19.8

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

Comment

The title compound, (I), was prepared as part of our ongoing studies of hydrogen-bonding interactions in the crystal structures of (protonated) amine phosphates (Demir *et al.*, 2003), phosphites (Harrison, 2003), selenites (Ritchie & Harrison, 2003) and arsenates (Lee & Harrison, 2003*a*,*b*,*c*; Wilkinson & Harrison, 2004).



(I)

The asymmetric unit of (I) contains one $C_3H_{12}N_2^{2+}$ cation, one SeO_2^{2-} anion and a water molecule (Fig. 1). The geometric parameters for the organic cation are unexceptional (Lee & Harrison, 2003*a*). This species is chiral (C1 has *S* configuration in the selected asymmetric unit), but crystal symmetry generates a 50:50 mix of enantiomers, consistent

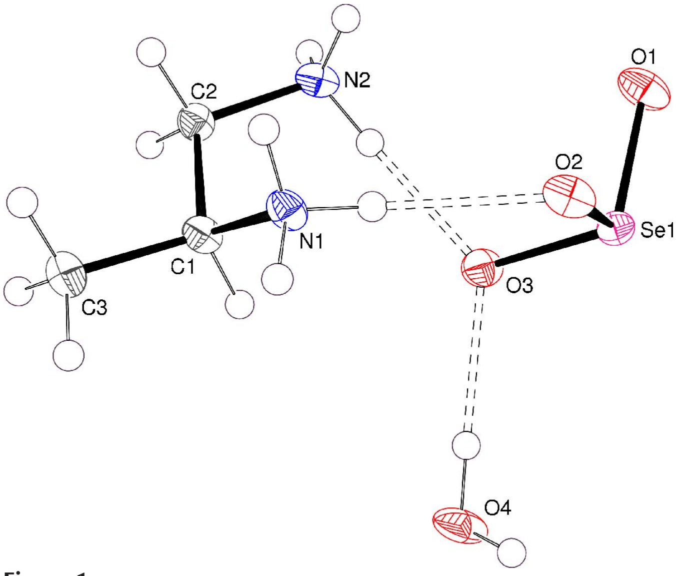


Figure 1
Asymmetric unit of (I), showing 50% displacement ellipsoids (arbitrary spheres for H atoms). Hydrogen bonds are indicated by dashed lines.

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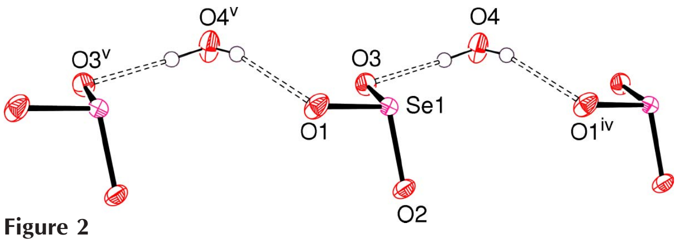

Figure 2
Detail of a hydrogen-bonded selenite/water chain in (I). Symmetry codes are as in Table 2 [additionally: (v) x, $1 + y$, z]. Hydrogen bonds are indicated by dashed lines.

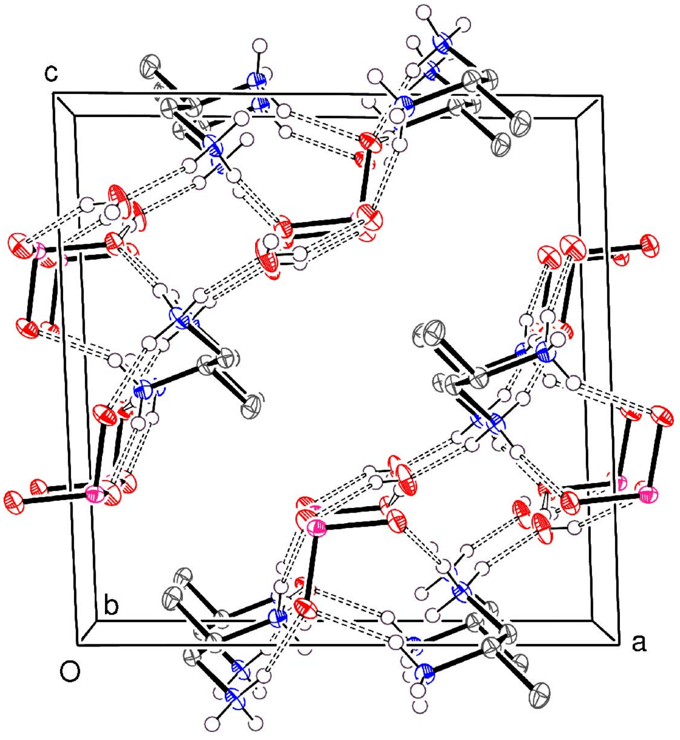

Figure 3
[010] projection of the packing for (I). C-bound H atoms have been omitted for clarity and hydrogen bonds are indicated by dashed lines.

with the racemic starting material. The selenite group in (I) shows its standard (Lee & Harrison, 2003) pyramidal geometry (Table 1) [average Se—O = 1.687 (2) Å], with the Se atom displaced from the plane of its three attached O atoms by 0.7213 (12) Å.

As well as electrostatic attractions, the component species in (I) interact by means of a network of N—H···O and O—H···O hydrogen bonds (Table 2). The selenite anions and water molecules are linked into a polymeric chain in the [010] direction by hydrogen bonds (Fig. 2). The organic species interacts with the selenite/water chains by way of N—H···O hydrogen bonds (Table 2). All six of the –NH_3^+ H atoms are involved in these links [mean H···O = 1.89 Å, N—H···O = 165° and N···O = 2.777 (3) Å]. These interactions result in (101) selenite/water/aminium layers sandwiched between the carbon backbones of the organic groups (Fig. 3), which themselves interact by way of van der Waals forces.

Propane-1,2-diaminium hydrogenarsenate monohydrate, $C_3H_{12}N_2^{2+}\cdot HAsO_4^{2-}\cdot H_2O$ (Lee & Harrison, 2003*a*), has an equivalent stoichiometry to (I). As might be expected, where the oxo anion has hydrogen-bonding capability (*i.e.* as As—OH···O links), a quite different overall structure arises. An interesting difference also arises for the organic cation; in (I), the –NH_3^+ and –CH_3 groups are *trans* about their linking C—C bond (Table 1), whereas in the hydrogenarsenate, they are *gauche* [C—C—C—N = −54.09 (18)°].

Experimental

An aqueous 0.5 *M* propane-1,2-diamine solution (10 ml) was added to aqueous 0.5 *M* H_2SeO_3 solution (10 ml, dissolved SeO_2) to result in a clear solution. A mass of colourless platy crystals of (I), with a pale-pink tinge arising from a surface coating, grew as the water evaporated over the course of a few days.

Crystal data

$C_3H_{12}N_2^{2+}\cdot SeO_3^{2-}\cdot H_2O$
$M_r = 221.12$
Monoclinic, $P2/n$
$a = 11.5494$ (7) Å
$b = 6.1399$ (4) Å
$c = 11.6601$ (6) Å
$\beta = 92.213$ (3)°
$V = 826.23$ (8) Å^3
$Z = 4$

$D_x = 1.778$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1941 reflections
$\theta = 2.9$–$27.5°$
$\mu = 4.51$ mm^{-1}
$T = 120$ (2) K
Plate, colourless
0.12 × 0.10 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{\min} = 0.613$, $T_{\max} = 0.915$
8108 measured reflections
1882 independent reflections

1617 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.044$
$\theta_{\max} = 27.5°$
$h = -12 \rightarrow 15$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.068$
$S = 1.07$
1882 reflections
95 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.5437P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.98$ e Å^{-3}
$\Delta\rho_{\min} = -0.51$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0026 (7)

Table 1
Selected geometric parameters (Å, °).

Se1—O1	1.673 (2)	Se1—O2	1.7052 (18)
Se1—O3	1.6826 (19)		
N1—C1—C2—N2	55.2 (3)	C3—C1—C2—N2	176.9 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.91	1.88	2.779 (3)	171
N1—H2···O1^{ii}	0.91	1.81	2.701 (3)	165
N1—H3···O2	0.91	2.00	2.835 (3)	152
N2—H4···O4^{iii}	0.91	1.91	2.802 (3)	165
N2—H5···O3	0.91	1.87	2.777 (3)	173
N2—H6···O2^{ii}	0.91	1.88	2.766 (3)	164
O4—H13···O3	0.88	1.96	2.840 (3)	178
O4—H14···O1^{iv}	0.76	2.04	2.747 (3)	157

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

The non-standard $P2/n$ setting of the space group was chosen in preference to $P2/c$ to avoid a unit cell with a very obtuse β angle of 133.6°. The water H atoms were found in a difference map and refined as riding in their as-found relative positions (Table 2). H atoms bonded to C and N atoms were placed in idealized positions (C—H = 0.98–1.00 Å and N—H = 0.91 Å) and refined as riding, allowing for free rotation of the rigid $-X\mathrm{H}_3$ (X = C3, N1 and N2) groups. The constraint $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{carrier})$ or $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{methyl\ carrier})$ was applied as appropriate.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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