metal-organic compounds

Poly[propane-1,3-diyldiammonium tetra-μ-selenito-trizinc dihydrate]

Lyndsey K. Ritchie and William T. A. Harrison*

Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland
Correspondence e-mail: w.harrison@abdn.ac.uk

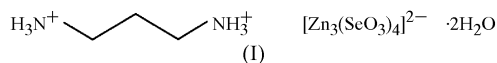The title compound, $(C_3H_{12}N_2)[Zn_3(SeO_3)_4]\cdot2H_2O$, is built up from organic cations, $\{[Zn_3(SeO_3)_4]^{2-}\}_n$ macroanionic sheets and water molecules. The inorganic component of the structure is notable for incorporating both octahedrally and tetrahedrally coordinated Zn atoms. A network of $N-H\cdots O$ and $O-H\cdots O$ hydrogen bonds helps to establish the layered structure. The six-coordinate Zn atom has site symmetry $\bar{1}$, and one C and the two water O atoms have site symmetry m.

Comment

Organically templated inorganic networks have been intensively studied in the last few years and a vast variety of new structures have been described (Cheetham *et al.*, 1999). Many zinc-containing compounds have been reported, with a large majority of these containing tetrahedral ZnO_4 groups in combination with phosphate, hydrogen phosphite, arsenate, selenite, *etc.*, oxo-anions (*e.g.* Ritchie & Harrison, 2004). Here, we describe the synthesis and structure of the title compound, $(C_3H_{12}N_2)[Zn_3(SeO_3)_4]\cdot2H_2O$, (I) (Fig. 1), which contains both octahdral and tetrahedral Zn centres. Compound (I) is quite distict from $(C_3H_{12}N_2)[Zn(SeO_3)_2]$ (Millange *et al.*, 2004), which contains chains built up from vertex-sharing ZnO_4 tetrahedra and SeO_3 pyramids.

$$H_3N^+ \text{———} NH_3^+ \qquad [Zn_3(SeO_3)_4]^{2-} \quad \cdot 2H_2O$$
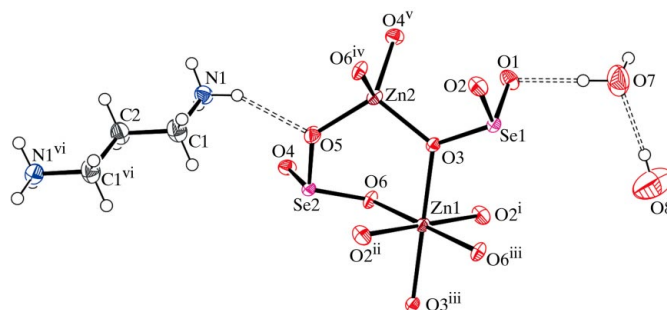$$(I)$$

There are two Zn sites in (I). Atom Zn1 (site symmetry $\bar{1}$) adopts a fairly regular octabedral coordination (Table 1) with a mean $Zn-O$ distance of 2.109 (2) Å [range of *cis* bond angles is 85.85 (9)–94.65 (9)°]. Atom Zn2 is the central atom of a somewhat distorted ZnO_4 tetrahedron, with a mean $Zn-O$ distance of 1.964 (2) Å and $O-Zn-O$ angles varying from 102.48 (10) to 122.01 (10)° (spread = 19.5°).

The two selenite groups in (I) show the usual pyramidal geometry, with mean $Se-O$ values of 1.695 (2) and 1.693 (2) Å for the Se1- and Se2-centred polyhedra, respectively. The $O-Se-O$ bond angles are clustered into the very
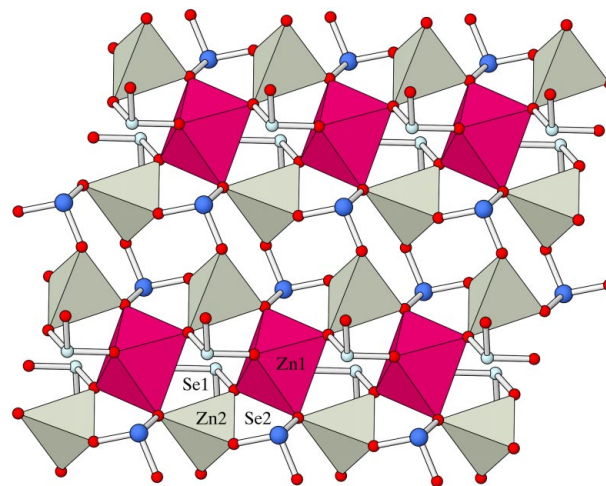
narrow range of 101.35 (12)–102.52 (11)° (spread = 1.2°). The unobserved lone pair of the Se^{IV} atom is presumed to point in the direction of the fourth tetrahedral vertex (Verma, 1999). Atoms Se1 and Se2 are displaced from the planes of their three attached O atoms by 0.7472 (14) and 0.7564 (14) Å, respectively.

There are six framework O atoms in (I). Atom O1 is terminal to Se1 and does not bond to Zn, whereas atoms O2, O4 and O5 are bicoordinate to one Se and one Zn atom, with a mean $Zn-O-Se$ angle of 128.1 (2)°. Finally, atoms O3 and O6 are tricoordinate to two Zn and one Se atom. The bond-angle sums for O3 and O6 are 359.5 and 353.6°, respectively. The $Se1-O1$ bond length is slightly shorter than the bonds between Se and O2, O4 and O5, whilst the $Se-O$ bond lengths for the tricoordinate O atoms are significantly longer.

The complete organic cation is generated by mirror symmetry, with atom C2 lying on the reflecting plane. Other-

Figure 1
View of a fragment of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $x + 1, y, z$; (ii) $-x, 1 - y, 1 - z$; (iii) $1 - x, 1 - y, 1 - z$; (iv) $x - 1, y, z$; (v) $1 - x, 1 - y, 2 - z$; (vi) $x, \frac{3}{2} - y, z$.]

Figure 2
A view of part of an (010) macroanionic layer in (I), with the ZnO_6 and ZnO_4 groups represented by polyhedra.

wise its geometrical parameters are normal. Two uncoordinated water molecules complete the structure of (I). Both water O atoms (O7 and O8) have site symmetry m. The H atoms attached to O8 also lie in the reflecting plane.

The polyhedral connectivity in (I) results in distinctive infinite macroanionic sheets of stoichiometry $[Zn_3(SeO_3)_4]_n^{2n-}$ which propagate in (010). Considered in isolation, the $Zn1O_6$ and $Zn2O_4$ groups form chains that propagate along [100]. Each $Zn1O_6$ octahedron is linked to two neighbouring $Zn1O_6$ moieties by a pair of $Zn2O_4$ tetrahdra, forming 'four-ring' (four-polyhedra) loops. The chains are crosslinked along [001] by the Se2 atoms, forming a sheet. Finally, the Se1–O1 fragments are attached to the four-ring loops, both above and below the plane (Fig. 3).

The organic cation and water molecules occupy the interlayer regions of the structure and interact with the inorganic sheets by way of N—H⋯O and O—H⋯O hydrogen bonds (Table 2). Each –NH$_3^+$ moiety makes two simple N—H⋯O links and one bifurcated N—H⋯(O,O) link, thus serving as a pillar or bridge between the (010) inorganic layers. This pillaring *via* hydrogen bonds is quite different from the direct ligand-like Zn—N bond that can occur in some networks containing Zn (Ritchie & Harrison, 2004).

The O7 water molecule in (I) also bridges the layers, in an O1⋯H—O7—H⋯O1($x, \frac{1}{2} - y, z$) configuration. Finally, the O8 water molecule behaves in a similar way, but the acceptor O atoms are parts of O7 water molecules and not framework O atoms. It is notable that the terminal (non-Zn bound) O1 atom accepts three hydrogen bonds.

Compound (I) complements a handful of other templated phases containing octahedral Zn atoms. The novel phase $(C_6H_{17}N_3)_2[Zn_7(PO_4)_6]$ (Kongshaug *et al.*, 2000) contains ZnO_6 groups incorporated into a chabazite-like tetrahdral ZnO_4/PO_4 framework $[C_6H_{17}N_3^{2+}$ is the 1-(2-aminoethyl)-piperazinium dication]. The partially cobalt-substituted phase $(C_4H_{12}N_2)[Zn_{3-x}Co_x(HPO_3)_4(H_2O)_2]$ ($x \simeq 0.83$; Shi *et al.*, 2004) contains *trans*-$Zn(H_2O)_2O_4$ octahedra as part of a three-dimensional architecture incorporating the organic cations $(C_4H_{12}N_2^{2+}$ is the piperazinium dication).

Experimental

A mixture of 1,3-diaminopropane (0.37 g, 5 mmol), aqueous 0.5 *M* 'H$_2$SeO$_3$' solution (*i.e.* dissolved SeO$_2$; 20 ml, 10 mmol) and ZnO (0.407 g, 5 mmol) was heated to 353 K for 2 d in a plastic bottle. Product recovery by vacuum filtration and rinsing with water and acetone yielded blocks of (I) accompanied by some white powder.

Crystal data

$(C_3H_{12}N_2)[Zn_3(SeO_3)_4]\cdot 2H_2O$	$Z = 2$
$M_r = 816.12$	$D_x = 2.941$ Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation
$a = 4.9345$ (3) Å	$\mu = 11.84$ mm^{-1}
$b = 22.9848$ (13) Å	$T = 293$ (2) K
$c = 8.3987$ (5) Å	Block, colourless
$\beta = 104.623$ (1)°	$0.21 \times 0.15 \times 0.06$ mm
$V = 921.71$ (9) Å^3	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	7902 measured reflections
ω scans	3219 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	2404 reflections with $I > 2\sigma(I)$
$T_{min} = 0.175$, $T_{max} = 0.494$	$R_{int} = 0.038$
	$\theta_{max} = 32.7°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.93$	$\Delta\rho_{max} = 1.08$ e Å^{-3}
3219 reflections	$\Delta\rho_{min} = -0.83$ e Å^{-3}
126 parameters	Extinction correction: *SHELXL97* (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.0040 (3)

Table 1
Selected geometric parameters (Å, °).

Zn1—O2^i	2.048 (2)	Se1—O1	1.674 (2)
Zn1—O3	2.136 (2)	Se1—O2	1.682 (2)
Zn1—O6	2.144 (2)	Se1—O3	1.730 (2)
Zn2—O4^{ii}	1.941 (2)	Se2—O4	1.681 (2)
Zn2—O5	1.946 (2)	Se2—O5	1.682 (2)
Zn2—O3	1.958 (2)	Se2—O6	1.715 (2)
Zn2—O6^{iii}	2.011 (2)		
Se1—O2—Zn1^{iii}	130.32 (13)	Se2—O5—Zn2	127.57 (14)
Se1—O3—Zn2	121.61 (12)	Se2—O6—Zn2^i	117.85 (11)
Se1—O3—Zn1	117.55 (11)	Se2—O6—Zn1	118.24 (11)
Zn2—O3—Zn1	120.34 (11)	Zn2^i—O6—Zn1	117.48 (11)
Se2—O4—Zn2^{ii}	126.44 (13)		

Symmetry codes: (i) $x + 1, y, z$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $x - 1, y, z$.
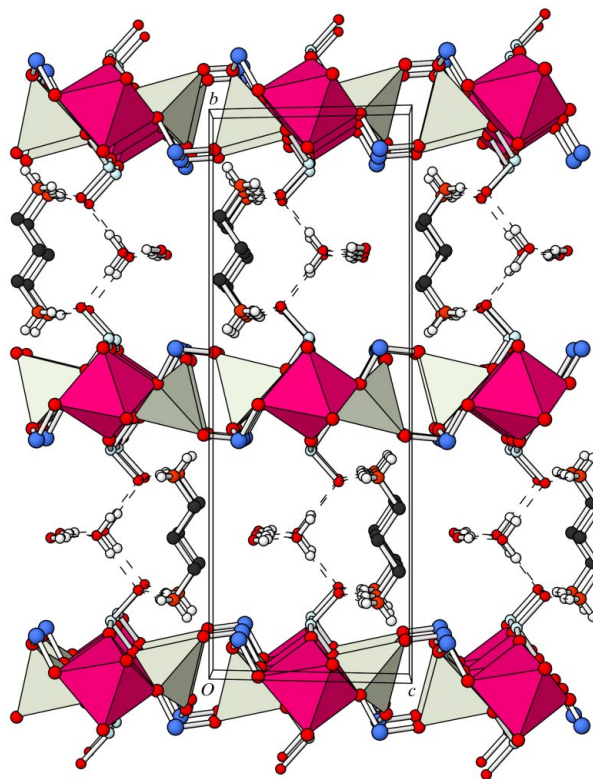

Figure 3
The unit-cell packing in (I), viewed down [100]. Polyhedral drawing conventions are as in Fig. 2. Hydrogen bonds are indicated by dashed lines.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1$\cdots$O5	0.89	2.26	3.081 (4)	153
N1—H1$\cdots$O4^{iii}	0.89	2.33	2.868 (4)	119
N1—H2$\cdots$O1^{iv}	0.89	2.11	2.974 (4)	165
N1—H3$\cdots$O1^{ii}	0.89	1.97	2.857 (4)	174
O7—H4$\cdots$O1	0.90	1.90	2.800 (4)	180
O8—H5$\cdots$O7	0.86	2.12	2.972 (9)	172
O8—H6$\cdots$O7^{i}	0.97	2.02	2.988 (8)	179

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

O-bound H atoms were located in a difference map and refined as riding in their as-found relative locations, with O—H distances in the range 0.86–0.97 Å. H atoms bonded to C or N atoms were placed in idealized locations, with C—H = 0.97 Å and N—H = 0.91 Å, and refined as riding, allowing the –NH$_3$ group to rotate but not tilt. The constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) was applied in all cases.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *ATOMS* (Dowty, 2002); software used to prepare material for publication: *SHELXL97*.

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supporting information

Poly[propane-1,3-diyldiammonium tetra-*μ*-selenito-trizinc dihydrate]

Lyndsey K. Ritchie and William T. A. Harrison

Computing details

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *ATOMS* (Dowty, 2002); software used to prepare material for publication: *SHELXL97*.

Propane-1,3-diyldiammonium tetra-*μ*-selenito-trizinc dihydrate

Crystal data

$(C_3H_{12}N_{20}[Zn_3(SeO_3)_4]\cdot 2H_2O$	$F(000) = 772$
$M_r = 816.12$	$D_x = 2.941$ Mg m^{-3}
Monoclinic $P2_1/m$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yb	Cell parameters from 2685 reflections
$a = 4.9345$ (3) Å	$\theta = 3.1–32.5°$
$b = 22.9848$ (13) Å	$\mu = 11.84$ mm^{-1}
$c = 8.3987$ (5) Å	$T = 293$ K
$\beta = 104.623$ (1)°	Block, colourless
$V = 921.71$ (9) Å^3	$0.21 \times 0.15 \times 0.06$ mm
$Z = 2$	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	7902 measured reflections
Radiation source: fine-focus sealed tube	3219 independent reflections
Graphite monochromator	2404 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.038$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	$\theta_{max} = 32.7°$, $\theta_{min} = 2.5°$
	$h = -7 \rightarrow 6$
	$k = -34 \rightarrow 29$
$T_{min} = 0.175$, $T_{max} = 0.494$	$l = -9 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2]$
$wR(F^2) = 0.064$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{max} = 0.001$
3219 reflections	$\Delta\rho_{max} = 1.08$ e Å^{-3}
126 parameters	$\Delta\rho_{min} = -0.83$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 1997), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0040 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.5000	0.5000	0.01443 (11)
Zn2	0.13449 (8)	0.489408 (17)	0.81307 (4)	0.01677 (10)
Se1	0.01254 (7)	0.401400 (14)	0.50464 (4)	0.01495 (8)
Se2	0.65495 (7)	0.579245 (14)	0.84141 (4)	0.01457 (8)
O1	0.0795 (5)	0.34728 (10)	0.6423 (3)	0.0248 (6)
O2	−0.3157 (5)	0.41983 (10)	0.5085 (3)	0.0226 (5)
O3	0.2089 (5)	0.45788 (10)	0.6117 (3)	0.0171 (5)
O4	0.8708 (5)	0.57246 (10)	1.0305 (3)	0.0211 (5)
O5	0.3453 (5)	0.56087 (11)	0.8768 (3)	0.0236 (5)
O6	0.7369 (5)	0.51810 (10)	0.7463 (3)	0.0178 (5)
N1	0.3533 (6)	0.64265 (13)	1.1687 (3)	0.0240 (6)
H1	0.3219	0.6115	1.1038	0.036*
H2	0.2447	0.6412	1.2386	0.036*
H3	0.5323	0.6433	1.2247	0.036*
C1	0.2884 (9)	0.69580 (16)	1.0670 (5)	0.0316 (9)
H1A	0.0919	0.6955	1.0084	0.038*
H1B	0.3981	0.6959	0.9861	0.038*
C2	0.3503 (12)	0.7500	1.1694 (6)	0.0290 (12)
H2A	0.5462	0.7500	1.2290	0.035*
H2B	0.2389	0.7500	1.2494	0.035*
O7	−0.0285 (11)	0.2500	0.4353 (6)	0.0576 (14)
H4	0.0058	0.2814	0.5013	0.069*
O8	0.3811 (14)	0.2500	0.2297 (7)	0.092 (2)
H5	0.2490	0.2500	0.2800	0.111*
H6	0.5740	0.2500	0.2953	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0146 (3)	0.0160 (3)	0.0128 (2)	−0.0005 (2)	0.00366 (17)	−0.00143 (19)
Zn2	0.0168 (2)	0.0197 (2)	0.01422 (18)	0.00056 (14)	0.00467 (13)	−0.00078 (14)
Se1	0.01639 (17)	0.01547 (16)	0.01322 (14)	0.00075 (12)	0.00417 (11)	−0.00126 (12)
Se2	0.01591 (17)	0.01570 (16)	0.01243 (14)	−0.00070 (12)	0.00418 (11)	−0.00056 (11)
O1	0.0292 (15)	0.0153 (12)	0.0274 (13)	0.0008 (10)	0.0024 (10)	0.0066 (10)
O2	0.0143 (12)	0.0179 (12)	0.0364 (14)	0.0023 (9)	0.0079 (10)	0.0009 (10)
O3	0.0189 (12)	0.0193 (12)	0.0146 (11)	−0.0045 (9)	0.0070 (8)	−0.0044 (9)

O4	0.0219 (13)	0.0262 (13)	0.0139 (11)	−0.0055 (10)	0.0020 (9)	0.0013 (9)
O5	0.0186 (13)	0.0258 (13)	0.0295 (13)	−0.0039 (10)	0.0119 (10)	−0.0088 (11)
O6	0.0163 (12)	0.0233 (12)	0.0132 (10)	0.0026 (9)	0.0024 (8)	−0.0056 (9)
N1	0.0259 (17)	0.0238 (16)	0.0208 (14)	−0.0047 (12)	0.0034 (12)	−0.0008 (12)
C1	0.040 (2)	0.025 (2)	0.026 (2)	0.0006 (16)	0.0015 (16)	0.0025 (15)
C2	0.037 (3)	0.024 (3)	0.023 (3)	0.000	0.002 (2)	0.000
O7	0.099 (4)	0.027 (2)	0.044 (3)	0.000	0.013 (3)	0.000
O8	0.082 (5)	0.144 (7)	0.056 (4)	0.000	0.027 (3)	0.000

Geometric parameters (Å, º)

Zn1—O2^i	2.048 (2)	Se2—O6	1.715 (2)
Zn1—O2^{ii}	2.048 (2)	N1—C1	1.479 (4)
Zn1—O3	2.136 (2)	N1—H1	0.8900
Zn1—O3^{iii}	2.136 (2)	N1—H2	0.8900
Zn1—O6	2.144 (2)	N1—H3	0.8900
Zn1—O6^{iii}	2.144 (2)	C1—C2	1.501 (4)
Zn2—O4^{iv}	1.941 (2)	C1—H1A	0.9700
Zn2—O5	1.946 (2)	C1—H1B	0.9700
Zn2—O3	1.958 (2)	C2—C1^{vi}	1.501 (4)
Zn2—O6^v	2.011 (2)	C2—H2A	0.9700
Se1—O1	1.674 (2)	C2—H2B	0.9700
Se1—O2	1.682 (2)	O7—H4	0.90
Se1—O3	1.730 (2)	O8—H5	0.86
Se2—O4	1.681 (2)	O8—H6	0.97
Se2—O5	1.682 (2)		
O2^i—Zn1—O2^{ii}	180.0	Se1—O3—Zn2	121.61 (12)
O2^i—Zn1—O3	94.65 (9)	Se1—O3—Zn1	117.55 (11)
O2^{ii}—Zn1—O3	85.35 (9)	Zn2—O3—Zn1	120.34 (11)
O2^i—Zn1—O3^{iii}	85.35 (9)	Se2—O4—Zn2^{iv}	126.44 (13)
O2^{ii}—Zn1—O3^{iii}	94.65 (9)	Se2—O5—Zn2	127.57 (14)
O3—Zn1—O3^{iii}	180.0	Se2—O6—Zn2^{ii}	117.85 (11)
O2^i—Zn1—O6	89.32 (9)	Se2—O6—Zn1	118.24 (11)
O2^{ii}—Zn1—O6	90.68 (9)	Zn2^{ii}—O6—Zn1	117.48 (11)
O3—Zn1—O6	85.85 (8)	C1—N1—H1	109.5
O3^{iii}—Zn1—O6	94.15 (8)	C1—N1—H2	109.5
O2^i—Zn1—O6^{iii}	90.68 (9)	H1—N1—H2	109.5
O2^{ii}—Zn1—O6^{iii}	89.32 (9)	C1—N1—H3	109.5
O3—Zn1—O6^{iii}	94.15 (8)	H1—N1—H3	109.5
O3^{iii}—Zn1—O6^{iii}	85.85 (8)	H2—N1—H3	109.5
O6—Zn1—O6^{iii}	180.0	N1—C1—C2	111.8 (3)
O4^{iv}—Zn2—O5	122.01 (10)	N1—C1—H1A	109.2
O4^{iv}—Zn2—O3	110.55 (10)	C2—C1—H1A	109.2
O5—Zn2—O3	110.25 (10)	N1—C1—H1B	109.2
O4^{iv}—Zn2—O6^v	104.50 (10)	C2—C1—H1B	109.2
O5—Zn2—O6^v	102.48 (10)	H1A—C1—H1B	107.9
O3—Zn2—O6^v	105.24 (9)	C1—C2—C1^{vi}	112.2 (4)

O1—Se1—O2	101.36 (13)	C1—C2—H2A	109.2
O1—Se1—O3	102.22 (11)	C1^{vi}—C2—H2A	109.2
O2—Se1—O3	102.52 (11)	C1—C2—H2B	109.2
O4—Se2—O5	101.35 (12)	C1^{vi}—C2—H2B	109.2
O4—Se2—O6	101.33 (11)	H2A—C2—H2B	107.9
O5—Se2—O6	102.01 (11)	H5—O8—H6	118.4
Se1—O2—Zn1^{v}	130.32 (13)		
O1—Se1—O2—Zn1^{v}	140.13 (17)	O5—Se2—O4—Zn2^{iv}	41.76 (19)
O3—Se1—O2—Zn1^{v}	34.7 (2)	O6—Se2—O4—Zn2^{iv}	−63.11 (19)
O1—Se1—O3—Zn2	−62.42 (16)	O4—Se2—O5—Zn2	−107.11 (17)
O2—Se1—O3—Zn2	42.33 (16)	O6—Se2—O5—Zn2	−2.78 (19)
O1—Se1—O3—Zn1	125.66 (14)	O4^{iv}—Zn2—O5—Se2	102.74 (18)
O2—Se1—O3—Zn1	−129.59 (13)	O3—Zn2—O5—Se2	−29.5 (2)
O4^{iv}—Zn2—O3—Se1	52.67 (16)	O6^{v}—Zn2—O5—Se2	−141.11 (16)
O5—Zn2—O3—Se1	−169.45 (13)	O4—Se2—O6—Zn2^{ii}	−33.08 (16)
O6^{v}—Zn2—O3—Se1	−59.62 (15)	O5—Se2—O6—Zn2^{ii}	−137.43 (14)
O4^{iv}—Zn2—O3—Zn1	−135.62 (12)	O4—Se2—O6—Zn1	175.73 (13)
O5—Zn2—O3—Zn1	2.26 (15)	O5—Se2—O6—Zn1	71.38 (15)
O6^{v}—Zn2—O3—Zn1	112.09 (12)	O2^{i}—Zn1—O6—Se2	8.82 (14)
O2^{i}—Zn1—O3—Se1	119.42 (13)	O2^{ii}—Zn1—O6—Se2	−171.18 (14)
O2^{ii}—Zn1—O3—Se1	−60.58 (13)	O3—Zn1—O6—Se2	−85.90 (14)
O6—Zn1—O3—Se1	−151.60 (13)	O3^{iii}—Zn1—O6—Se2	94.10 (14)
O6^{iii}—Zn1—O3—Se1	28.40 (13)	O2^{i}—Zn1—O6—Zn2^{ii}	−142.49 (13)
O2^{i}—Zn1—O3—Zn2	−52.61 (13)	O2^{ii}—Zn1—O6—Zn2^{ii}	37.51 (13)
O2^{ii}—Zn1—O3—Zn2	127.39 (13)	O3—Zn1—O6—Zn2^{ii}	122.80 (13)
O6—Zn1—O3—Zn2	36.37 (12)	O3^{iii}—Zn1—O6—Zn2^{ii}	−57.20 (13)
O6^{iii}—Zn1—O3—Zn2	−143.63 (12)	N1—C1—C2—C1^{vi}	179.3 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*−1, *y*, *z*; (vi) *x*, −*y*+3/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O5	0.89	2.26	3.081 (4)	153
N1—H1···O4^{v}	0.89	2.33	2.868 (4)	119
N1—H2···O1^{vii}	0.89	2.11	2.974 (4)	165
N1—H3···O1^{iv}	0.89	1.97	2.857 (4)	174
O7—H4···O1	0.90	1.90	2.800 (4)	180
O8—H5···O7	0.86	2.12	2.972 (9)	172
O8—H6···O7^{ii}	0.97	2.02	2.988 (8)	179

Symmetry codes: (ii) *x*+1, *y*, *z*; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*−1, *y*, *z*; (vii) −*x*, −*y*+1, −*z*+2.