

## Zinc mercury(II) tetrakis(selenocyanate)

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{N}-\text{C}) = 0.007$  Å;  $R$  factor = 0.026;  $wR$  factor = 0.053; data-to-parameter ratio = 37.7.

The title crystal,  $[\text{HgZn}(\text{NCSe})_4]_n$ , a coordination polymer, has a diamond-like network. In the crystal, the metal ions,  $\text{Zn}^{2+}$  and  $\text{Hg}^{2+}$ , are both located on fourfold inversion axes and mimic the role of C atoms in the structure of diamond, and the linear selenocyanate bridges replace the C–C bonds. The C–N–Zn unit is almost linear and the C–Se–Hg unit is nearly a right angle. Thus, the  $\text{HgZn}_4$  (or  $\text{ZnHg}_4$ ) arrangement is midway between a tetrahedron and a square plane, with two types of Hg–Zn–Hg (or Zn–Hg–Zn) angles of  $92.38$  (6) and  $156.45$  (6)°.

### Related literature

For background to coordination polymers, see: Batten *et al.* (2009). For diamond-like networks, see: Sun *et al.* (2006); Evans *et al.* (1999). For similar structures, see: Wang *et al.* (2001, 2007); Sun *et al.* (2005, 2006); Tian *et al.* (1999); Xu *et al.* (1999); Yan *et al.* (1999); Yuan *et al.* (1997).

### Experimental

#### Crystal data

$[\text{HgZn}(\text{NCSe})_4]$	$Z = 2$
$M_r = 685.88$	Mo $K\alpha$ radiation
Tetragonal, $I\bar{4}$	$\mu = 27.02$ mm <sup>-1</sup>
$a = 11.2716$ (1) Å	$T = 293$ K
$c = 4.6981$ (1) Å	$0.13 \times 0.12 \times 0.10$ mm
$V = 596.89$ (2) Å <sup>3</sup>	

#### Data collection

Bruker APEXII CCD area-detector diffractometer	2476 measured reflections
Absorption correction: multi-scan (APEX2; Bruker, 2005)	1244 independent reflections
$T_{\min} = 0.127$ , $T_{\max} = 0.173$	1113 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.029$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	$\Delta\rho_{\min} = -0.81$ e Å <sup>-3</sup>
$wR(F^2) = 0.053$	Absolute structure: Flack (1983),
$S = 0.86$	467 Friedel pairs
1244 reflections	Absolute structure parameter: 0.026
33 parameters	(10)
$\Delta\rho_{\max} = 1.35$ e Å <sup>-3</sup>	

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2230).

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## supporting information

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### S1. Comment

Coordination polymers, which contain ions linked by coordinated ligands into an infinite array, have extensive applications such as porosity, magnetism, non-linear optical activity, reactive networks, heterogenous catalysis and luminescence (Batten *et al.* 2009).  $[AB(SCN)_4]_n$  and  $[AB(SeCN)_4]_n$  (where A and B = Zn, Cd, Hg or Mn) are coordination polymers that have non-linear optical property (Wang *et al.*, 2007, 2001; Sun *et al.*, 2006, 2005; Yuan *et al.* 1997).

$[ZnHg(SeCN)_4]_n$  is a new member of this group.

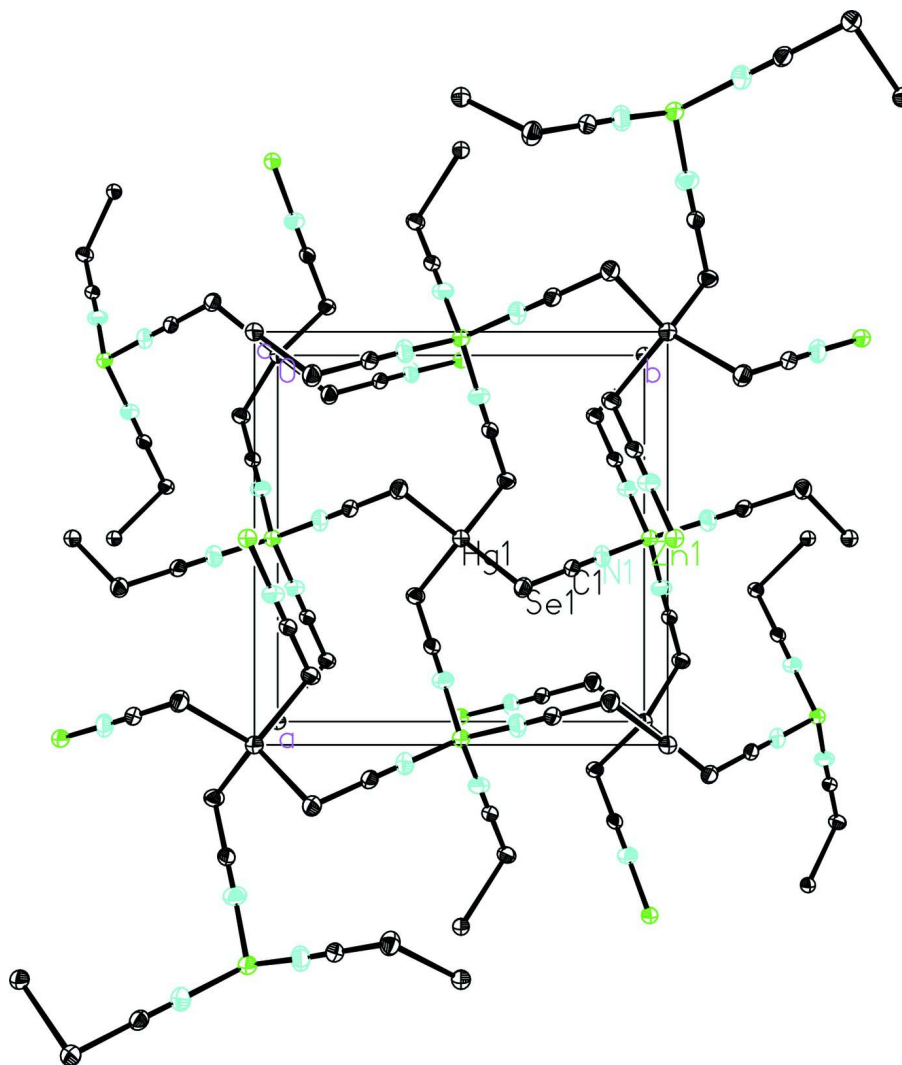
All the  $[AB(SCN)_4]_n$  and  $[AB(SeCN)_4]_n$  have similar structure. The  $[ZnHg(SeCN)_4]_n$  is of no exception. The Zn and Hg atoms are connected by SeCN<sup>-</sup> ions, forming an infinite three-dimensional network (see Fig. 1). Each Zn or Hg node is 4-coordinated with Zn—N or Hg—Se bond. The ZnN<sub>4</sub> and HgSe<sub>4</sub> tetrahedra are slightly distorted from an ideal one. The Zn—N—C—Se is nearly linear, but the C—Se—Hg is bent. The whole structure might be defined as a diamond-like network with Zn and Hg nodes and bent bonds. The HgZn<sub>4</sub> (or ZnHg<sub>4</sub>) tetrahedra have a significant distortion from an ideal one, with two types of Hg—Zn—Hg (or Zn—Hg—Zn) angles, 92.38 (6)° and 156.45 (6)°. Along the c-direction there are irregular octagon channels.

### S2. Experimental

Sodium metasilicate nonahydrate (Na<sub>2</sub>SiO<sub>3</sub>·9H<sub>2</sub>O), ZnCl<sub>2</sub> and KSeCN solution were mixed together with stirring for 1 h. Then the sol is put into a test tube. Glacial acetic acid was added to adjust pH to 3.1. The above solution was sealed and gelled on standing for 72 h. Then some HgCl<sub>2</sub> solution was added on top of the gel. Within 20 d the ZMSC crystal grew in the gel medium.

### S3. Refinement

The unusually large residual electron density (1.347 e Å<sup>-3</sup>) is found near the Hg atoms.

**Figure 1**

Packing diagram of  $[\text{ZnHg}(\text{NCSe})_4]_n$  (viewed down the  $c$  axis), with displacement ellipsoids drawn at the 50% probability level.

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#### Crystal data

$[\text{HgZn}(\text{NCSe})_4]$   
 $M_r = 685.88$   
 Tetragonal,  $\bar{I}4$   
 Hall symbol: I -4  
 $a = 11.2716$  (1) Å  
 $c = 4.6981$  (1) Å  
 $V = 596.89$  (2) Å<sup>3</sup>  
 $Z = 2$   
 $F(000) = 596$

$D_x = 3.816$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 1556 reflections  
 $\theta = 2.6\text{--}34.8^\circ$   
 $\mu = 27.02$  mm<sup>-1</sup>  
 $T = 293$  K  
 Prism, colourless  
 $0.13 \times 0.12 \times 0.10$  mm

Data collection

Bruker APEXII CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (APEX2; Bruker, 2005)  
 $T_{\min} = 0.127$ ,  $T_{\max} = 0.173$

2476 measured reflections  
 1244 independent reflections  
 1113 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$   
 $\theta_{\max} = 38.1^\circ$ ,  $\theta_{\min} = 2.6^\circ$   
 $h = -16 \rightarrow 19$   
 $k = -17 \rightarrow 11$   
 $l = -6 \rightarrow 7$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.053$   
 $S = 0.86$   
 1244 reflections  
 33 parameters  
 0 restraints  
 Primary atom site location: isomorphous  
 structure methods

Secondary atom site location: difference Fourier  
 map  
 $w = 1/[\sigma^2(F_o^2)]$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 1.35 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.81 \text{ e } \text{Å}^{-3}$   
 Extinction correction: SHELXL97 (Sheldrick,  
 2008),  $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0047 (3)  
 Absolute structure: Flack (1983), 467 Friedel  
 pairs  
 Absolute structure parameter: 0.026 (10)

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 ( $\text{Å}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.0000	0.0000	0.0000	0.02909 (11)
Se1	0.12160 (4)	0.15390 (4)	0.31572 (11)	0.03115 (13)
Zn1	0.0000	0.5000	-0.2500	0.0289 (2)
N1	0.0462 (4)	0.3643 (3)	-0.0118 (16)	0.0374 (9)
C1	0.0756 (4)	0.2818 (4)	0.1106 (10)	0.0280 (9)

Atomic displacement parameters ( $\text{Å}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Hg1	0.02405 (11)	0.02405 (11)	0.0392 (2)	0.000	0.000	0.000
Se1	0.0322 (2)	0.0250 (2)	0.0363 (3)	-0.00208 (18)	-0.0073 (2)	0.00031 (19)
Zn1	0.0242 (3)	0.0242 (3)	0.0382 (6)	0.000	0.000	0.000
N1	0.040 (2)	0.0242 (16)	0.048 (2)	0.0011 (14)	-0.004 (3)	-0.004 (2)
C1	0.0241 (19)	0.0219 (18)	0.038 (2)	-0.0019 (15)	0.0023 (17)	-0.0046 (17)

Geometric parameters (Å, °)

Hg1—Se1	2.6623 (5)	Zn1—N1 <sup>iv</sup>	1.966 (6)
Hg1—Se1 <sup>i</sup>	2.6623 (5)	Zn1—N1 <sup>v</sup>	1.966 (6)
Hg1—Se1 <sup>ii</sup>	2.6623 (5)	Zn1—N1 <sup>vi</sup>	1.966 (6)
Hg1—Se1 <sup>iii</sup>	2.6623 (5)	Zn1—N1	1.966 (6)
Se1—C1	1.810 (5)	N1—C1	1.141 (7)
Se1—Hg1—Se1 <sup>i</sup>	108.084 (11)	N1 <sup>iv</sup> —Zn1—N1 <sup>vi</sup>	110.6 (4)
Se1—Hg1—Se1 <sup>ii</sup>	112.28 (2)	N1 <sup>v</sup> —Zn1—N1 <sup>vi</sup>	108.91 (18)
Se1 <sup>i</sup> —Hg1—Se1 <sup>ii</sup>	108.084 (11)	N1 <sup>iv</sup> —Zn1—N1	108.91 (18)
Se1—Hg1—Se1 <sup>iii</sup>	108.084 (11)	N1 <sup>v</sup> —Zn1—N1	110.6 (4)
Se1 <sup>i</sup> —Hg1—Se1 <sup>iii</sup>	112.28 (2)	N1 <sup>vi</sup> —Zn1—N1	108.91 (18)
Se1 <sup>ii</sup> —Hg1—Se1 <sup>iii</sup>	108.084 (11)	C1—N1—Zn1	175.5 (6)
C1—Se1—Hg1	94.29 (14)	N1—C1—Se1	178.1 (5)
N1 <sup>iv</sup> —Zn1—N1 <sup>v</sup>	108.91 (18)		
Se1 <sup>i</sup> —Hg1—Se1—C1	-14.76 (14)	N1 <sup>iv</sup> —Zn1—N1—C1	69 (5)
Se1 <sup>ii</sup> —Hg1—Se1—C1	-133.89 (14)	N1 <sup>vi</sup> —Zn1—N1—C1	-52 (5)
Se1 <sup>iii</sup> —Hg1—Se1—C1	106.99 (14)	Hg1—Se1—C1—N1	140 (12)

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