



Synthesis and structure of an arylselenium(II) cation, $[\text{C}_{34}\text{H}_{41}\text{N}_4\text{Se}^+]_2[\text{Hg}(\text{SeCN})_4]^{2-}$, based on a 5-*tert*-butyl-1,3-bis(1-pentyl-1*H*-benzimidazol-2-yl)benzene scaffold

Varsha Rani,^a Harkesh B. Singh^a and Ray J. Butcher^{b*}

Received 16 March 2018

Accepted 25 April 2018

Edited by M. Zeller, Purdue University, USA

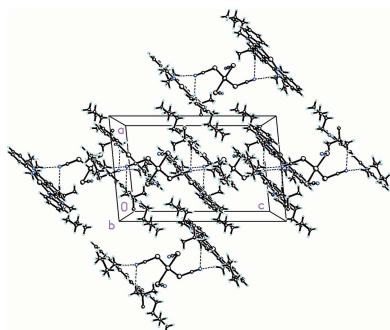
Keywords: crystal structure; arylselenium(II) cation; tetraselenocyanatomercury(II) anion.**CCDC reference:** 1839609**Supporting information:** this article has supporting information at journals.iucr.org/e^aDepartment of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India, and ^bDepartment of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA. *Correspondence e-mail: rbutter99@yahoo.com

In the title salt, bis{[5-*tert*-butyl-1,3-bis(1-pentyl-1*H*-benzimidazol-2-yl)benzene]selenium} tetrakis(selenocyanato)mercury, $(\text{C}_{34}\text{H}_{41}\text{N}_4\text{Se})_2[\text{Hg}(\text{SeCN})_4]$, the arylselenium cations, $[\text{C}_{34}\text{H}_{41}\text{N}_4\text{Se}]^+$, are linked through $[\text{Hg}(\text{SeCN})_4]^{2-}$ anions by C—H...N hydrogen bonds. In the cation, the geometry around the Se atom in the 5-*tert*-butyl-1,3-bis(1-pentyl-1*H*-benzimidazol-2-yl)benzene scaffold is T-shaped, resulting from the coordination of Se by the C atom of the central aromatic ring and the N atoms of both of the benzimidazole moieties. The *trans* Se—N bond lengths are almost equal [2.087 (3) and 2.099 (3) Å] and the Se—C bond length is 1.886 (3) Å. The N—Se—N angle is 159.29 (11)°. The geometry around the Hg^{II} atom in the $[\text{Hg}(\text{SeCN})_4]^{2-}$ anion is distorted tetrahedral, with Se—Hg—Se angles ranging from 88.78 (3) to 126.64 (2)°. In $[\text{Hg}(\text{SeCN})_4]^{2-}$, the Hg—Se bonds are unsymmetrical [2.5972 (4) and 2.7242 (5) Å]. One of the pentyl substituents is disordered over two equivalent conformations, with occupancies of 0.852 (8) and 0.148 (8).

1. Chemical context

Over the past two decades, organochalcogen chemistry has gained the attention of synthetic chemists because of its promising utility in biomimetic chemistry (Mugesh & Singh, 2000; Zhao *et al.*, 2012; Bhuyan & Mugesh, 2012), synthetic organic chemistry (Back 1999; Singh & Wirth, 2012; Chivers & Laitinen, 2015) and material science (Manjare *et al.*, 2014; Kremer *et al.*, 2015). The first stable selenium cation complex, $[2,6-(\text{Me}_2\text{NCH}_2)_2\text{C}_6\text{H}_3\text{Se}]^+[\text{PF}_6]^-$, was isolated while attempting the synthesis of the respective oxides from the reaction of 2,6-bis[(dimethylamino)methyl]phenyl methyl selenide with *t*-BuOCl (Fujihara *et al.*, 1995). In the literature, examples of arylselenium(II) cations are limited to a basic scaffold, the [2,6-bis(dimethylaminomethyl)phenyl]selenium moiety, which is stabilized by different counter-anions $[\text{Cl}^-$, Br^- , I^- (Pop *et al.*, 2014) and HF_2^- (Poleschner & Seppelt, 2004)].

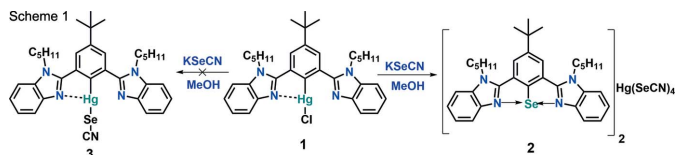
Our group has been active in the area of synthesis and isolation of novel, unstable arylchalcogen derivatives featuring intramolecular interactions ($E \cdots D$; $E = \text{S, Se, Te}$ and $D = \text{N, O}$) between chalcogen heteroatoms by using either one or two coordinating groups (Zade *et al.*, 2004*a,b*; Selvakumar *et al.*, 2011*a,b,c,d*; Singh *et al.*, 2011; Prasad *et al.*, 2016). Recently, and for the first time, we have shown the use of the bis-benzimidazole group to isolate an organometallic deriva-



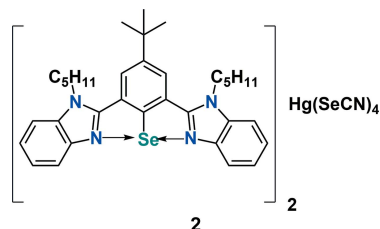
tive of a non-transition metal where 1,3-bis(N-substituted benzimidazol-2'-yl)benzene has been used as a pincer ligand with chalcogens (Rani *et al.*, 2018a).

As far as the synthesis of transition metal complexes with the bis-benzimidazole group is concerned, there are several reports in the literature for platinum(II) pincer complexes with similar kinds of scaffolds. Some of these were investigated for their photoluminescence properties (Wang *et al.*, 2014; Dorazco-González, 2014; Chan *et al.*, 2016). Recently, we also reported some palladium(II) pincer complexes with a 1,3-bis(N-substituted benzimidazol-2'-yl)benzene-based ligand. In all the cases, we found that the transition metal complexes were quite stable and in no case was auto-ionization observed (Rani *et al.*, 2018b).

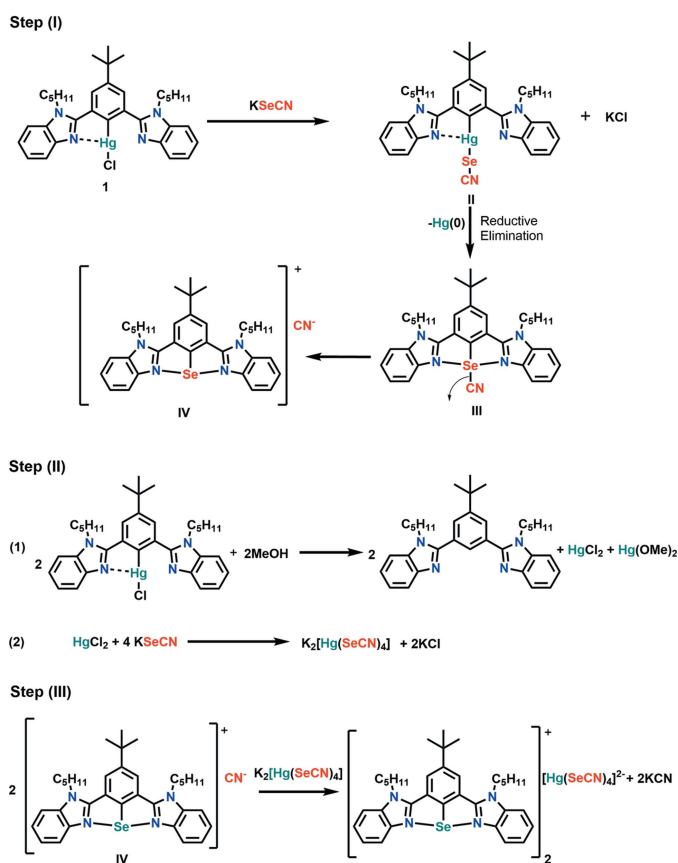
In an attempt to synthesize {4-(*tert*-butyl)-2,6-bis(1-pentyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl}(selenocyanato)mercury (3), [4-*tert*-butyl-2,6-bis(1-pentyl-1*H*-benzimidazol-2-yl)phenyl]mercury(II) chloride (1) was reacted with potassium selenocyanate in 1,4-dioxane under reflux conditions. It was observed that, instead of the formation of the desired compound, the reaction leads to the isolation of an aryl-selenium(II) cation *via* auto-ionization (Scheme 1). The procedure for the synthesis of complex 1 will be reported elsewhere. A plausible mechanism for the formation of complex 2 is shown in Scheme 2. Organomercury complex 1 reacts with potassium selenocyanate to form the desired product 3 with potassium chloride as a by-product. However, if complex II is unstable, mercury may be eliminated in elemental form *via* a reductive elimination pathway to form intermediate III. Strong secondary bonding interactions between Se...N atoms may facilitate auto-ionization and the formation of an arylselenium cation with CN[−] as the counter-anion IV. In the presence of a polar protic solvent, there is the possibility of decomposition of organomercury complex 1 to give the free ligand along with HgCl₂ and Hg(OMe)₂ as by-products.



HgCl₂ reacts with an excess of KSeCN to form K₂[Hg(SeCN)₄] (Space & Armeanu, 1930). Two selenium cations can then associate with the [Hg(SeCN)₄]^{2−} anion to form complex 2. Since we only used one equivalent of potassium selenocyanate for the reaction, the product was obtained in low yield (11%).



Scheme 2



2. Structural commentary

The title compound, 2, crystallizes in the monoclinic space group *C2/c*. The asymmetric unit contains a selenium cation along with half of a [Hg(SeCN)₄]^{2−} anion with the Hg atom located on a crystallographic twofold axis (Fig. 1). In the cation, the coordination geometry around Se is T-shaped with each Se atom bonded to the central carbon atom of the aromatic ring and intramolecularly coordinated to the two N atoms. This coordination gives rise to a heptacyclic framework. The tetracyanoselenomercurate anion [Hg(SeCN)₄]^{2−} is sandwiched between two arylselenium cationic units. The observed Se—C bond length is 1.886 (3) Å, which is comparable with that found for a NCN pincer-based selenium cation [2,6-(Me₂NCH₂)₂C₆H₃Se]⁺[PF₆][−] (1.874 Å; Furukawa *et al.*, 1995), and an OCN pincer-based selenium cation [2-NO₂-6-(C₆H₅N=CH)C₆H₃Se]⁺[Br₃][−] (1.84 Å). The Se3—N1 and Se3—N2 bond lengths are almost equal [2.087 (3) and 2.099 (3) Å]. The Se—N distances are shorter than the sum of the van der Waals radii for Se and N [$\Sigma_{\text{rvdW}}(\text{Se},\text{N})$ 3.45 Å] and longer than the covalent radii [$\Sigma_{\text{rcov}}(\text{Se},\text{N})$ 1.91 Å] (Bondi, 1964). This implies stronger intramolecular Se...N interactions in the selenium cation. The N1—Se3—N2 bond angle is found to be 159.29 (11)°. In related molecules (Rani *et al.*, 2017a,b,c), in the absence of coordinated Hg or Se atoms, the benzimidazole arms are twisted significantly out of the plane of the central phenyl ring. However, in the present

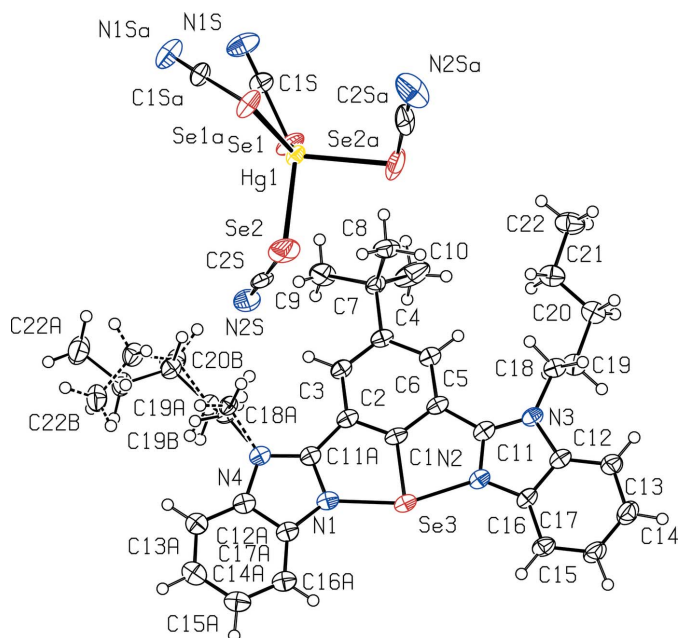


Figure 1
A view of the structure of the title compound, showing the atom-labelling scheme and the disorder in the pentyl side chain. Displacement ellipsoids are drawn at the 50% probability level. Symmetry code for generating equivalent atoms: $1 - x, y, \frac{3}{2} - z$.

structure, as a result of the interaction with Se, the two benzimidazole arms are almost in the plane of the central

phenyl ring [dihedral angles of $3.10(16)$ and $7.18(19)^\circ$]. The Se atom is displaced by $0.116(4)$ Å from the plane of the central phenyl ring. The atoms involved in the chelating system (N2, C11, C6, C1, C2, C11A, N1) form a plane (r.m.s deviation for fitted atoms of 0.0182 Å) with the Se in this plane [deviation from the plane of $0.011(2)$ Å].

In the anion, the mercury atom is coordinated by four selenocyanate anions (two are crystallographically unique) and the geometry around the mercury atom is distorted tetrahedral with Se–Hg–Se angles ranging from $88.78(3)$ to $126.64(2)^\circ$. The tetracyanoselenomercurate anion $[\text{Hg}(\text{SeCN})_4]^{2-}$ acts as a bridging moiety between two selenium cationic units. The $\text{Se}3 \cdots \text{Se}2(-x, -y, 1 - z)$ distance is $4.189(2)$ Å and the $\text{C}1 - \text{Se}3 \cdots \text{Se}2(-x, -y, 1 - z)$ angle is $163.40(9)^\circ$, which indicates that there is a weak secondary interaction between the two different kinds of Se atoms in the cation and anion (Se3 and Se2). In the $[\text{Hg}(\text{SeCN})_4]^{2-}$ anion, two sets of Hg–Se bonds exist. One set is shorter [$2.5972(4)$ Å] and the other set is longer [$2.7242(5)$ Å]. The Hg–SeCN moieties are not linear, with Hg–Se–C angles of $101.31(14)$ and $101.43(11)^\circ$.

3. Supramolecular features

In the crystal, the molecules are arranged in a parallel fashion along the *b*-axis direction as shown in Fig. 2. These parallel units are stacked together by $\text{C}18 - \text{H}18A \cdots \text{N}1\text{S}$ and $\text{C}18A -$

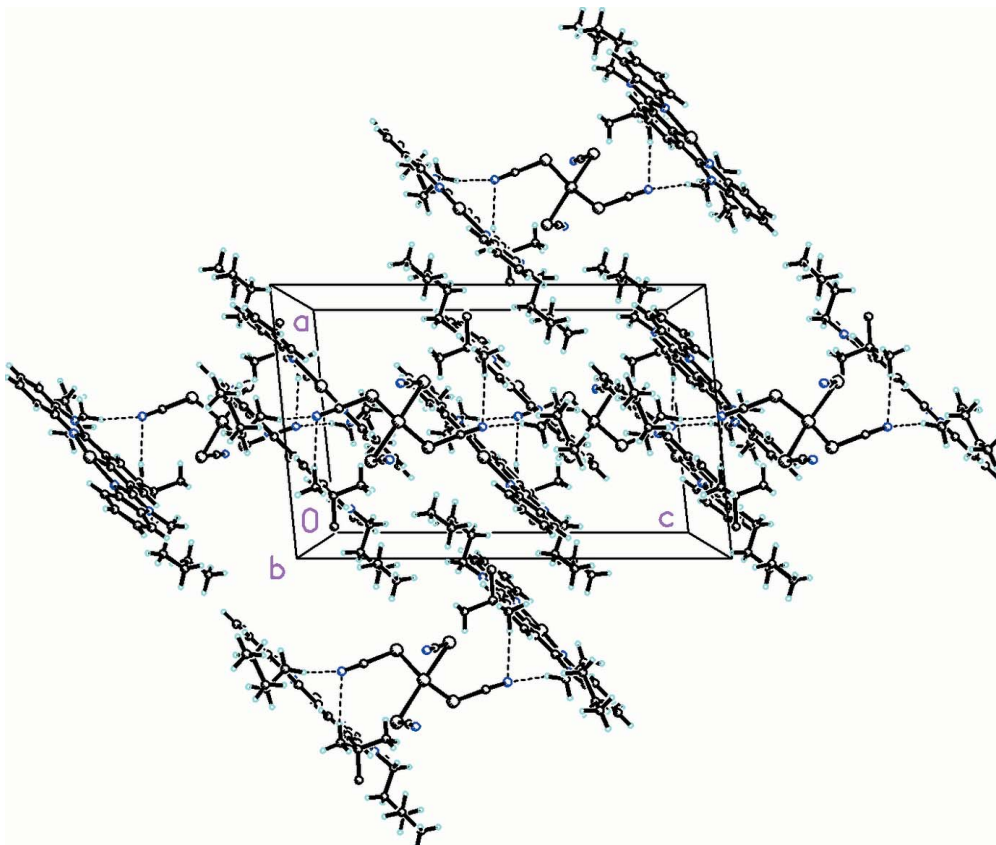


Figure 2
Packing diagram viewed along the *b* axis. C–H \cdots N interactions linking the cations and anions are shown as dashed lines. Only the major disorder component is shown for clarity.

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C18—H18A \cdots N1S ⁱ	0.99	2.62	3.568 (5)	160
C18A—H18C \cdots N2S	0.99	2.38	3.324 (8)	159
C18B—H18F \cdots N2S	0.99	2.22	3.06 (6)	142

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

H18C \cdots N2S interactions (numerical details are given in Table 1) and π - π stacking interactions between the benzimidazole rings (centroid-centroid distances = 3.535 Å).

4. Database survey

There are no structural reports in the literature on a [phenylenebis(benzimidazole)]selenium cation. However, there have been several reports of structures containing [Hg(SeCN)_x]²⁻ moieties [CICLOP, Brodersen *et al.* 1984; LENHES, Li *et al.*, 2006a; LENHES01, Sun *et al.*, 2005; MURQOH, Li *et al.*, 2006b; PUMVAU, Kushch, *et al.*, 1998; WUYGUU, Sun *et al.*, 2013; YIHKUV, Shibaeva *et al.* 1994; YIHKUV01, Shibaeva *et al.* 1997]

5. Synthesis and crystallization

To a solution of **1** (0.2 g, 0.269 mmol) in 1,4-dioxane (30 ml) was added potassium selenocyanate (0.039 g, 0.270 mmol) dissolved in MeOH. The reaction mixture was stirred for 6 h under a nitrogen atmosphere and refluxed. The reaction mixture was filtered and the precipitate was washed with dioxane. Colourless prism-shaped crystals of **2** were obtained by layering a MeOH solution with diethyl ether at room temperature.

Yield 11% (0.058 g, 0.036 mmol); m. p. turned blackish after 423 K was reached. FT-IR (KBr) (cm⁻¹): 3059 (*w*), 2957 (*s*), 2931 (*s*), 2869 (*s*), 2124 (*s*, needle-like, C≡N), 1614 (*m*), 1464 (*s*), 1458 (*s*), 1440 (*s*), 1330 (*w*), 1288 (*w*), 1273 (*w*), 1154 (*w*), 1137 (*w*), 1011 (*w*), 892 (*w*), 746 (*s*). ESI-MS: *m/z* calculated for C₃₄H₄₁N₄Se: 585.2496. Found: 585.2552.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances ranging from 0.95 to 0.99 Å. $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H atoms and 1.2 for all other C-bound H atoms. One of the pentyl substituents is disordered with an occupancy ratio of 0.852 (8):0.148 (8). It was refined as two equivalent conformations using SAME and SIMU instructions (SAME 0.01 and SIMU 0.01).

Funding information

RJB is grateful for NSF award 1205608, to the Partnership for Reduced Dimensional Materials for partial funding of this

Table 2

Experimental details.

Crystal data	
Chemical formula	(C ₃₄ H ₄₁ N ₄ Se) ₂ [Hg(CNSe) ₄]
M_r	1789.84
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	100
a, b, c (Å)	12.7788 (15), 27.276 (3), 20.180 (3)
β (°)	95.591 (2)
V (Å ³)	7000.4 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	5.37
Crystal size (mm)	0.24 × 0.23 × 0.19
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2002)
$T_{\text{min}}, T_{\text{max}}$	0.267, 0.336
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46553, 9030, 8196
R_{int}	0.095
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.040, 0.097, 1.03
No. of reflections	9030
No. of parameters	463
No. of restraints	147
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.97, -2.10

Computer programs: APEX2 (Bruker, 2005), SAINT and XPREP (Bruker, 2002), SHELXT (Sheldrick, 2015a), SHELXL2018 (Sheldrick, 2015b) and SHELXTL (Sheldrick, 2008).

research, to Howard University's Nanoscience Facility for access to liquid nitrogen, and the NSF-MRI program (grant No. CHE0619278) for funds to purchase the X-ray diffractometer. HBS is grateful to the DST, New Delhi, for a J. C. Bose National Fellowship. VR gratefully acknowledges the Council of Scientific and Industrial Research (CSIR), New Delhi, for a Senior Research Fellowship.

References

- Back, T. G. (1999). *Organoselenium Chemistry: A Practical Approach*. Oxford University Press.
- Bhuyan, B. J. & Mughes, G. (2012). *Biological and Biochemical Aspects of Selenium Compounds*. In *Organoselenium Chemistry: Synthesis and Reactions* edited by T. Wirth, p. 361. Weinheim: Wiley-VCH.
- Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
- Brodersen, K., Cygan, M. & Hummel, H.-U. (1984). *Z. Naturforschung, Teil B*, **39**, 582–5.
- Bruker (2002). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2005). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chan, M. H.-Y., Wong, H.-L. & Yam, V. W.-W. (2016). *Inorg. Chem.* **55**, 5570–5577.
- Chivers, T. & Laitinen, R. S. (2015). *Chem. Soc. Rev.* **44**, 1725–1739.
- Dorazco-González, A. (2014). *Organometallics*, **33**, 868–875.
- Fujihara, H., Mima, H. & Furukawa, N. (1995). *J. Am. Chem. Soc.* **117**, 10153–10154.
- Fujihara, H., Mima, H. & Furukawa, H. (1995). *J. Am. Chem. Soc.* **117**, 10153–10154.

- Kremer, A., Aurisicchio, C., De Leo, F., Ventura, B., Wouters, J., Armaroli, N., Barbieri, A. & Bonifazi, D. (2015). *Chem. Eur. J.* **21**, 15377–15387.
- Kushch, N. D., Buravov, L. I., Pesotskii, S. I., Lyubovskii, R. B., Yagubskii, E. B., Kaplunov, M. G., Golubev, E. V., Narymbetov, B. Zh., Khasanov, S. S., Zorina, L. V., Rozenberg, L. P., Shibaeva, R. P., Kobayashi, A. & Kobayashi, H. (1998). *J. Mater. Chem.* **8**, 897–901.
- Li, S.-L., Fun, H.-K., Chantrapromma, S., Wu, J.-Y. & Tian, Y.-P. (2006a). *Acta Cryst.* **E62**, i47–i49.
- Li, S.-L., Wu, J.-Y., Tian, Y.-P., Ming, H., Wang, P., Jiang, M.-H. & Fun, H.-K. (2006b). *Eur. J. Inorg. Chem.* pp. 2900–2907.
- Manjare, S. T., Kim, Y. & Churchill, D. G. (2014). *Acc. Chem. Res.* **47**, 2985–2998.
- Mugesh, G. & Singh, H. B. (2000). *Chem. Soc. Rev.* **29**, 347–357.
- Poleschner, H. & Seppelt, K. (2004). *Chem. Eur. J.* **10**, 6565–6574.
- Pop, A., Silvestru, A., Juárez-Pérez, E. J., Arca, M., Lippolis, V. & Silvestru, C. (2014). *Dalton Trans.* **43**, 2221–2233.
- Prasad, P. R., Selvakumar, K., Singh, H. B. & Butcher, R. J. (2016). *J. Org. Chem.* **81**, 3214–3226.
- Rani, V., Singh, H. B. & Butcher, R. J. (2017a). *Acta Cryst.* **E73**, 341–344.
- Rani, V., Singh, H. B. & Butcher, R. J. (2017b). *IUCrData*, **2**, x171746.
- Rani, V., Singh, H. B. & Butcher, R. J. (2017c). *Organometallics*, **36**, 4741–4752.
- Rani, V., Singh, H. B. & Butcher, R. J. (2018a). *Acta Cryst.* **E74**, 390–393.
- Rani, V., Singh, H. B. & Butcher, R. J. (2018b). *J. Organomet. Chem.* **859**, 33–43.
- Selvakumar, K., Shah, P., Singh, H. B. & Butcher, R. J. (2011a). *Chem. Eur. J.* **17**, 12741–12755.
- Selvakumar, K., Singh, H. B. & Butcher, R. J. (2011b). *Tetrahedron Lett.* **52**, 6831–6834.
- Selvakumar, K., Singh, H. B., Goel, N. & Singh, U. P. (2011c). *Organometallics*, **30**, 3892–3896.
- Selvakumar, K., Singh, V. P., Shah, P. & Singh, H. B. (2011d). *Main Group Chemistry*, **10**, 141–152.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Shibaeva, R. P., Khasanov, S. S., Rozenberg, L. P., Kushch, N. D., Yagubskii, E. B. & Canadell, E. (1997). *Kristallografiya*, **42**, 846–850.
- Shibaeva, R. P., Rozenberg, L. P., Kushch, N. D. & Yagubskii, E. B. (1994). *Kristallografiya*, **39**, 825–831.
- Singh, V. P., Singh, H. B. & Butcher, R. J. (2011). *Chem. Commun.* **47**, 7221–7223.
- Singh, F. V. & Wirth, T. (2012). *Selenium Compounds as Ligands and Catalysts*. In *Organoselenium Chemistry: Synthesis and Reactions* edited by T. Wirth, pp. 321–334. Weinheim: Wiley-VCH.
- Space, G. & Armeanu, V. (1930). *Bul. Soc. Stiinte Cluj*, **5**, 294–318.
- Sun, H.-Q., Wang, X.-Q. & Zhang, W.-W. (2013). *Acta Cryst.* **E69**, i59.
- Sun, H.-Q., Yu, W.-T., Yuan, D.-R., Wang, X.-Q. & Xue, G. (2005). *Acta Cryst.* **E61**, i111–i112.
- Wang, Z., Sun, Z., Hao, X.-Q., Niu, J.-L., Wei, D., Tu, T., Gong, J.-F. & Song, M.-P. (2014). *Organometallics*, **33**, 1563–1573.
- Zade, S. S., Panda, S., Tripathi, S. K., Singh, H. B. & Wolmershäuser, G. (2004a). *Eur. J. Org. Chem.* pp. 3857–3864.
- Zade, S. S., Singh, H. B. & Butcher, R. J. (2004b). *Angew. Chem. Int. Ed.* **43**, 4513–4515.
- Zhao, L., Li, J., Li, Y., Liu, J., Wirth, T. & Li, Z. (2012). *Bioorg. Med. Chem.* **20**, 2558–2563.

supporting information

Acta Cryst. (2018). E74, 786-790 [https://doi.org/10.1107/S2056989018006394]

Synthesis and structure of an arylselenium(II) cation, $[\text{C}_{34}\text{H}_{41}\text{N}_4\text{Se}^+]_2[\text{Hg}(\text{SeCN})_4]^{2-}$, based on a 5-*tert*-butyl-1,3-bis(1-pentyl-1*H*-benzimidazol-2-yl)benzene scaffold

Varsha Rani, Harkesh B. Singh and Ray J. Butcher

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *S SAINT* (Bruker, 2002); data reduction: *S SAINT*, *SADABS* and *XPREP* (Bruker, 2002); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Bis{[5-*tert*-butyl-1,3-bis(1-pentyl-1*H*-benzimidazol-2-yl)benzene]selenium} tetrakis(selenocyanato)mercury

Crystal data

$(\text{C}_{34}\text{H}_{41}\text{N}_4\text{Se})_2[\text{Hg}(\text{CNSe})_4]$

$M_r = 1789.84$

Monoclinic, *C2/c*

$a = 12.7788$ (15) Å

$b = 27.276$ (3) Å

$c = 20.180$ (3) Å

$\beta = 95.591$ (2)°

$V = 7000.4$ (15) Å³

$Z = 4$

$F(000) = 3528$

$D_x = 1.698$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9623 reflections

$\theta = 2.4\text{--}28.8^\circ$

$\mu = 5.37$ mm⁻¹

$T = 100$ K

Prism, colorless

0.24 × 0.23 × 0.19 mm

Data collection

Bruker APEXII CCD
diffractometer

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2002)

$T_{\min} = 0.267$, $T_{\max} = 0.336$

46553 measured reflections

9030 independent reflections

8196 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.095$

$\theta_{\max} = 28.7^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -17 \rightarrow 17$

$k = -36 \rightarrow 36$

$l = -26 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.097$

$S = 1.03$

9030 reflections

463 parameters

147 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 29.0826P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.97$ e Å⁻³

$\Delta\rho_{\min} = -2.10$ e Å⁻³

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Hg1	0.500000	0.26306 (2)	0.750000	0.02668 (6)	
Se1	0.34755 (3)	0.22031 (2)	0.67740 (2)	0.03961 (11)	
Se2	0.60087 (4)	0.33443 (2)	0.68639 (3)	0.06039 (16)	
C1S	0.3559 (3)	0.15796 (14)	0.7105 (2)	0.0329 (8)	
N1S	0.3565 (3)	0.11791 (14)	0.7281 (2)	0.0530 (11)	
C2S	0.5511 (4)	0.32426 (16)	0.6025 (3)	0.0527 (14)	
N2S	0.5206 (5)	0.3180 (2)	0.5468 (3)	0.0818 (18)	
Se3	0.35746 (3)	0.55143 (2)	0.44746 (2)	0.02529 (8)	
C1	0.3163 (3)	0.49229 (12)	0.48583 (17)	0.0246 (7)	
N1	0.4520 (2)	0.50194 (11)	0.40157 (15)	0.0268 (6)	
N2	0.2460 (2)	0.57747 (10)	0.50876 (15)	0.0266 (6)	
C2	0.3607 (3)	0.44802 (12)	0.46652 (17)	0.0253 (7)	
N3	0.1405 (2)	0.56201 (11)	0.58694 (16)	0.0266 (6)	
C3	0.3253 (3)	0.40392 (13)	0.49273 (18)	0.0274 (7)	
H3	0.355121	0.373771	0.480319	0.033*	
N4	0.5031 (2)	0.42500 (11)	0.39049 (15)	0.0258 (6)	
C4	0.2474 (3)	0.40351 (12)	0.53656 (18)	0.0268 (7)	
C5	0.2061 (3)	0.44847 (12)	0.55594 (18)	0.0264 (7)	
H5	0.153811	0.448618	0.586325	0.032*	
C6	0.2404 (3)	0.49287 (12)	0.53141 (17)	0.0244 (7)	
C7	0.2071 (3)	0.35552 (12)	0.56442 (19)	0.0289 (7)	
C8	0.2489 (4)	0.35045 (15)	0.6371 (2)	0.0415 (10)	
H8A	0.220563	0.320554	0.655474	0.062*	
H8B	0.227426	0.378964	0.661992	0.062*	
H8C	0.325862	0.348547	0.640679	0.062*	
C9	0.2425 (5)	0.31052 (15)	0.5271 (3)	0.0593 (15)	
H9A	0.319392	0.310115	0.528966	0.089*	
H9B	0.212572	0.311945	0.480534	0.089*	
H9C	0.218126	0.280689	0.547898	0.089*	
C10	0.0862 (4)	0.35594 (18)	0.5592 (4)	0.0672 (18)	
H10A	0.060786	0.324118	0.573535	0.101*	
H10B	0.058519	0.362129	0.513002	0.101*	
H10C	0.062382	0.381828	0.587900	0.101*	
C11	0.2057 (3)	0.54262 (12)	0.54487 (18)	0.0253 (7)	
C12	0.1378 (3)	0.61244 (13)	0.57613 (19)	0.0276 (7)	
C13	0.0821 (3)	0.64909 (14)	0.6057 (2)	0.0352 (8)	
H13	0.038815	0.642379	0.640317	0.042*	
C14	0.0942 (3)	0.69620 (15)	0.5809 (2)	0.0417 (10)	
H14	0.057845	0.722574	0.599213	0.050*	

C15	0.1576 (3)	0.70585 (14)	0.5305 (2)	0.0389 (9)	
H15	0.162170	0.738592	0.514960	0.047*	
C16	0.2146 (3)	0.66971 (13)	0.5018 (2)	0.0325 (8)	
H16	0.258323	0.676713	0.467486	0.039*	
C17	0.2036 (3)	0.62215 (12)	0.52651 (19)	0.0266 (7)	
C18	0.0780 (3)	0.53739 (13)	0.63476 (18)	0.0275 (7)	
H18A	0.078020	0.557671	0.675445	0.033*	
H18B	0.110525	0.505402	0.647584	0.033*	
C19	-0.0355 (3)	0.52925 (14)	0.60471 (18)	0.0317 (8)	
H19C	-0.069910	0.561405	0.595627	0.038*	
H19D	-0.035131	0.511632	0.561841	0.038*	
C20	-0.0988 (3)	0.49959 (14)	0.65154 (19)	0.0336 (8)	
H20C	-0.084659	0.512629	0.697324	0.040*	
H20D	-0.174743	0.503795	0.637724	0.040*	
C21	-0.0724 (3)	0.44565 (15)	0.6518 (2)	0.0376 (9)	
H21C	0.003550	0.441622	0.665720	0.045*	
H21D	-0.085951	0.432855	0.605869	0.045*	
C22	-0.1347 (3)	0.41508 (18)	0.6977 (2)	0.0482 (11)	
H22D	-0.125713	0.428832	0.742783	0.072*	
H22E	-0.108927	0.381218	0.698705	0.072*	
H22F	-0.209348	0.415560	0.681153	0.072*	
C11A	0.4382 (3)	0.45556 (13)	0.42009 (17)	0.0257 (7)	
C12A	0.5610 (3)	0.45354 (14)	0.35008 (18)	0.0276 (7)	
C13A	0.6369 (3)	0.44094 (15)	0.30797 (18)	0.0303 (8)	
H13A	0.658408	0.407932	0.302826	0.036*	
C14A	0.6792 (3)	0.47904 (16)	0.2740 (2)	0.0360 (9)	
H14A	0.731050	0.472026	0.244678	0.043*	
C15A	0.6474 (3)	0.52805 (16)	0.2819 (2)	0.0355 (9)	
H15A	0.678307	0.553194	0.257699	0.043*	
C16A	0.5729 (3)	0.54032 (15)	0.3238 (2)	0.0325 (8)	
H16A	0.552318	0.573426	0.329275	0.039*	
C17A	0.5288 (3)	0.50248 (13)	0.35761 (18)	0.0278 (7)	
C18A	0.5203 (10)	0.3728 (3)	0.3997 (3)	0.0244 (14)	0.852 (8)
H18C	0.510020	0.364134	0.446248	0.029*	0.852 (8)
H18D	0.594009	0.365117	0.392479	0.029*	0.852 (8)
C19A	0.4470 (8)	0.3412 (3)	0.3527 (5)	0.0277 (9)	0.852 (8)
H19A	0.450494	0.352300	0.306284	0.033*	0.852 (8)
H19B	0.373681	0.345283	0.363775	0.033*	0.852 (8)
C20A	0.4781 (4)	0.2871 (3)	0.3588 (4)	0.0309 (12)	0.852 (8)
H20A	0.478389	0.276876	0.405842	0.037*	0.852 (8)
H20B	0.424614	0.267235	0.332065	0.037*	0.852 (8)
C21A	0.5855 (4)	0.27671 (18)	0.3354 (3)	0.0380 (11)	0.852 (8)
H21A	0.640296	0.291481	0.367370	0.046*	0.852 (8)
H21B	0.589821	0.292579	0.291671	0.046*	0.852 (8)
C22A	0.6079 (5)	0.2223 (2)	0.3291 (3)	0.0549 (16)	0.852 (8)
H22A	0.604420	0.206332	0.372400	0.082*	0.852 (8)
H22B	0.678187	0.217741	0.314583	0.082*	0.852 (8)
H22C	0.555409	0.207595	0.296356	0.082*	0.852 (8)

C18B	0.517 (6)	0.3685 (19)	0.411 (3)	0.025 (3)	0.148 (8)
H18E	0.592583	0.359205	0.414384	0.031*	0.148 (8)
H18F	0.490086	0.362428	0.454562	0.031*	0.148 (8)
C19B	0.455 (5)	0.3390 (17)	0.356 (3)	0.028 (3)	0.148 (8)
H19E	0.379655	0.348402	0.354008	0.034*	0.148 (8)
H19F	0.480373	0.347037	0.312626	0.034*	0.148 (8)
C20B	0.4652 (19)	0.2838 (16)	0.368 (2)	0.031 (3)	0.148 (8)
H20E	0.431322	0.275516	0.409056	0.037*	0.148 (8)
H20F	0.426915	0.266244	0.330620	0.037*	0.148 (8)
C21B	0.5777 (19)	0.2659 (10)	0.3768 (12)	0.036 (3)	0.148 (8)
H21E	0.577496	0.230268	0.386154	0.043*	0.148 (8)
H21F	0.614890	0.282350	0.415953	0.043*	0.148 (8)
C22B	0.639 (2)	0.2747 (12)	0.3169 (13)	0.042 (5)	0.148 (8)
H22G	0.700518	0.253336	0.319720	0.064*	0.148 (8)
H22H	0.661217	0.309070	0.316499	0.064*	0.148 (8)
H22I	0.593579	0.267534	0.275995	0.064*	0.148 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02158 (9)	0.01884 (9)	0.03905 (12)	0.000	-0.00001 (7)	0.000
Se1	0.03104 (19)	0.02352 (18)	0.0598 (3)	-0.00375 (14)	-0.01827 (18)	0.00848 (17)
Se2	0.0556 (3)	0.0361 (2)	0.0907 (4)	-0.0220 (2)	0.0137 (3)	0.0094 (3)
C1S	0.0283 (17)	0.0288 (18)	0.040 (2)	-0.0052 (14)	-0.0040 (15)	0.0027 (16)
N1S	0.061 (3)	0.0317 (19)	0.061 (3)	-0.0115 (17)	-0.018 (2)	0.0078 (18)
C2S	0.053 (3)	0.031 (2)	0.080 (4)	0.0182 (19)	0.033 (3)	0.033 (2)
N2S	0.110 (4)	0.076 (3)	0.066 (3)	0.052 (3)	0.038 (3)	0.045 (3)
Se3	0.02258 (15)	0.02116 (16)	0.03000 (18)	-0.00393 (12)	-0.00818 (13)	0.00354 (13)
C1	0.0241 (15)	0.0218 (15)	0.0252 (16)	-0.0042 (12)	-0.0106 (13)	0.0045 (13)
N1	0.0242 (13)	0.0267 (14)	0.0279 (15)	-0.0031 (11)	-0.0055 (11)	0.0037 (12)
N2	0.0218 (13)	0.0233 (13)	0.0332 (16)	-0.0014 (11)	-0.0054 (11)	0.0018 (12)
C2	0.0263 (16)	0.0235 (16)	0.0239 (16)	-0.0023 (13)	-0.0086 (13)	0.0013 (13)
N3	0.0264 (14)	0.0214 (13)	0.0309 (15)	-0.0033 (11)	-0.0034 (11)	0.0008 (12)
C3	0.0312 (17)	0.0218 (15)	0.0278 (17)	-0.0018 (13)	-0.0048 (14)	-0.0008 (13)
N4	0.0255 (13)	0.0251 (14)	0.0250 (14)	-0.0026 (11)	-0.0060 (11)	-0.0002 (11)
C4	0.0305 (17)	0.0209 (15)	0.0270 (17)	-0.0064 (13)	-0.0068 (13)	0.0006 (13)
C5	0.0267 (16)	0.0242 (16)	0.0265 (17)	-0.0043 (13)	-0.0062 (13)	-0.0007 (13)
C6	0.0232 (15)	0.0226 (15)	0.0250 (16)	-0.0017 (12)	-0.0106 (12)	0.0028 (13)
C7	0.0363 (18)	0.0184 (15)	0.0319 (18)	-0.0026 (13)	0.0025 (14)	-0.0024 (14)
C8	0.062 (3)	0.0283 (19)	0.034 (2)	-0.0092 (18)	0.0025 (19)	0.0041 (16)
C9	0.108 (4)	0.0217 (19)	0.054 (3)	-0.021 (2)	0.037 (3)	-0.0152 (19)
C10	0.036 (2)	0.039 (2)	0.123 (5)	-0.015 (2)	-0.010 (3)	0.028 (3)
C11	0.0218 (15)	0.0236 (15)	0.0282 (17)	-0.0026 (12)	-0.0103 (13)	-0.0001 (13)
C12	0.0273 (16)	0.0226 (16)	0.0309 (18)	-0.0013 (13)	-0.0067 (13)	0.0013 (14)
C13	0.040 (2)	0.0285 (18)	0.038 (2)	-0.0022 (16)	0.0052 (16)	0.0005 (16)
C14	0.045 (2)	0.0262 (18)	0.055 (3)	0.0020 (17)	0.0071 (19)	-0.0025 (18)
C15	0.038 (2)	0.0216 (17)	0.057 (3)	-0.0031 (15)	0.0064 (19)	0.0032 (17)
C16	0.0283 (17)	0.0247 (17)	0.044 (2)	-0.0057 (14)	-0.0006 (15)	0.0043 (16)

C17	0.0242 (15)	0.0202 (15)	0.0336 (18)	-0.0017 (12)	-0.0062 (13)	-0.0014 (13)
C18	0.0272 (16)	0.0271 (17)	0.0264 (17)	-0.0041 (13)	-0.0066 (13)	0.0012 (14)
C19	0.0244 (16)	0.039 (2)	0.0294 (18)	-0.0047 (14)	-0.0076 (14)	0.0019 (16)
C20	0.0272 (17)	0.043 (2)	0.0294 (18)	-0.0078 (15)	-0.0048 (14)	-0.0012 (16)
C21	0.0316 (19)	0.043 (2)	0.037 (2)	-0.0084 (16)	-0.0023 (16)	0.0050 (17)
C22	0.039 (2)	0.054 (3)	0.051 (3)	-0.012 (2)	0.0008 (19)	0.013 (2)
C11A	0.0243 (15)	0.0275 (16)	0.0236 (16)	-0.0007 (13)	-0.0061 (12)	0.0011 (13)
C12A	0.0242 (15)	0.0329 (18)	0.0234 (16)	-0.0031 (13)	-0.0100 (13)	0.0001 (14)
C13A	0.0249 (16)	0.039 (2)	0.0251 (17)	0.0003 (14)	-0.0074 (13)	0.0012 (15)
C14A	0.0230 (16)	0.053 (2)	0.0300 (19)	-0.0047 (16)	-0.0060 (14)	0.0019 (17)
C15A	0.0292 (18)	0.044 (2)	0.0311 (19)	-0.0082 (16)	-0.0074 (15)	0.0083 (17)
C16A	0.0280 (17)	0.0344 (19)	0.0331 (19)	-0.0037 (15)	-0.0071 (14)	0.0056 (16)
C17A	0.0234 (15)	0.0304 (17)	0.0274 (17)	-0.0021 (13)	-0.0084 (13)	0.0027 (14)
C18A	0.026 (2)	0.024 (2)	0.022 (3)	0.0008 (18)	-0.005 (3)	0.004 (2)
C19A	0.026 (2)	0.028 (2)	0.028 (2)	0.0015 (16)	-0.0036 (17)	-0.0035 (18)
C20A	0.034 (2)	0.027 (2)	0.030 (3)	-0.0015 (18)	-0.0016 (18)	-0.0035 (19)
C21A	0.043 (3)	0.037 (2)	0.034 (2)	0.013 (2)	0.002 (2)	-0.001 (2)
C22A	0.069 (4)	0.049 (3)	0.047 (3)	0.024 (3)	0.004 (3)	-0.005 (3)
C18B	0.026 (6)	0.024 (6)	0.026 (6)	0.003 (6)	-0.001 (6)	0.000 (6)
C19B	0.028 (5)	0.028 (5)	0.027 (5)	0.002 (5)	-0.004 (5)	-0.002 (5)
C20B	0.033 (5)	0.030 (5)	0.029 (5)	0.005 (5)	0.000 (5)	-0.004 (5)
C21B	0.039 (5)	0.034 (5)	0.033 (5)	0.005 (5)	-0.002 (5)	-0.004 (5)
C22B	0.042 (10)	0.048 (10)	0.037 (10)	0.011 (9)	0.003 (9)	-0.008 (9)

Geometric parameters (Å, °)

Hg1—Se1	2.5972 (4)	C18—C19	1.533 (4)
Hg1—Se1 ⁱ	2.5972 (4)	C18—H18A	0.9900
Hg1—Se2	2.7242 (5)	C18—H18B	0.9900
Hg1—Se2 ⁱ	2.7242 (5)	C19—C20	1.533 (5)
Se1—C1S	1.826 (4)	C19—H19C	0.9900
Se2—C2S	1.771 (7)	C19—H19D	0.9900
C1S—N1S	1.149 (5)	C20—C21	1.509 (5)
C2S—N2S	1.165 (8)	C20—H20C	0.9900
Se3—C1	1.886 (3)	C20—H20D	0.9900
Se3—N1	2.087 (3)	C21—C22	1.527 (5)
Se3—N2	2.099 (3)	C21—H21C	0.9900
C1—C6	1.400 (5)	C21—H21D	0.9900
C1—C2	1.405 (5)	C22—H22D	0.9800
N1—C11A	1.336 (4)	C22—H22E	0.9800
N1—C17A	1.386 (5)	C22—H22F	0.9800
N2—C11	1.332 (5)	C12A—C13A	1.393 (5)
N2—C17	1.395 (4)	C12A—C17A	1.410 (5)
C2—C3	1.406 (5)	C13A—C14A	1.384 (6)
C2—C11A	1.443 (5)	C13A—H13A	0.9500
N3—C11	1.353 (5)	C14A—C15A	1.410 (6)
N3—C12	1.393 (4)	C14A—H14A	0.9500
N3—C18	1.473 (5)	C15A—C16A	1.375 (6)

C3—C4	1.394 (5)	C15A—H15A	0.9500
C3—H3	0.9500	C16A—C17A	1.387 (5)
N4—C11A	1.355 (5)	C16A—H16A	0.9500
N4—C12A	1.392 (5)	C18A—C19A	1.530 (5)
N4—C18A	1.450 (9)	C18A—H18C	0.9900
N4—C18B	1.60 (5)	C18A—H18D	0.9900
C4—C5	1.406 (5)	C19A—C20A	1.530 (5)
C4—C7	1.534 (5)	C19A—H19A	0.9900
C5—C6	1.395 (5)	C19A—H19B	0.9900
C5—H5	0.9500	C20A—C21A	1.520 (6)
C6—C11	1.461 (5)	C20A—H20A	0.9900
C7—C8	1.517 (6)	C20A—H20B	0.9900
C7—C9	1.531 (5)	C21A—C22A	1.520 (6)
C7—C10	1.537 (6)	C21A—H21A	0.9900
C8—H8A	0.9800	C21A—H21B	0.9900
C8—H8B	0.9800	C22A—H22A	0.9800
C8—H8C	0.9800	C22A—H22B	0.9800
C9—H9A	0.9800	C22A—H22C	0.9800
C9—H9B	0.9800	C18B—C19B	1.531 (9)
C9—H9C	0.9800	C18B—H18E	0.9900
C10—H10A	0.9800	C18B—H18F	0.9900
C10—H10B	0.9800	C19B—C20B	1.529 (9)
C10—H10C	0.9800	C19B—H19E	0.9900
C12—C13	1.394 (5)	C19B—H19F	0.9900
C12—C17	1.394 (5)	C20B—C21B	1.512 (10)
C13—C14	1.393 (6)	C20B—H20E	0.9900
C13—H13	0.9500	C20B—H20F	0.9900
C14—C15	1.387 (6)	C21B—C22B	1.519 (10)
C14—H14	0.9500	C21B—H21E	0.9900
C15—C16	1.386 (6)	C21B—H21F	0.9900
C15—H15	0.9500	C22B—H22G	0.9800
C16—C17	1.402 (5)	C22B—H22H	0.9800
C16—H16	0.9500	C22B—H22I	0.9800
Se1—Hg1—Se1 ⁱ	126.637 (19)	H19C—C19—H19D	108.0
Se1—Hg1—Se2	114.732 (19)	C21—C20—C19	112.7 (3)
Se1 ⁱ —Hg1—Se2	102.907 (18)	C21—C20—H20C	109.1
Se1—Hg1—Se2 ⁱ	102.908 (18)	C19—C20—H20C	109.1
Se1 ⁱ —Hg1—Se2 ⁱ	114.732 (19)	C21—C20—H20D	109.1
Se2—Hg1—Se2 ⁱ	88.78 (3)	C19—C20—H20D	109.1
C1S—Se1—Hg1	101.43 (11)	H20C—C20—H20D	107.8
C2S—Se2—Hg1	101.31 (14)	C20—C21—C22	113.9 (4)
N1S—C1S—Se1	175.7 (4)	C20—C21—H21C	108.8
N2S—C2S—Se2	178.3 (5)	C22—C21—H21C	108.8
C1—Se3—N1	79.95 (14)	C20—C21—H21D	108.8
C1—Se3—N2	79.34 (14)	C22—C21—H21D	108.8
N1—Se3—N2	159.29 (11)	H21C—C21—H21D	107.7
C6—C1—C2	121.1 (3)	C21—C22—H22D	109.5

C6—C1—Se3	119.9 (3)	C21—C22—H22E	109.5
C2—C1—Se3	119.0 (3)	H22D—C22—H22E	109.5
C11A—N1—C17A	108.1 (3)	C21—C22—H22F	109.5
C11A—N1—Se3	113.0 (2)	H22D—C22—H22F	109.5
C17A—N1—Se3	138.9 (2)	H22E—C22—H22F	109.5
C11—N2—C17	107.6 (3)	N1—C11A—N4	110.9 (3)
C11—N2—Se3	113.7 (2)	N1—C11A—C2	115.8 (3)
C17—N2—Se3	138.6 (2)	N4—C11A—C2	133.4 (3)
C1—C2—C3	118.5 (3)	N4—C12A—C13A	131.4 (4)
C1—C2—C11A	112.3 (3)	N4—C12A—C17A	106.8 (3)
C3—C2—C11A	129.2 (3)	C13A—C12A—C17A	121.8 (4)
C11—N3—C12	107.2 (3)	C14A—C13A—C12A	116.5 (4)
C11—N3—C18	129.7 (3)	C14A—C13A—H13A	121.8
C12—N3—C18	123.1 (3)	C12A—C13A—H13A	121.8
C4—C3—C2	121.4 (3)	C13A—C14A—C15A	121.7 (4)
C4—C3—H3	119.3	C13A—C14A—H14A	119.2
C2—C3—H3	119.3	C15A—C14A—H14A	119.2
C11A—N4—C12A	107.3 (3)	C16A—C15A—C14A	121.6 (4)
C11A—N4—C18A	129.7 (5)	C16A—C15A—H15A	119.2
C12A—N4—C18A	122.8 (5)	C14A—C15A—H15A	119.2
C11A—N4—C18B	122 (3)	C15A—C16A—C17A	117.4 (4)
C12A—N4—C18B	129 (3)	C15A—C16A—H16A	121.3
C3—C4—C5	118.7 (3)	C17A—C16A—H16A	121.3
C3—C4—C7	121.7 (3)	N1—C17A—C16A	132.1 (4)
C5—C4—C7	119.6 (3)	N1—C17A—C12A	107.0 (3)
C6—C5—C4	121.3 (4)	C16A—C17A—C12A	121.0 (4)
C6—C5—H5	119.4	N4—C18A—C19A	113.4 (6)
C4—C5—H5	119.4	N4—C18A—H18C	108.9
C5—C6—C1	119.0 (3)	C19A—C18A—H18C	108.9
C5—C6—C11	129.0 (3)	N4—C18A—H18D	108.9
C1—C6—C11	112.0 (3)	C19A—C18A—H18D	108.9
C8—C7—C9	108.0 (4)	H18C—C18A—H18D	107.7
C8—C7—C4	109.4 (3)	C18A—C19A—C20A	110.8 (4)
C9—C7—C4	112.2 (3)	C18A—C19A—H19A	109.5
C8—C7—C10	108.9 (4)	C20A—C19A—H19A	109.5
C9—C7—C10	108.4 (4)	C18A—C19A—H19B	109.5
C4—C7—C10	109.9 (3)	C20A—C19A—H19B	109.5
C7—C8—H8A	109.5	H19A—C19A—H19B	108.1
C7—C8—H8B	109.5	C21A—C20A—C19A	113.0 (5)
H8A—C8—H8B	109.5	C21A—C20A—H20A	109.0
C7—C8—H8C	109.5	C19A—C20A—H20A	109.0
H8A—C8—H8C	109.5	C21A—C20A—H20B	109.0
H8B—C8—H8C	109.5	C19A—C20A—H20B	109.0
C7—C9—H9A	109.5	H20A—C20A—H20B	107.8
C7—C9—H9B	109.5	C20A—C21A—C22A	113.0 (5)
H9A—C9—H9B	109.5	C20A—C21A—H21A	109.0
C7—C9—H9C	109.5	C22A—C21A—H21A	109.0
H9A—C9—H9C	109.5	C20A—C21A—H21B	109.0

H9B—C9—H9C	109.5	C22A—C21A—H21B	109.0
C7—C10—H10A	109.5	H21A—C21A—H21B	107.8
C7—C10—H10B	109.5	C21A—C22A—H22A	109.5
H10A—C10—H10B	109.5	C21A—C22A—H22B	109.5
C7—C10—H10C	109.5	H22A—C22A—H22B	109.5
H10A—C10—H10C	109.5	C21A—C22A—H22C	109.5
H10B—C10—H10C	109.5	H22A—C22A—H22C	109.5
N2—C11—N3	111.0 (3)	H22B—C22A—H22C	109.5
N2—C11—C6	114.9 (3)	C19B—C18B—N4	106 (3)
N3—C11—C6	134.1 (3)	C19B—C18B—H18E	110.5
N3—C12—C13	130.3 (4)	N4—C18B—H18E	110.5
N3—C12—C17	107.0 (3)	C19B—C18B—H18F	110.5
C13—C12—C17	122.7 (3)	N4—C18B—H18F	110.5
C14—C13—C12	115.4 (4)	H18E—C18B—H18F	108.7
C14—C13—H13	122.3	C20B—C19B—C18B	111.6 (13)
C12—C13—H13	122.3	C20B—C19B—H19E	109.3
C15—C14—C13	122.1 (4)	C18B—C19B—H19E	109.3
C15—C14—H14	118.9	C20B—C19B—H19F	109.3
C13—C14—H14	118.9	C18B—C19B—H19F	109.3
C16—C15—C14	122.7 (4)	H19E—C19B—H19F	108.0
C16—C15—H15	118.6	C21B—C20B—C19B	113.8 (13)
C14—C15—H15	118.6	C21B—C20B—H20E	108.8
C15—C16—C17	115.7 (4)	C19B—C20B—H20E	108.8
C15—C16—H16	122.1	C21B—C20B—H20F	108.8
C17—C16—H16	122.1	C19B—C20B—H20F	108.8
C12—C17—N2	107.2 (3)	H20E—C20B—H20F	107.7
C12—C17—C16	121.3 (3)	C20B—C21B—C22B	114.6 (13)
N2—C17—C16	131.5 (4)	C20B—C21B—H21E	108.6
N3—C18—C19	111.1 (3)	C22B—C21B—H21E	108.6
N3—C18—H18A	109.4	C20B—C21B—H21F	108.6
C19—C18—H18A	109.4	C22B—C21B—H21F	108.6
N3—C18—H18B	109.4	H21E—C21B—H21F	107.6
C19—C18—H18B	109.4	C21B—C22B—H22G	109.5
H18A—C18—H18B	108.0	C21B—C22B—H22H	109.5
C20—C19—C18	111.6 (3)	H22G—C22B—H22H	109.5
C20—C19—H19C	109.3	C21B—C22B—H22I	109.5
C18—C19—H19C	109.3	H22G—C22B—H22I	109.5
C20—C19—H19D	109.3	H22H—C22B—H22I	109.5
C18—C19—H19D	109.3		
N1—Se3—C1—C6	-179.9 (3)	Se3—N2—C17—C16	8.2 (6)
N2—Se3—C1—C6	0.1 (2)	C15—C16—C17—C12	1.0 (5)
N1—Se3—C1—C2	-1.6 (2)	C15—C16—C17—N2	178.2 (4)
N2—Se3—C1—C2	178.3 (3)	C11—N3—C18—C19	-96.6 (4)
C6—C1—C2—C3	1.5 (5)	C12—N3—C18—C19	80.9 (4)
Se3—C1—C2—C3	-176.6 (2)	N3—C18—C19—C20	174.9 (3)
C6—C1—C2—C11A	-179.1 (3)	C18—C19—C20—C21	-76.2 (4)
Se3—C1—C2—C11A	2.7 (4)	C19—C20—C21—C22	-179.7 (3)

C1—C2—C3—C4	0.5 (5)	C17A—N1—C11A—N4	0.3 (4)
C11A—C2—C3—C4	-178.7 (3)	Se3—N1—C11A—N4	-178.3 (2)
C2—C3—C4—C5	-1.7 (5)	C17A—N1—C11A—C2	179.7 (3)
C2—C3—C4—C7	178.9 (3)	Se3—N1—C11A—C2	1.1 (4)
C3—C4—C5—C6	1.0 (5)	C12A—N4—C11A—N1	-0.7 (4)
C7—C4—C5—C6	-179.6 (3)	C18A—N4—C11A—N1	175.0 (5)
C4—C5—C6—C1	1.0 (5)	C18B—N4—C11A—N1	171 (3)
C4—C5—C6—C11	178.9 (3)	C12A—N4—C11A—C2	-179.9 (3)
C2—C1—C6—C5	-2.3 (5)	C18A—N4—C11A—C2	-4.3 (7)
Se3—C1—C6—C5	175.9 (2)	C18B—N4—C11A—C2	-9 (3)
C2—C1—C6—C11	179.5 (3)	C1—C2—C11A—N1	-2.3 (4)
Se3—C1—C6—C11	-2.3 (4)	C3—C2—C11A—N1	176.9 (3)
C3—C4—C7—C8	106.9 (4)	C1—C2—C11A—N4	176.9 (3)
C5—C4—C7—C8	-72.5 (4)	C3—C2—C11A—N4	-3.9 (6)
C3—C4—C7—C9	-13.0 (5)	C11A—N4—C12A—C13A	-178.7 (3)
C5—C4—C7—C9	167.7 (4)	C18A—N4—C12A—C13A	5.3 (6)
C3—C4—C7—C10	-133.6 (4)	C18B—N4—C12A—C13A	11 (3)
C5—C4—C7—C10	47.0 (5)	C11A—N4—C12A—C17A	0.8 (3)
C17—N2—C11—N3	-1.5 (4)	C18A—N4—C12A—C17A	-175.3 (5)
Se3—N2—C11—N3	175.4 (2)	C18B—N4—C12A—C17A	-170 (3)
C17—N2—C11—C6	178.7 (3)	N4—C12A—C13A—C14A	179.5 (3)
Se3—N2—C11—C6	-4.4 (3)	C17A—C12A—C13A—C14A	0.2 (5)
C12—N3—C11—N2	1.0 (4)	C12A—C13A—C14A—C15A	0.2 (5)
C18—N3—C11—N2	178.8 (3)	C13A—C14A—C15A—C16A	0.1 (5)
C12—N3—C11—C6	-179.3 (3)	C14A—C15A—C16A—C17A	-0.7 (5)
C18—N3—C11—C6	-1.5 (6)	C11A—N1—C17A—C16A	180.0 (4)
C5—C6—C11—N2	-173.6 (3)	Se3—N1—C17A—C16A	-2.0 (6)
C1—C6—C11—N2	4.4 (4)	C11A—N1—C17A—C12A	0.2 (4)
C5—C6—C11—N3	6.7 (6)	Se3—N1—C17A—C12A	178.2 (2)
C1—C6—C11—N3	-175.3 (3)	C15A—C16A—C17A—N1	-178.6 (3)
C11—N3—C12—C13	179.1 (4)	C15A—C16A—C17A—C12A	1.2 (5)
C18—N3—C12—C13	1.1 (6)	N4—C12A—C17A—N1	-0.6 (3)
C11—N3—C12—C17	-0.2 (4)	C13A—C12A—C17A—N1	178.9 (3)
C18—N3—C12—C17	-178.1 (3)	N4—C12A—C17A—C16A	179.6 (3)
N3—C12—C13—C14	-177.4 (4)	C13A—C12A—C17A—C16A	-0.9 (5)
C17—C12—C13—C14	1.7 (6)	C11A—N4—C18A—C19A	90.1 (8)
C12—C13—C14—C15	-0.2 (6)	C12A—N4—C18A—C19A	-94.9 (10)
C13—C14—C15—C16	-1.0 (7)	N4—C18A—C19A—C20A	172.9 (7)
C14—C15—C16—C17	0.6 (6)	C18A—C19A—C20A—C21A	-65.4 (11)
N3—C12—C17—N2	-0.7 (4)	C19A—C20A—C21A—C22A	-169.3 (5)
C13—C12—C17—N2	179.9 (3)	C11A—N4—C18B—C19B	104 (4)
N3—C12—C17—C16	177.1 (3)	C12A—N4—C18B—C19B	-87 (6)
C13—C12—C17—C16	-2.2 (5)	N4—C18B—C19B—C20B	178 (4)
C11—N2—C17—C12	1.3 (4)	C18B—C19B—C20B—C21B	-55 (7)
Se3—N2—C17—C12	-174.3 (2)	C19B—C20B—C21B—C22B	-60 (4)
C11—N2—C17—C16	-176.1 (4)		

Symmetry code: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C18—H18 <i>A</i> ···N1 <i>S</i> ⁱⁱ	0.99	2.62	3.568 (5)	160
C18 <i>A</i> —H18 <i>C</i> ···N2 <i>S</i>	0.99	2.38	3.324 (8)	159
C18 <i>B</i> —H18 <i>F</i> ···N2 <i>S</i>	0.99	2.22	3.06 (6)	142

Symmetry code: (ii) $-x+1/2, y+1/2, -z+3/2$.