# Tetrakis(1,2-dimethoxyethane-$\kappa^2O,O'$)-ytterbium(II) bis($\mu_2$-phenylselenolato-$\kappa^2Se$:Se)bis[bis(phenylselenolato-$\kappa Se$)-mercurate(II)]

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The title salt, $[Yb(C_4H_{10}O_2)_4][Hg_2(C_6H_5Se)_6]$, consists of eight-coordinate homoleptic $[Yb(DME)_4]^{2+}$ dications (DME is 1,2-dimethoxyethane) countered with $[Hg_2(SePh)_6]^{2-}$ dianions. The cations and anions have twofold rotation and inversion symmetry, respectively. The Yb centre displays a square-antiprismatic coordination geometry and the Hg centre has a distorted tetrahedral coordination environment. One phenylselenolate anion and one methyl group of a DME ligand are disordered over two positions with equal occupancies. This structure is unique in that it represents a less common molecular lanthanide species in which the lanthanide ion is not directly bonded to an anionic ligand. There are no occurrences of the $[Hg_2(SePh)_6]^{2-}$ dianion in the Cambridge Structural Database (Version of November 2007), but there are similar oligomeric and polymeric $Hg_x(SePh)_y$ species. The crystal structure is characterized by alternating layers of cations and anions stacked along the $c$ axis.

## Related literature

For the synthesis and crystal structures of related compounds see: Berardini *et al.* (1995); Bettenhausen & Fenske (1998); Deacon *et al.* (2001); Evans *et al.* (2000); Freedman *et al.* (1997); Hyeon & Edelmann (2003); Hakansson *et al.* (1999); Kim & Kanatzidis (1991); Magull *et al.* (1991); Melman *et al.* (2002); Allen (2002); Allen *et al.* (1991).
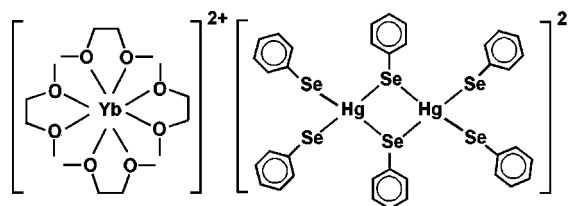


## Experimental

### Crystal data

| | |
|---|---|
| $[Yb(C_4H_{10}O_2)_4][Hg_2(C_6H_5Se)_6]$ | $V$ = 5839.1 (14) Å³ |
| $M_r$ = 1871.06 | $Z$ = 4 |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| $a$ = 22.688 (3) Å | $\mu$ = 10.62 mm⁻¹ |
| $b$ = 12.354 (2) Å | $T$ = 100 (2) K |
| $c$ = 22.843 (3) Å | 0.17 × 0.14 × 0.02 mm |
| $\beta$ = 114.218 (3)° | |

### Data collection

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 26008 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2003) | 5956 independent reflections |
| $T_{min}$ = 0.18, $T_{max}$ = 0.81 | 4806 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.052 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.028 | 734 restraints |
| $wR(F^2)$ = 0.064 | H-atom parameters constrained |
| $S$ = 1.00 | $\Delta\rho_{max}$ = 1.50 e Å⁻³ |
| 5956 reflections | $\Delta\rho_{min}$ = −0.73 e Å⁻³ |
| 389 parameters | |

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Yb1—O2 | 2.469 (4) | Hg1—Se1 | 2.5683 (7) |
| Yb1—O3 | 2.489 (3) | Hg1—Se3A | 2.635 (3) |
| Yb1—O1 | 2.534 (4) | Hg1—Se2 | 2.6747 (6) |
| Yb1—O4 | 2.555 (4) | Hg1—Se2ii | 2.8667 (6) |
| Hg1—Se3B | 2.544 (3) | | |

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

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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# supporting information

# Tetrakis(1,2-dimethoxyethane-*κ²O,O′*)ytterbium(II) bis(*μ₂*-phenylselenolato-*κ²Se:Se*)bis[bis(phenylselenolato-*κSe*)mercurate(II)]

**Michael D. Romanelli, Thomas J. Emge and John G. Brennan**

## S1. Comment

Lanthanide (Ln) ion salts, in which the Ln metal itself is surrounded only by neutral donor ligands and oxidized only by a non-bonded anionic molecule, make up a small portion of less common Ln complexes. It is more likely for the Ln metal to be oxidized by direct coordination of an anionic species (EPh⁻, $X^-$, Cp⁻, *etc.*. where E = S, Se, Te, $X$ = Cl, Br, I) with the metal (Hyeon *et al.*, 2003, Melman *et al.*, 2002). Similar species to the one described herein exist, such as, tris(1,2-di-methoxyethane-*O,O′*)-diiododysprosium(II) (Evans *et al.*, 2000), rac-diiodo-tris(dimethoxyethane)samarium (Hakansson *et al.*, 1999), and tris(1,2-dimethoxyethane)-bis(isothiocyanato)ytterbium(II) (Deacon *et al.*, 2001). These structures differ from the species reported here by their having direct oxidation of the lanthanide metal with anionic coordinating ligands.

In this communication, we report the structure of a unique $[Yb(DME)_4]^{2+}[Hg_2(SePh)_6]^{2-}$ molecular salt (Fig 1.). The 8-coordinate $[Yb(DME)_4]^{2+}$ dication in this study has approximate D-42*m* (Td) symmetry giving rise to square antiprism geometry similar to U(acac)₄. Yb—O bonds of the dication range from 2.465 (4) Å to 2.561 (4) Å and are consistent with the range found for divalent ytterbium(II)—O$R_2$ species, having an associated average of 2.45 Å (Cambridge Structural Database; Allen *et al.*, 1991). Consistent with the general trend, trivalent ytterbium(III)—O$R_2$ bond distances average noticeably shorter at 2.35 Å. Like the dication, the Hg—Se bond geometries of the dianion in this study are consistent with the Hg—Se bonds found in similar oligomeric or polymeric structures (Berardini *et al.*, 1995; Bettenhausen *et al.*, 1998; Freedman *et al.*, 1997; Kim *et al.*, 1991; Magull *et al.*,1991), which average 2.68 Å. It should be noted that these types of anions are not common and no reports of the dimeric form presented here are found in the Cambridge Structure Database (Nov 2007 version; Allen, 2002). In this Hg dianion, the doubly bridging selenolates bond to the Hg with bond lengths of 2.6746 (5) Å and 2.8664 (6) Å, while the terminal Hg—Se bond lengths are 2.545 (2), 2.5691 (6) and 2.625 (2) Å for Hg1—Se3B, Hg1—Se1 and Hg1—Se3A, respectively. Packing of the cation/anion pair in this sturcture is consistent with other molecular salts in that there are alternating planes of cations and anions repeated along the crystallographic *c* axis (Fig. 2).

## S2. Experimental

All synthesis were carried out under high purity nitrogen (Welco Praxair) using standard Schlenk and glovebox techniques. Solvents (Aldrich) were purified with a dual column Solv-Tek Solvent Purification System. Lanthanide metals were purchased from Strem. The reported structure, $[Yb(DME)_4]^{2+}[Hg_2(SePh)_6]^{2-}$ was synthesized by the reaction of 1 mmol Yb metal with 1.5 mmol PhSeSePh and 40 mg elemental Hg in 30 ml DME. After 14 days, the deep red solution was filtered and concentrated from approximately 20 ml down to 5 ml. The saturated solution was held at -5 C for 7 days to afford yellow crystals of the title compound.

### S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93–0.97 Å and refined as riding with $U_{iso}(H) = 1.2\ U_{eq}(C)$ or $1.5\ U_{eq}(C)$ for methyl H atoms. The Se3/C21—C26 phenylselenolato anion and the C4 methyl carbon atom are disordered over two positions with equal site-occupancy factors of 0.5 and refined using SIMU, SADI and DELU restraints. To improve refinement stability, restraints (DELU and SIMU) were applied to the displacement parameters of all non-H atoms.
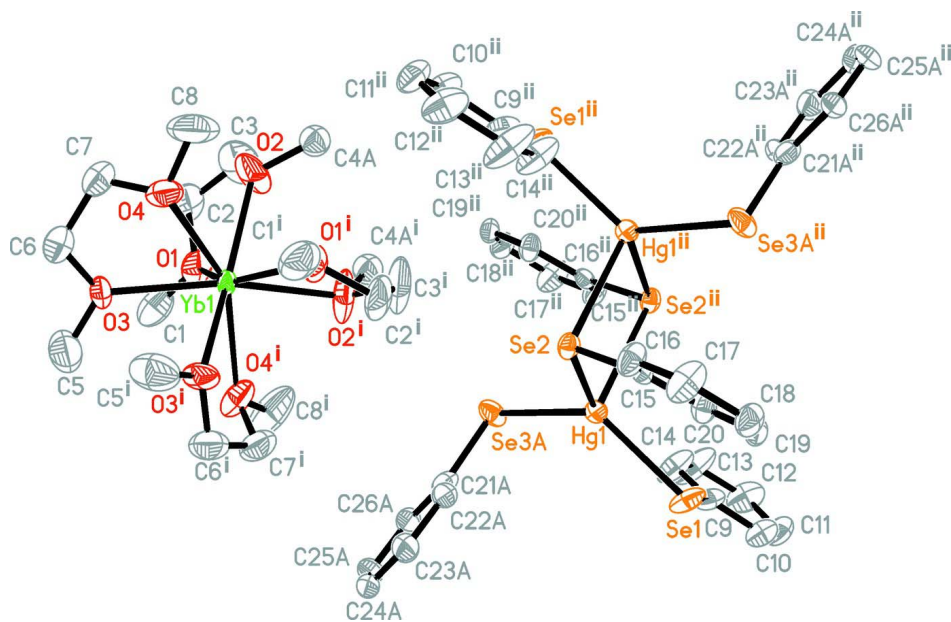


**Figure 1**

*ORTEP* drawing of the title compound with thermal ellipsoids drawn at 50% probability. Hydrogen atoms are omitted for clarity. Only one component of disorder is shown. Symmetry codes: i = -*x*, *y*, 1/2 - *z*; ii = -*x*, 1 - *y*, 1 - *z*.
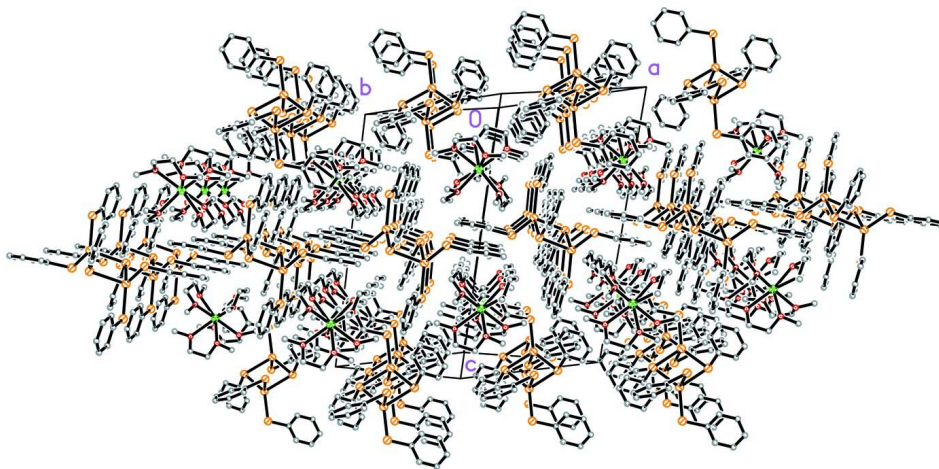


**Figure 2**

Packing diagram of the title compound showing alternating layers of cations and anions stacking along the c direction. Hydrogen atoms are omitted for clarity. Only one component of disorder is shown.

**tetrakis(1,2-dimethoxyethane-$\kappa^2O,O'$)ytterbium(II) bis($\mu_2$-phenylselenolato-$\kappa^2Se:Se$)bis[bis(phenylselenolato-$\kappa Se$)mercurate(II)]**

*Crystal data*

| | |
|---|---|
| [Yb(C$_4$H$_{10}$O$_2$)$_4$][Hg$_2$(C$_6$H$_5$Se)$_6$] | $F(000) = 3520$ |
| $M_r = 1871.06$ | $D_x = 2.128$ Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -C 2yc | Cell parameters from 7567 reflections |
| $a = 22.688$ (3) Å | $\theta = 2.4$–$30.5°$ |
| $b = 12.354$ (2) Å | $\mu = 10.62$ mm$^{-1}$ |
| $c = 22.843$ (3) Å | $T = 100$ K |
| $\beta = 114.218$ (3)° | Plate, yellow |
| $V = 5839.1$ (14) Å$^3$ | $0.17 \times 0.14 \times 0.02$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD diffractometer | 26008 measured reflections |
| Radiation source: fine-focus sealed tube | 5956 independent reflections |
| Graphite monochromator | 4806 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.052$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2003) | $\theta_{max} = 26.4°$, $\theta_{min} = 1.9°$ |
| $T_{min} = 0.18$, $T_{max} = 0.81$ | $h = -28 \rightarrow 28$ |
| | $k = -15 \rightarrow 15$ |
| | $l = -28 \rightarrow 28$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.064$ | |
| $S = 1.00$ | H-atom parameters constrained |
| 5956 reflections | $w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 0.9P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 389 parameters | |
| 734 restraints | $(\Delta/\sigma)_{max} = 0.001$ |
| 280 constraints | $\Delta\rho_{max} = 1.50$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.73$ e Å$^{-3}$ |

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Yb1 | 0.0000 | 0.07701 (2) | 0.2500 | 0.02876 (8) | |
| O1 | 0.0836 (2) | 0.1319 (3) | 0.20857 (19) | 0.0506 (10) | |
| O2 | −0.0312 (2) | 0.2322 (3) | 0.1753 (2) | 0.0707 (13) | |

| | | | | | |
|---|---|---|---|---|---|
| O3 | 0.00913 (18) | −0.0821 (3) | 0.18739 (19) | 0.0439 (9) | |
| O4 | −0.10668 (19) | 0.0251 (3) | 0.15775 (19) | 0.0533 (10) | |
| C1 | 0.1380 (3) | 0.0671 (6) | 0.2132 (3) | 0.0624 (17) | |
| H1A | 0.1530 | 0.0255 | 0.2521 | 0.094* | |
| H1B | 0.1722 | 0.1135 | 0.2136 | 0.094* | |
| H1C | 0.1253 | 0.0192 | 0.1770 | 0.094* | |
| C2 | 0.0571 (4) | 0.1880 (5) | 0.1486 (3) | 0.0626 (16) | |
| H2A | 0.0339 | 0.1374 | 0.1144 | 0.075* | |
| H2B | 0.0918 | 0.2194 | 0.1398 | 0.075* | |
| C3 | 0.0133 (4) | 0.2736 (6) | 0.1501 (4) | 0.0793 (19) | |
| H3A | 0.0380 | 0.3327 | 0.1768 | 0.095* | |
| H3B | −0.0107 | 0.3013 | 0.1071 | 0.095* | |
| C4A | −0.0602 (8) | 0.3280 (10) | 0.1864 (9) | 0.061 (4) | 0.50 |
| H4A | −0.0897 | 0.3089 | 0.2053 | 0.092* | 0.50 |
| H4B | −0.0833 | 0.3646 | 0.1464 | 0.092* | 0.50 |
| H4C | −0.0272 | 0.3748 | 0.2151 | 0.092* | 0.50 |
| C4B | −0.0863 (6) | 0.3006 (13) | 0.1677 (10) | 0.075 (4) | 0.50 |
| H4D | −0.1145 | 0.2622 | 0.1823 | 0.113* | 0.50 |
| H4E | −0.1094 | 0.3191 | 0.1232 | 0.113* | 0.50 |
| H4F | −0.0713 | 0.3654 | 0.1925 | 0.113* | 0.50 |
| C5 | 0.0553 (3) | −0.1652 (5) | 0.2109 (4) | 0.070 (2) | |
| H5A | 0.0924 | −0.1389 | 0.2469 | 0.105* | |
| H5B | 0.0682 | −0.1881 | 0.1777 | 0.105* | |
| H5C | 0.0369 | −0.2254 | 0.2242 | 0.105* | |
| C6 | −0.0454 (3) | −0.1146 (5) | 0.1329 (3) | 0.0596 (16) | |
| H6A | −0.0664 | −0.1746 | 0.1440 | 0.072* | |
| H6B | −0.0319 | −0.1392 | 0.0999 | 0.072* | |
| C7 | −0.0926 (3) | −0.0226 (5) | 0.1071 (3) | 0.0565 (15) | |
| H7A | −0.0745 | 0.0320 | 0.0887 | 0.068* | |
| H7B | −0.1322 | −0.0491 | 0.0734 | 0.068* | |
| C8 | −0.1610 (4) | 0.0929 (7) | 0.1291 (4) | 0.091 (3) | |
| H8A | −0.1694 | 0.1295 | 0.1620 | 0.137* | |
| H8B | −0.1979 | 0.0500 | 0.1035 | 0.137* | |
| H8C | −0.1527 | 0.1453 | 0.1024 | 0.137* | |
| Hg1 | 0.072118 (8) | 0.426875 (14) | 0.561656 (9) | 0.02549 (6) | |
| Se1 | 0.10648 (3) | 0.44945 (5) | 0.68300 (2) | 0.03980 (14) | |
| Se2 | −0.04871 (2) | 0.35961 (3) | 0.49222 (2) | 0.02268 (10) | |
| C9 | 0.1760 (2) | 0.5511 (4) | 0.7052 (2) | 0.0340 (11) | |
| C10 | 0.2013 (2) | 0.5948 (4) | 0.7657 (3) | 0.0398 (12) | |
| H10 | 0.1856 | 0.5718 | 0.7954 | 0.048* | |
| C11 | 0.2492 (3) | 0.6718 (5) | 0.7837 (3) | 0.0434 (13) | |
| H11 | 0.2654 | 0.7002 | 0.8250 | 0.052* | |
| C12 | 0.2731 (2) | 0.7066 (5) | 0.7412 (3) | 0.0505 (14) | |
| H12 | 0.3046 | 0.7603 | 0.7528 | 0.061* | |
| C13 | 0.2501 (3) | 0.6611 (6) | 0.6810 (3) | 0.0590 (17) | |
| H13 | 0.2671 | 0.6827 | 0.6521 | 0.071* | |
| C14 | 0.2019 (3) | 0.5837 (5) | 0.6629 (3) | 0.0496 (15) | |
| H14 | 0.1868 | 0.5536 | 0.6220 | 0.060* | |

| | | | | |
|---|---|---|---|---|
| C15 | −0.0921 (2) | 0.3620 (3) | 0.5486 (2) | 0.0213 (9) | |
| C16 | −0.1494 (2) | 0.3053 (4) | 0.5311 (2) | 0.0330 (11) | |
| H16 | −0.1666 | 0.2694 | 0.4919 | 0.040* | |
| C17 | −0.1812 (2) | 0.3015 (5) | 0.5714 (3) | 0.0439 (13) | |
| H17 | −0.2204 | 0.2652 | 0.5583 | 0.053* | |
| C18 | −0.1556 (2) | 0.3506 (4) | 0.6302 (2) | 0.0342 (11) | |
| H18 | −0.1765 | 0.3456 | 0.6576 | 0.041* | |
| C19 | −0.0986 (2) | 0.4075 (4) | 0.6484 (2) | 0.0291 (10) | |
| H19 | −0.0811 | 0.4417 | 0.6881 | 0.035* | |
| C20 | −0.0677 (2) | 0.4141 (4) | 0.6079 (2) | 0.0281 (10) | |
| H20 | −0.0298 | 0.4540 | 0.6203 | 0.034* | |
| Se3A | 0.14624 (15) | 0.36619 (19) | 0.50396 (14) | 0.0311 (4) | 0.50 |
| C21A | 0.1583 (3) | 0.2179 (5) | 0.5311 (4) | 0.0246 (18) | 0.50 |
| C22A | 0.1111 (4) | 0.1562 (5) | 0.5387 (4) | 0.027 (2) | 0.50 |
| H22A | 0.0721 | 0.1891 | 0.5325 | 0.032* | 0.50 |
| C23A | 0.1193 (4) | 0.0471 (5) | 0.5553 (4) | 0.0345 (19) | 0.50 |
| H23A | 0.0866 | 0.0076 | 0.5601 | 0.041* | 0.50 |
| C24A | 0.1772 (4) | −0.0007 (6) | 0.5643 (4) | 0.036 (2) | 0.50 |
| H24A | 0.1836 | −0.0736 | 0.5753 | 0.044* | 0.50 |
| C25A | 0.2267 (4) | 0.0574 (6) | 0.5572 (4) | 0.036 (2) | 0.50 |
| H25A | 0.2656 | 0.0242 | 0.5634 | 0.043* | 0.50 |
| C26A | 0.2163 (3) | 0.1663 (6) | 0.5406 (4) | 0.0273 (18) | 0.50 |
| H26A | 0.2489 | 0.2059 | 0.5358 | 0.033* | 0.50 |
| Se3B | 0.14874 (15) | 0.3380 (2) | 0.52023 (15) | 0.0452 (6) | 0.50 |
| C21B | 0.1398 (4) | 0.1869 (5) | 0.5340 (4) | 0.034 (2) | 0.50 |
| C22B | 0.0823 (4) | 0.1404 (6) | 0.5287 (4) | 0.039 (2) | 0.50 |
| H22B | 0.0465 | 0.1849 | 0.5196 | 0.047* | 0.50 |
| C23B | 0.0758 (4) | 0.0299 (6) | 0.5365 (4) | 0.048 (2) | 0.50 |
| H23B | 0.0366 | 0.0005 | 0.5327 | 0.057* | 0.50 |
| C24B | 0.1294 (5) | −0.0345 (6) | 0.5500 (4) | 0.055 (2) | 0.50 |
| H24B | 0.1259 | −0.1085 | 0.5553 | 0.066* | 0.50 |
| C25B | 0.1886 (5) | 0.0073 (7) | 0.5559 (5) | 0.050 (2) | 0.50 |
| H25B | 0.2242 | −0.0375 | 0.5650 | 0.059* | 0.50 |
| C26B | 0.1928 (4) | 0.1183 (7) | 0.5477 (4) | 0.046 (2) | 0.50 |
| H26B | 0.2319 | 0.1475 | 0.5515 | 0.055* | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Yb1 | 0.05749 (19) | 0.01481 (14) | 0.01899 (16) | 0.000 | 0.02075 (14) | 0.000 |
| O1 | 0.083 (3) | 0.044 (2) | 0.039 (2) | −0.0086 (18) | 0.040 (2) | 0.0020 (18) |
| O2 | 0.130 (3) | 0.037 (2) | 0.076 (3) | 0.029 (2) | 0.073 (3) | 0.028 (2) |
| O3 | 0.053 (2) | 0.0304 (18) | 0.042 (2) | 0.0060 (15) | 0.0138 (18) | −0.0135 (16) |
| O4 | 0.059 (2) | 0.064 (2) | 0.032 (2) | 0.0202 (19) | 0.0129 (19) | 0.0095 (19) |
| C1 | 0.069 (4) | 0.083 (5) | 0.043 (4) | −0.006 (3) | 0.030 (3) | −0.005 (3) |
| C2 | 0.107 (4) | 0.056 (4) | 0.049 (3) | 0.000 (3) | 0.057 (3) | 0.009 (3) |
| C3 | 0.132 (5) | 0.057 (4) | 0.074 (4) | 0.013 (3) | 0.068 (4) | 0.030 (3) |
| C4A | 0.110 (9) | 0.033 (6) | 0.050 (8) | 0.025 (6) | 0.041 (7) | 0.011 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4B | 0.108 (8) | 0.042 (7) | 0.072 (10) | 0.033 (6) | 0.033 (7) | 0.002 (6) |
| C5 | 0.066 (4) | 0.051 (4) | 0.079 (5) | 0.012 (3) | 0.016 (3) | −0.019 (3) |
| C6 | 0.070 (4) | 0.050 (3) | 0.047 (4) | 0.000 (3) | 0.011 (3) | −0.014 (3) |
| C7 | 0.073 (4) | 0.056 (3) | 0.034 (3) | 0.004 (3) | 0.016 (3) | −0.007 (3) |
| C8 | 0.082 (4) | 0.125 (6) | 0.057 (5) | 0.058 (4) | 0.020 (4) | 0.025 (4) |
| Hg1 | 0.02478 (9) | 0.02907 (10) | 0.02306 (11) | 0.00644 (7) | 0.01028 (8) | 0.00076 (8) |
| Se1 | 0.0472 (3) | 0.0482 (3) | 0.0198 (3) | −0.0124 (2) | 0.0094 (2) | 0.0091 (2) |
| Se2 | 0.0279 (2) | 0.0224 (2) | 0.0226 (3) | −0.00359 (17) | 0.0153 (2) | −0.00224 (19) |
| C9 | 0.026 (2) | 0.047 (3) | 0.023 (2) | 0.0002 (19) | 0.0041 (19) | 0.006 (2) |
| C10 | 0.040 (3) | 0.051 (3) | 0.027 (3) | −0.004 (2) | 0.013 (2) | 0.004 (2) |
| C11 | 0.043 (3) | 0.056 (3) | 0.026 (3) | −0.006 (2) | 0.009 (2) | −0.007 (2) |
| C12 | 0.031 (3) | 0.071 (4) | 0.040 (3) | −0.017 (3) | 0.005 (2) | 0.000 (3) |
| C13 | 0.045 (3) | 0.099 (5) | 0.030 (3) | −0.031 (3) | 0.014 (3) | −0.001 (3) |
| C14 | 0.037 (3) | 0.084 (4) | 0.026 (3) | −0.020 (3) | 0.010 (2) | −0.002 (3) |
| C15 | 0.025 (2) | 0.019 (2) | 0.025 (2) | 0.0055 (16) | 0.0151 (19) | 0.0036 (18) |
| C16 | 0.025 (2) | 0.051 (3) | 0.026 (3) | −0.002 (2) | 0.013 (2) | −0.006 (2) |
| C17 | 0.023 (2) | 0.076 (4) | 0.033 (3) | −0.013 (2) | 0.013 (2) | −0.010 (3) |
| C18 | 0.029 (2) | 0.051 (3) | 0.029 (3) | 0.002 (2) | 0.018 (2) | −0.002 (2) |
| C19 | 0.041 (2) | 0.025 (2) | 0.024 (3) | −0.0010 (19) | 0.016 (2) | −0.0046 (19) |
| C20 | 0.034 (2) | 0.025 (2) | 0.030 (3) | −0.0068 (18) | 0.017 (2) | −0.0047 (19) |
| Se3A | 0.0342 (7) | 0.0292 (10) | 0.0414 (11) | 0.0113 (7) | 0.0273 (7) | 0.0129 (7) |
| C21A | 0.028 (4) | 0.029 (3) | 0.020 (4) | 0.003 (3) | 0.013 (3) | −0.001 (3) |
| C22A | 0.028 (4) | 0.028 (4) | 0.024 (4) | 0.006 (3) | 0.011 (4) | 0.004 (4) |
| C23A | 0.050 (4) | 0.029 (4) | 0.029 (4) | 0.009 (3) | 0.022 (4) | 0.003 (3) |
| C24A | 0.054 (4) | 0.032 (4) | 0.026 (4) | 0.016 (3) | 0.019 (4) | 0.006 (4) |
| C25A | 0.040 (4) | 0.035 (4) | 0.029 (4) | 0.018 (3) | 0.011 (4) | 0.000 (4) |
| C26A | 0.027 (4) | 0.034 (4) | 0.020 (4) | 0.008 (3) | 0.010 (3) | 0.002 (4) |
| Se3B | 0.0400 (9) | 0.0440 (14) | 0.069 (2) | 0.0054 (9) | 0.0405 (13) | −0.0030 (10) |
| C21B | 0.041 (5) | 0.038 (4) | 0.020 (4) | 0.015 (3) | 0.010 (4) | −0.003 (4) |
| C22B | 0.055 (5) | 0.039 (4) | 0.026 (5) | 0.008 (4) | 0.019 (5) | 0.007 (4) |
| C23B | 0.068 (5) | 0.044 (4) | 0.036 (5) | 0.011 (4) | 0.026 (5) | 0.006 (4) |
| C24B | 0.082 (5) | 0.050 (5) | 0.036 (5) | 0.022 (4) | 0.027 (5) | 0.007 (4) |
| C25B | 0.066 (4) | 0.048 (4) | 0.031 (5) | 0.032 (4) | 0.017 (4) | −0.003 (4) |
| C26B | 0.052 (4) | 0.051 (4) | 0.029 (4) | 0.017 (3) | 0.009 (4) | −0.009 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Yb1—O2 | 2.469 (4) | Se2—C15 | 1.917 (4) |
| Yb1—O2$^i$ | 2.469 (4) | C9—C10 | 1.372 (7) |
| Yb1—O3 | 2.489 (3) | C9—C14 | 1.381 (7) |
| Yb1—O3$^i$ | 2.489 (3) | C10—C11 | 1.374 (7) |
| Yb1—O1 | 2.534 (4) | C10—H10 | 0.9300 |
| Yb1—O1$^i$ | 2.534 (4) | C11—C12 | 1.360 (8) |
| Yb1—O4$^i$ | 2.554 (4) | C11—H11 | 0.9300 |
| Yb1—O4 | 2.555 (4) | C12—C13 | 1.375 (8) |
| O1—C2 | 1.430 (7) | C12—H12 | 0.9300 |
| O1—C1 | 1.439 (7) | C13—C14 | 1.382 (8) |
| O2—C4A | 1.427 (8) | C13—H13 | 0.9300 |

| | | | |
|---|---|---|---|
| O2—C3 | 1.445 (7) | C14—H14 | 0.9300 |
| O2—C4B | 1.459 (9) | C15—C16 | 1.383 (6) |
| O3—C5 | 1.407 (7) | C15—C20 | 1.392 (6) |
| O3—C6 | 1.407 (7) | C16—C17 | 1.383 (7) |
| O4—C8 | 1.410 (7) | C16—H16 | 0.9300 |
| O4—C7 | 1.447 (7) | C17—C18 | 1.368 (7) |
| C1—H1A | 0.9600 | C17—H17 | 0.9300 |
| C1—H1B | 0.9600 | C18—C19 | 1.378 (6) |
| C1—H1C | 0.9600 | C18—H18 | 0.9300 |
| C2—C3 | 1.462 (9) | C19—C20 | 1.372 (6) |
| C2—H2A | 0.9700 | C19—H19 | 0.9300 |
| C2—H2B | 0.9700 | C20—H20 | 0.9300 |
| C3—H3A | 0.9700 | Se3A—C21A | 1.917 (5) |
| C3—H3B | 0.9700 | C21A—C22A | 1.384 (6) |
| C4A—H4A | 0.9600 | C21A—C26A | 1.396 (6) |
| C4A—H4B | 0.9600 | C22A—C23A | 1.392 (6) |
| C4A—H4C | 0.9600 | C22A—H22A | 0.9300 |
| C4B—H4D | 0.9600 | C23A—C24A | 1.377 (6) |
| C4B—H4E | 0.9600 | C23A—H23A | 0.9300 |
| C4B—H4F | 0.9600 | C24A—C25A | 1.396 (7) |
| C5—H5A | 0.9600 | C24A—H24A | 0.9300 |
| C5—H5B | 0.9600 | C25A—C26A | 1.392 (6) |
| C5—H5C | 0.9600 | C25A—H25A | 0.9300 |
| C6—C7 | 1.506 (8) | C26A—H26A | 0.9300 |
| C6—H6A | 0.9700 | Se3B—C21B | 1.917 (6) |
| C6—H6B | 0.9700 | C21B—C22B | 1.386 (6) |
| C7—H7A | 0.9700 | C21B—C26B | 1.396 (6) |
| C7—H7B | 0.9700 | C22B—C23B | 1.393 (6) |
| C8—H8A | 0.9600 | C22B—H22B | 0.9300 |
| C8—H8B | 0.9600 | C23B—C24B | 1.379 (6) |
| C8—H8C | 0.9600 | C23B—H23B | 0.9300 |
| Hg1—Se3B | 2.544 (3) | C24B—C25B | 1.393 (7) |
| Hg1—Se1 | 2.5683 (7) | C24B—H24B | 0.9300 |
| Hg1—Se3A | 2.635 (3) | C25B—C26B | 1.392 (7) |
| Hg1—Se2 | 2.6747 (6) | C25B—H25B | 0.9300 |
| Hg1—Se2ii | 2.8667 (6) | C26B—H26B | 0.9300 |
| Se1—C9 | 1.914 (5) | | |
| | | | |
| O2—Yb1—O2i | 78.1 (2) | H8A—C8—H8B | 109.5 |
| O2—Yb1—O3 | 106.50 (14) | O4—C8—H8C | 109.5 |
| O2i—Yb1—O3 | 160.44 (15) | H8A—C8—H8C | 109.5 |
| O2—Yb1—O3i | 160.44 (15) | H8B—C8—H8C | 109.5 |
| O2i—Yb1—O3i | 106.50 (14) | Se3B—Hg1—Se1 | 119.81 (7) |
| O3—Yb1—O3i | 75.68 (18) | Se3B—Hg1—Se3A | 10.79 (6) |
| O2—Yb1—O1 | 65.21 (14) | Se1—Hg1—Se3A | 126.67 (7) |
| O2i—Yb1—O1 | 90.22 (13) | Se3B—Hg1—Se2 | 109.62 (8) |
| O3—Yb1—O1 | 75.25 (13) | Se1—Hg1—Se2 | 117.211 (17) |
| O3i—Yb1—O1 | 132.63 (13) | Se3A—Hg1—Se2 | 108.91 (8) |

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|---|---|---|---|
| O2—Yb1—O1[i] | 90.22 (13) | Se3B—Hg1—Se2[ii] | 105.78 (5) |
| O2[i]—Yb1—O1[i] | 65.21 (14) | Se1—Hg1—Se2[ii] | 106.512 (17) |
| O3—Yb1—O1[i] | 132.63 (13) | Se3A—Hg1—Se2[ii] | 95.21 (4) |
| O3[i]—Yb1—O1[i] | 75.25 (13) | Se2—Hg1—Se2[ii] | 93.839 (14) |
| O1—Yb1—O1[i] | 148.96 (18) | C9—Se1—Hg1 | 102.10 (15) |
| O2—Yb1—O4[i] | 132.16 (15) | C15—Se2—Hg1 | 106.31 (13) |
| O2[i]—Yb1—O4[i] | 73.67 (16) | C15—Se2—Hg1[ii] | 102.62 (12) |
| O3—Yb1—O4[i] | 90.09 (13) | Hg1—Se2—Hg1[ii] | 86.163 (14) |
| O3[i]—Yb1—O4[i] | 66.53 (12) | C10—C9—C14 | 117.9 (5) |
| O1—Yb1—O4[i] | 76.96 (13) | C10—C9—Se1 | 119.0 (4) |
| O1[i]—Yb1—O4[i] | 111.10 (13) | C14—C9—Se1 | 123.1 (4) |
| O2—Yb1—O4 | 73.66 (16) | C9—C10—C11 | 121.7 (5) |
| O2[i]—Yb1—O4 | 132.16 (15) | C9—C10—H10 | 119.1 |
| O3—Yb1—O4 | 66.53 (12) | C11—C10—H10 | 119.1 |
| O3[i]—Yb1—O4 | 90.09 (13) | C12—C11—C10 | 120.3 (5) |
| O1—Yb1—O4 | 111.10 (13) | C12—C11—H11 | 119.9 |
| O1[i]—Yb1—O4 | 76.96 (13) | C10—C11—H11 | 119.9 |
| O4[i]—Yb1—O4 | 150.91 (18) | C11—C12—C13 | 119.0 (5) |
| C2—O1—C1 | 110.5 (4) | C11—C12—H12 | 120.5 |
| C2—O1—Yb1 | 113.8 (4) | C13—C12—H12 | 120.5 |
| C1—O1—Yb1 | 125.1 (3) | C12—C13—C14 | 120.8 (5) |
| C4A—O2—C3 | 103.0 (8) | C12—C13—H13 | 119.6 |
| C3—O2—C4B | 116.8 (10) | C14—C13—H13 | 119.6 |
| C4A—O2—Yb1 | 122.9 (8) | C9—C14—C13 | 120.3 (6) |
| C3—O2—Yb1 | 120.1 (4) | C9—C14—H14 | 119.9 |
| C4B—O2—Yb1 | 121.4 (10) | C13—C14—H14 | 119.9 |
| C5—O3—C6 | 112.1 (4) | C16—C15—C20 | 117.8 (4) |
| C5—O3—Yb1 | 125.5 (4) | C16—C15—Se2 | 118.6 (3) |
| C6—O3—Yb1 | 118.9 (3) | C20—C15—Se2 | 123.5 (3) |
| C8—O4—C7 | 108.0 (5) | C15—C16—C17 | 120.6 (5) |
| C8—O4—Yb1 | 125.9 (5) | C15—C16—H16 | 119.7 |
| C7—O4—Yb1 | 108.5 (3) | C17—C16—H16 | 119.7 |
| O1—C1—H1A | 109.5 | C18—C17—C16 | 120.8 (5) |
| O1—C1—H1B | 109.5 | C18—C17—H17 | 119.6 |
| H1A—C1—H1B | 109.5 | C16—C17—H17 | 119.6 |
| O1—C1—H1C | 109.5 | C17—C18—C19 | 119.3 (4) |
| H1A—C1—H1C | 109.5 | C17—C18—H18 | 120.3 |
| H1B—C1—H1C | 109.5 | C19—C18—H18 | 120.3 |
| O1—C2—C3 | 110.5 (5) | C20—C19—C18 | 120.2 (5) |
| O1—C2—H2A | 109.6 | C20—C19—H19 | 119.9 |
| C3—C2—H2A | 109.6 | C18—C19—H19 | 119.9 |
| O1—C2—H2B | 109.6 | C19—C20—C15 | 121.3 (4) |
| C3—C2—H2B | 109.6 | C19—C20—H20 | 119.4 |
| H2A—C2—H2B | 108.1 | C15—C20—H20 | 119.4 |
| O2—C3—C2 | 110.3 (5) | C21A—Se3A—Hg1 | 98.4 (2) |
| O2—C3—H3A | 109.6 | C22A—C21A—C26A | 117.2 (6) |
| C2—C3—H3A | 109.6 | C22A—C21A—Se3A | 123.5 (5) |
| O2—C3—H3B | 109.6 | C26A—C21A—Se3A | 119.2 (5) |

| | | | |
|---|---|---|---|
| C2—C3—H3B | 109.6 | C21A—C22A—C23A | 122.9 (6) |
| H3A—C3—H3B | 108.1 | C21A—C22A—H22A | 118.5 |
| O2—C4A—H4A | 109.5 | C23A—C22A—H22A | 118.5 |
| O2—C4A—H4B | 109.5 | C24A—C23A—C22A | 118.0 (7) |
| H4A—C4A—H4B | 109.5 | C24A—C23A—H23A | 121.0 |
| O2—C4A—H4C | 109.5 | C22A—C23A—H23A | 121.0 |
| H4A—C4A—H4C | 109.5 | C23A—C24A—C25A | 121.7 (7) |
| H4B—C4A—H4C | 109.5 | C23A—C24A—H24A | 119.1 |
| O2—C4B—H4D | 109.5 | C25A—C24A—H24A | 119.1 |
| O2—C4B—H4E | 109.5 | C26A—C25A—C24A | 118.3 (7) |
| H4D—C4B—H4E | 109.5 | C26A—C25A—H25A | 120.9 |
| O2—C4B—H4F | 109.5 | C24A—C25A—H25A | 120.9 |
| H4D—C4B—H4F | 109.5 | C25A—C26A—C21A | 121.9 (6) |
| H4E—C4B—H4F | 109.5 | C25A—C26A—H26A | 119.1 |
| O3—C5—H5A | 109.5 | C21A—C26A—H26A | 119.1 |
| O3—C5—H5B | 109.5 | C21B—Se3B—Hg1 | 103.0 (3) |
| H5A—C5—H5B | 109.5 | C22B—C21B—C26B | 117.4 (6) |
| O3—C5—H5C | 109.5 | C22B—C21B—Se3B | 123.2 (5) |
| H5A—C5—H5C | 109.5 | C26B—C21B—Se3B | 119.3 (6) |
| H5B—C5—H5C | 109.5 | C21B—C22B—C23B | 122.7 (7) |
| O3—C6—C7 | 110.9 (5) | C21B—C22B—H22B | 118.6 |
| O3—C6—H6A | 109.5 | C23B—C22B—H22B | 118.6 |
| C7—C6—H6A | 109.5 | C24B—C23B—C22B | 117.7 (7) |
| O3—C6—H6B | 109.5 | C24B—C23B—H23B | 121.2 |
| C7—C6—H6B | 109.5 | C22B—C23B—H23B | 121.2 |
| H6A—C6—H6B | 108.0 | C23B—C24B—C25B | 122.3 (7) |
| O4—C7—C6 | 110.5 (5) | C23B—C24B—H24B | 118.8 |
| O4—C7—H7A | 109.6 | C25B—C24B—H24B | 118.8 |
| C6—C7—H7A | 109.6 | C26B—C25B—C24B | 118.0 (7) |
| O4—C7—H7B | 109.6 | C26B—C25B—H25B | 121.0 |
| C6—C7—H7B | 109.6 | C24B—C25B—H25B | 121.0 |
| H7A—C7—H7B | 108.1 | C25B—C26B—C21B | 121.9 (7) |
| O4—C8—H8A | 109.5 | C25B—C26B—H26B | 119.1 |
| O4—C8—H8B | 109.5 | C21B—C26B—H26B | 119.1 |
| | | | |
| O2—Yb1—O1—C2 | −24.1 (4) | O1—C2—C3—O2 | −48.0 (8) |
| O2$^i$—Yb1—O1—C2 | −100.9 (4) | C5—O3—C6—C7 | −177.5 (5) |
| O3—Yb1—O1—C2 | 92.3 (4) | Yb1—O3—C6—C7 | 22.1 (7) |
| O3$^i$—Yb1—O1—C2 | 146.2 (4) | C8—O4—C7—C6 | −166.9 (6) |
| O1$^i$—Yb1—O1—C2 | −64.7 (4) | Yb1—O4—C7—C6 | 53.8 (6) |
| O4$^i$—Yb1—O1—C2 | −174.1 (4) | O3—C6—C7—O4 | −51.4 (7) |
| O4—Yb1—O1—C2 | 35.2 (4) | Se3B—Hg1—Se1—C9 | 66.62 (17) |
| O2—Yb1—O1—C1 | −165.2 (5) | Se3A—Hg1—Se1—C9 | 56.65 (17) |
| O2$^i$—Yb1—O1—C1 | 118.0 (5) | Se2—Hg1—Se1—C9 | −156.51 (15) |
| O3—Yb1—O1—C1 | −48.7 (4) | Se2$^{ii}$—Hg1—Se1—C9 | −53.16 (15) |
| O3$^i$—Yb1—O1—C1 | 5.1 (5) | Se3B—Hg1—Se2—C15 | 149.70 (14) |
| O1$^i$—Yb1—O1—C1 | 154.2 (5) | Se1—Hg1—Se2—C15 | 8.74 (13) |
| O4$^i$—Yb1—O1—C1 | 44.9 (4) | Se3A—Hg1—Se2—C15 | 161.11 (13) |

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|---|---|---|---|
| O4—Yb1—O1—C1 | −105.9 (4) | Se2ⁱⁱ—Hg1—Se2—C15 | −102.04 (13) |
| O2ⁱ—Yb1—O2—C4A | −39.6 (8) | Se3B—Hg1—Se2—Hg1ⁱⁱ | −108.26 (5) |
| O3—Yb1—O2—C4A | 160.0 (9) | Se1—Hg1—Se2—Hg1ⁱⁱ | 110.779 (18) |
| O3ⁱ—Yb1—O2—C4A | 66.4 (10) | Se3A—Hg1—Se2—Hg1ⁱⁱ | −96.85 (4) |
| O1—Yb1—O2—C4A | −135.4 (9) | Se2ⁱⁱ—Hg1—Se2—Hg1ⁱⁱ | 0.0 |
| O1ⁱ—Yb1—O2—C4A | 25.0 (9) | Hg1—Se1—C9—C10 | 171.1 (4) |
| O4ⁱ—Yb1—O2—C4A | −94.3 (9) | Hg1—Se1—C9—C14 | −8.3 (5) |
| O4—Yb1—O2—C4A | 101.3 (9) | C14—C9—C10—C11 | 2.4 (8) |
| O2ⁱ—Yb1—O2—C3 | 93.7 (5) | Se1—C9—C10—C11 | −177.0 (4) |
| O3—Yb1—O2—C3 | −66.7 (5) | C9—C10—C11—C12 | −0.2 (9) |
| O3ⁱ—Yb1—O2—C3 | −160.3 (5) | C10—C11—C12—C13 | −2.1 (9) |
| O1—Yb1—O2—C3 | −2.2 (5) | C11—C12—C13—C14 | 2.1 (10) |
| O1ⁱ—Yb1—O2—C3 | 158.2 (5) | C10—C9—C14—C13 | −2.4 (9) |
| O4ⁱ—Yb1—O2—C3 | 39.0 (5) | Se1—C9—C14—C13 | 177.1 (5) |
| O4—Yb1—O2—C3 | −125.4 (5) | C12—C13—C14—C9 | 0.1 (10) |
| O2ⁱ—Yb1—O2—C4B | −71.0 (9) | Hg1—Se2—C15—C16 | −163.3 (3) |
| O3—Yb1—O2—C4B | 128.6 (9) | Hg1ⁱⁱ—Se2—C15—C16 | 107.0 (3) |
| O3ⁱ—Yb1—O2—C4B | 35.0 (10) | Hg1—Se2—C15—C20 | 13.8 (4) |
| O1—Yb1—O2—C4B | −166.9 (9) | Hg1ⁱⁱ—Se2—C15—C20 | −75.9 (4) |
| O1ⁱ—Yb1—O2—C4B | −6.5 (9) | C20—C15—C16—C17 | 0.4 (7) |
| O4ⁱ—Yb1—O2—C4B | −125.7 (9) | Se2—C15—C16—C17 | 177.7 (4) |
| O4—Yb1—O2—C4B | 69.9 (9) | C15—C16—C17—C18 | −2.2 (8) |
| O2—Yb1—O3—C5 | 143.0 (5) | C16—C17—C18—C19 | 2.2 (8) |
| O2ⁱ—Yb1—O3—C5 | 41.9 (7) | C17—C18—C19—C20 | −0.5 (8) |
| O3ⁱ—Yb1—O3—C5 | −57.2 (4) | C18—C19—C20—C15 | −1.3 (7) |
| O1—Yb1—O3—C5 | 85.0 (5) | C16—C15—C20—C19 | 1.3 (7) |
| O1ⁱ—Yb1—O3—C5 | −110.9 (5) | Se2—C15—C20—C19 | −175.8 (4) |
| O4ⁱ—Yb1—O3—C5 | 8.5 (5) | Se3B—Hg1—Se3A—C21A | 16.5 (7) |
| O4—Yb1—O3—C5 | −153.6 (5) | Se1—Hg1—Se3A—C21A | 70.0 (3) |
| O2—Yb1—O3—C6 | −59.5 (4) | Se2—Hg1—Se3A—C21A | −79.1 (3) |
| O2ⁱ—Yb1—O3—C6 | −160.6 (5) | Se2ⁱⁱ—Hg1—Se3A—C21A | −175.0 (3) |
| O3ⁱ—Yb1—O3—C6 | 100.4 (4) | Hg1—Se3A—C21A—C22A | 35.3 (5) |
| O1—Yb1—O3—C6 | −117.4 (4) | Hg1—Se3A—C21A—C26A | −148.2 (4) |
| O1ⁱ—Yb1—O3—C6 | 46.7 (5) | C26A—C21A—C22A—C23A | 0.00 (3) |
| O4ⁱ—Yb1—O3—C6 | 166.1 (4) | Se3A—C21A—C22A—C23A | 176.6 (6) |
| O4—Yb1—O3—C6 | 3.9 (4) | C21A—C22A—C23A—C24A | 0.00 (3) |
| O2—Yb1—O4—C8 | −43.4 (5) | C22A—C23A—C24A—C25A | 0.00 (7) |
| O2ⁱ—Yb1—O4—C8 | 13.0 (6) | C23A—C24A—C25A—C26A | −0.01 (9) |
| O3—Yb1—O4—C8 | −160.1 (5) | C24A—C25A—C26A—C21A | 0.01 (9) |
| O3ⁱ—Yb1—O4—C8 | 125.6 (5) | C22A—C21A—C26A—C25A | −0.01 (7) |
| O1—Yb1—O4—C8 | −97.8 (5) | Se3A—C21A—C26A—C25A | −176.8 (6) |
| O1ⁱ—Yb1—O4—C8 | 50.8 (5) | Se1—Hg1—Se3B—C21B | 77.9 (3) |
| O4ⁱ—Yb1—O4—C8 | 160.9 (5) | Se3A—Hg1—Se3B—C21B | −150.0 (10) |
| O2—Yb1—O4—C7 | 86.7 (4) | Se2—Hg1—Se3B—C21B | −61.9 (3) |
| O2ⁱ—Yb1—O4—C7 | 143.0 (3) | Se2ⁱⁱ—Hg1—Se3B—C21B | −162.0 (3) |
| O3—Yb1—O4—C7 | −30.1 (3) | Hg1—Se3B—C21B—C22B | 34.0 (5) |
| O3ⁱ—Yb1—O4—C7 | −104.4 (4) | Hg1—Se3B—C21B—C26B | −148.4 (4) |
| O1—Yb1—O4—C7 | 32.2 (4) | C26B—C21B—C22B—C23B | 0.00 (3) |

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| O1$^i$—Yb1—O4—C7 | −179.2 (4) | Se3B—C21B—C22B—C23B | 177.6 (7) |
| O4$^i$—Yb1—O4—C7 | −69.1 (3) | C21B—C22B—C23B—C24B | 0.00 (3) |
| C1—O1—C2—C3 | −165.6 (6) | C22B—C23B—C24B—C25B | 0.00 (7) |
| Yb1—O1—C2—C3 | 47.6 (7) | C23B—C24B—C25B—C26B | 0.00 (9) |
| C4A—O2—C3—C2 | 168.1 (9) | C24B—C25B—C26B—C21B | 0.01 (9) |
| C4B—O2—C3—C2 | −167.7 (10) | C22B—C21B—C26B—C25B | −0.01 (7) |
| Yb1—O2—C3—C2 | 26.9 (8) | Se3B—C21B—C26B—C25B | −177.7 (6) |

Symmetry codes: (i) −*x*, *y*, −*z*+1/2; (ii) −*x*, −*y*+1, −*z*+1.