Bis(μ-cobaltoceniumselenolate-1:2κ²Se:Se)bis-[bis(cobaltoceniumselenolate-κSe)mercury(II)] tetrakis(hexafluoridophosphate) acetonitrile disolvate

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The title compound, \([\text{Co}_6\text{Hg}_2(\text{C}_5\text{H}_5)_6(\text{C}_5\text{H}_4\text{Se})_6][\text{PF}_6]_4\cdot2\text{CH}_3\text{CN}\) or \([\text{Hg}_2(\text{CcSe})_6][\text{PF}_6]_4\cdot2\text{CH}_3\text{CN}\) (Cc = \(\text{C}_{10}\text{H}_9\text{Co}\)), was obtained as bright-orange needle-shaped crystals. It is a salt containing a tetracationic dimercury species with six cobaltoceniumselenolate ligands, four hexafluoridophosphate counterions and two acetonitrile solvent molecules. The cation (point group \(\bar{1}\)) has a bitetrahedral \([\text{Hg}_2\text{Se}_6]\) core with two bridging Se atoms and four terminal Se atoms.

Structure description

Zwitterionic cobaltoceniumselenolate is a versatile ligand for forming organometallic coordination compounds (Vanicek et al., 2018). The title salt, \([\text{Hg}_2(\text{CcSe})_6][\text{PF}_6]_4\cdot2\text{CH}_3\text{CN}\) (Cc = \(\text{C}_{10}\text{H}_9\text{Co}\)), was synthesized starting from the recently reported cobaltocenium selenolate gold(I) triphenylphosphine hexafluoridophosphate (Menia et al., 2021) using elemental mercury in dry ortho-dichlorobenzene. It was crystallized as an acetonitrile solvate showing positional disorder of the solvent molecule and of one of the \(\text{PF}_6^-\) anions.

The cation lies about a crystallographic inversion center and has a bitetrahedral \([\text{Hg}_2\text{Se}_6]\) core formed by edge-sharing of two \(\text{HgSe}_4\) tetrahedra and has two bridging Se2 atoms and four terminal Se1 and Se3 atoms (Fig. 1). The Se2—Hg1—Se2' angle between the bridging Se atoms is 91.509 (10)', resulting in an Hg1—Se1—Hg1' angle of 88.491 (10)' [symmetry code: (i) \(-x + 1, -y + 1, -z + 1\)]. The four \(\text{Cipso—Se—Hg1}\) angles are slightly compressed, ranging from 98.79 (7) to 106.04 (7)', as was also observed for cobaltocenium selenolate gold complexes (Menia et al., 2021). The terminal Se—Hg1 bonds...
bond lengths are 2.5476 (3) Å (Se1—Hg1) and 2.5451 (3) Å (Se3—Hg1), whereas the bridging Se2—Hg1 bond lengths differ considerably with 2.6254 (3) Å for Se2—Hg1 and 3.1537 (4) Å for Se2—Hg1'. With an average Se—C distance of 1.89 Å between the selenolate and the cobaltocenium residues, these bond lengths are comparable with other recently reported cobaltocenium selenolates (Menia et al., 2021).

The sole comparable compound found in the literature is [Yb(C6H10O2)4][Hg2(C6H5Se)6] (Romanelli et al., 2008). Here, instead of the cationic cobaltocenium species the selenium atoms are bonded to phenyl residues, which makes the Hg species a dianion. With an average Se—Hg bond length of 2.81 Å in the title compound, bonds are elongated in comparison with the dianion of Romanelli et al. (2.68 Å).

Since the packing of the molecules (Fig. 2) shows no remarkable hydrogen bonding or π-stacking interactions, the cohesion within the crystal structure is dominated by van der Waals forces.

Synthesis and crystallization

In a 50 ml Schlenk flask, 11.1 mg of [(CeSe)(PPh3)Au]PF6 (1 eq., 0.013 mmol) were suspended in 5 ml of dry ortho-dichlorobenzene. Approximately 0.1 ml of liquid mercury was added and the mixture stirred for 48 h. This reaction was originally carried out with the aim of removing selenium from the desired compound. The bright-orange precipitate was filtered off, washed with two portions of 10 ml of diethyl ether and dissolved in 5 ml of acetonitrile. This orange solution was concentrated to about 1 ml. Bright-orange needle-shaped crystals were obtained by diffusion-crystallization with diethyl ether at 253 K. 1H NMR (300 MHz, CD3CN): δ 5.70 (t, J = 2.0 Hz, 2H), 5.51 (t, J = 2.0 Hz, 2H), 5.46 (s, 5H).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. One of the two PF6 anions (P2) shows disorder of four fluorine atoms over two sets of sites in a 2:1 ratio for F7, F8, F9, F10 and F7A, F8A, F9A, F10A. Another positional disorder occurs for the complete acetonitrile solvent molecule in a 1:1 ratio. All disordered atoms were refined with anisotropic displacement parameters without further restraints, but with fixed occupation factors.
Table 1
Experimental details.

| Crystal data                  | Chemical formula |
|-------------------------------|------------------|
| Chemical formula              | \([\text{Co}_6\text{Hg}_2(\text{C}_5\text{H}_5)_3(\text{C}_5\text{H}_4\text{Se})_6](\text{PF}_6)_4\) |
| \(M_r\)                      | 2665.54          |
| Crystal system, space group  | Triclinic, \(P\bar{1}\) |
| Temperature (K)              | 183              |
| \(a, b, c\) (\(\text{Å}\))   | 10.2933 (8), 14.3271 (12), 15.1087 (12) |
| \(\alpha, \beta, \gamma\) (\(^\circ\)) | 109.744 (3), 109.764 (2), 95.306 (3) |
| \(V\) (\(\text{Å}^3\))       | 1919.1 (3)       |
| \(Z\)                        | 1               |
| Radiation type               | Mo K\(\alpha\)   |
| \(\mu\) (mm\(^{-1}\))       | 8.28             |
| Crystal size (mm)            | 0.18 \(\times\) 0.09 \(\times\) 0.04 |

Data collection

| Diffractometer               | Bruker D8 QUEST PHOTON 100 |
|------------------------------|-----------------------------|
| Absorption correction       | Multi-scan (SADABS: Krause et al., 2015) |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.574, 0.837 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 69321, 7546, 7005 |
| \(R_{\text{int}}\)          | 0.038                       |
| \(\sin(\theta/\lambda)_{\text{max}}\) (\(\text{Å}^{-1}\)) | 0.617                        |

Refinement

| \(R[F^2 > 2\sigma(F^2)]\), \(wR(F^2), S\) | 0.017, 0.042, 1.04 |
| No. of reflections             | 7546 |
| No. of parameters              | 553  |
| H-atom treatment               | H-atom parameters constrained |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (e \(\text{Å}^{-3}\)) | 0.77, -0.80 |

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full crystallographic data

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Crystal data

[Co₆Hg₂(C₅H₅)(C₅H₄Se)₆](PF₆)₄·2C₂H₃N

Mr = 2665.54

Triclinic, P1

a = 10.2933 (8) Å

b = 14.3271 (12) Å

c = 15.1087 (12) Å

α = 109.744 (3)°

β = 109.764 (2)°

γ = 95.306 (3)°

V = 1919.1 (3) Å³

Z = 1

F(000) = 1260

Dx = 2.306 Mg m⁻³

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 9672 reflections

θ = 2.3–26.4°

µ = 8.28 mm⁻¹

T = 183 K

Prism, orange

0.18 × 0.09 × 0.04 mm

Data collection

Bruker D8 QUEST PHOTON 100
diffractometer

Radiation source: Incoatec Microfocus

Multi layered optics monochromator

Detector resolution: 10.4 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause et al., 2015)

Tmin = 0.574, Tmax = 0.837

69321 measured reflections

7546 independent reflections

7005 reflections with I > 2σ(I)

Rint = 0.038

θmax = 26.0°, θmin = 2.2°

hk=−12→12

kl=−17→17

ilm=−18→18

Refinement

Refinement on F²

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.017

wR(F²) = 0.042

S = 1.04

7546 reflections

553 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ(Fc⁻²) + (0.0197P)² + 1.8079P]

where P = (Fc⁻² + 2Fc²)/3

(Δσ)max = 0.003

Δρmax = 0.77 e Å⁻³

Δρmin = −0.80 e Å⁻³

Extinction correction: SHELXL2014/7 (Sheldrick, 2015b),

Fc*=kFc[1+0.001xFc²λ/sin(2θ)]⁻¹/⁴

Extinction coefficient: 0.00230 (10)
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.

Refinement. C-bound hydrogen atoms were placed in calculated positions and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ and a C—H distance of 0.95 Å for aromatic H atoms. Positonal disorder of same flourine atoms at P2 in ratio 2:1 for F7-F10 : F7a-F10a and for solvent acetonitrile C32-C31-N1 : C32a-C31a-N1a in ratio 1:1, respectively.

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

|    | x           | y           | z           | $U_{iso}/U_{eq}$ | Occ. (<1) |
|----|-------------|-------------|-------------|-----------------|-----------|
| Hg1| 0.31028 (2) | 0.47867 (2) | 0.51180 (2) | 0.02781 (4)     |           |
| Se1| 0.32480 (3) | 0.45328 (2) | 0.67355 (2) | 0.02603 (6)     |           |
| Se2| 0.40933 (3) | 0.35008 (2) | 0.39551 (2) | 0.02572 (6)     |           |
| Se3| 0.13272 (3) | 0.56435 (2) | 0.42414 (2) | 0.02556 (6)     |           |
| Co1| 0.51168 (3) | 0.26149 (2) | 0.69145 (3) | 0.02302 (8)     |           |
| Co2| 0.21259 (4) | 0.23319 (2) | 0.12527 (3) | 0.02438 (8)     |           |
| Co3| 0.18455 (3) | 0.79863 (2) | 0.63293 (3) | 0.02143 (7)     |           |
| C1 | 0.4091 (3)  | 0.1559 (2)  | 0.7209 (3)  | 0.0462 (8)      |           |
| H1 | 0.4018      | 0.1660      | 0.7843      | 0.055           |           |
| C2 | 0.5175 (3)  | 0.1204 (2)  | 0.6918 (3)  | 0.0416 (7)      |           |
| H2 | 0.5954      | 0.1018      | 0.7320      | 0.050           |           |
| C3 | 0.4906 (4)  | 0.1174 (2)  | 0.5936 (3)  | 0.0482 (8)      |           |
| H3 | 0.5471      | 0.0967      | 0.5554      | 0.058           |           |
| C4 | 0.3634 (4)  | 0.1508 (2)  | 0.5614 (3)  | 0.058 (11)      |           |
| H4 | 0.3197      | 0.1566      | 0.4977      | 0.070           |           |
| C5 | 0.3142 (3)  | 0.1739 (2)  | 0.6405 (3)  | 0.0519 (10)     |           |
| H5 | 0.2308      | 0.1976      | 0.6395      | 0.062           |           |
| C6 | 0.5531 (3)  | 0.3958 (2)  | 0.8092 (2)  | 0.0312 (6)      |           |
| H6 | 0.5136      | 0.4081      | 0.8594      | 0.037           |           |
| C7 | 0.6793 (3)  | 0.3613 (2)  | 0.8153 (2)  | 0.0337 (6)      |           |
| H7 | 0.7394      | 0.3473      | 0.8703      | 0.040           |           |
| C8 | 0.6998 (3)  | 0.3516 (2)  | 0.7255 (2)  | 0.0312 (6)      |           |
| H8 | 0.7763      | 0.3297      | 0.7093      | 0.037           |           |
| C9 | 0.5863 (3)  | 0.38023 (19)| 0.6631 (2)  | 0.0267 (5)      |           |
| H9 | 0.5737      | 0.3801      | 0.5978      | 0.032           |           |
| C10| 0.4948 (3)  | 0.40899 (17)| 0.71494 (19)| 0.0233 (5)      |           |
| C11| 0.1956 (3)  | 0.0996 (2)  | 0.1453 (2)  | 0.0393 (7)      |           |
| H11| 0.2363      | 0.0915      | 0.2080      | 0.047           |           |
| C12| 0.2595 (3)  | 0.0951 (2)  | 0.0760 (2)  | 0.0402 (7)      |           |
| H12| 0.3511      | 0.0831      | 0.0835      | 0.048           |           |
| C13| 0.1648 (4)  | 0.1113 (2)  | 0.0067 (2)  | 0.0411 (7)      |           |
| H13| 0.1816      | 0.1126      | 0.0644      | 0.049           |           |
| C14| 0.0411 (3)  | 0.1252 (2)  | 0.0110 (2)  | 0.0438 (8)      |           |
| H14| 0.1451      | 0.1371      | 0.0328      | 0.053           |           |
| C15| 0.0598 (3)  | 0.1183 (2)  | 0.1054 (3)  | 0.0437 (8)      |           |
|   |   |   |   |   |
|---|---|---|---|---|
| H15 | −0.0069 | 0.1250 | 0.1365 | 0.052* |
| C16 | 0.3985 (3) | 0.34072 (19) | 0.1954 (2) | 0.0338 (6) |
| H16 | 0.4904 | 0.3277 | 0.2072 | 0.041* |
| C17 | 0.3071 (4) | 0.3502 (2) | 0.1062 (2) | 0.0482 (9) |
| H17 | 0.3276 | 0.3454 | 0.0483 | 0.058* |
| C18 | 0.1804 (4) | 0.3679 (2) | 0.1184 (2) | 0.0474 (9) |
| H18 | 0.1010 | 0.3775 | 0.0702 | 0.057* |
| C19 | 0.1920 (3) | 0.36898 (19) | 0.2153 (2) | 0.0323 (6) |
| H19 | 0.1211 | 0.3780 | 0.2425 | 0.039* |
| C20 | 0.3288 (3) | 0.35406 (17) | 0.26440 (19) | 0.0241 (5) |
| C21 | 0.3979 (3) | 0.8491 (2) | 0.6884 (3) | 0.0446 (8) |
| H21 | 0.4663 | 0.8112 | 0.7061 | 0.053* |
| C22 | 0.3452 (3) | 0.9115 (2) | 0.7541 (2) | 0.0368 (7) |
| H22 | 0.3713 | 0.9237 | 0.8243 | 0.044* |
| C23 | 0.2474 (3) | 0.9533 (2) | 0.6989 (3) | 0.0456 (8) |
| H23 | 0.1953 | 0.9988 | 0.7249 | 0.055* |
| C24 | 0.2399 (4) | 0.9162 (3) | 0.5986 (3) | 0.0642 (12) |
| H24 | 0.1818 | 0.9318 | 0.5442 | 0.077* |
| C25 | 0.3341 (4) | 0.8515 (3) | 0.5931 (3) | 0.0603 (12) |
| H25 | 0.3509 | 0.8156 | 0.5339 | 0.072* |
| C26 | 0.1367 (3) | 0.65878 (18) | 0.6361 (2) | 0.0279 (6) |
| H26 | 0.2027 | 0.6255 | 0.6669 | 0.033* |
| C27 | 0.0690 (3) | 0.7278 (2) | 0.6860 (2) | 0.0373 (7) |
| H27 | 0.0805 | 0.7476 | 0.7554 | 0.045* |
| C28 | −0.0186 (3) | 0.7617 (2) | 0.6146 (3) | 0.0439 (8) |
| H28 | −0.0767 | 0.8081 | 0.6275 | 0.053* |
| C29 | −0.0046 (3) | 0.7144 (2) | 0.5202 (2) | 0.0350 (6) |
| H29 | −0.0500 | 0.7252 | 0.4594 | 0.042* |
| C30 | 0.0896 (3) | 0.64768 (18) | 0.5321 (2) | 0.0242 (5) |
| P1 | 0.94494 (10) | 0.11818 (8) | 0.70615 (7) | 0.0506 (2) |
| F1 | 0.9016 (3) | 0.1795 (2) | 0.79546 (19) | 0.0935 (9) |
| F2 | 0.9873 (3) | 0.0561 (2) | 0.61544 (18) | 0.0837 (8) |
| F3 | 0.7858 (3) | 0.0741 (3) | 0.6318 (2) | 0.1244 (14) |
| F4 | 1.1077 (3) | 0.1638 (2) | 0.7786 (2) | 0.0832 (7) |
| F5 | 0.9538 (3) | 0.0274 (2) | 0.7437 (2) | 0.0931 (9) |
| F6 | 0.9436 (4) | 0.2112 (3) | 0.6708 (3) | 0.1183 (12) |
| P2 | 0.65318 (11) | 0.20499 (8) | 1.02043 (7) | 0.0507 (2) |
| F11 | 0.5820 (5) | 0.2828 (3) | 0.9804 (3) | 0.1310 (14) |
| F12 | 0.7338 (3) | 0.13036 (18) | 1.06292 (17) | 0.0688 (6) |
| N1 | 0.6305 (9) | 0.5411 (7) | 1.0496 (6) | 0.077 (2) |
| C31 | 0.7429 (13) | 0.5419 (11) | 1.0966 (8) | 0.058 (3) |
| C32 | 0.8832 (15) | 0.5370 (17) | 1.1525 (14) | 0.077 (4) |
| H32A | 0.8795 | 0.4739 | 1.1644 | 0.115* |
| H32B | 0.9248 | 0.5957 | 1.2183 | 0.115* |
| H32C | 0.9415 | 0.5381 | 1.1131 | 0.115* |
| N1A | 0.9757 (6) | 0.5167 (5) | 1.0373 (5) | 0.0523 (14) |
| C31A | 0.9058 (7) | 0.5274 (6) | 1.0817 (5) | 0.0459 (15) |
| C32A | 0.8167 (17) | 0.5410 (13) | 1.1386 (14) | 0.087 (6) |
| Atom   | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|--------|-----------|-----------|-----------|-----------|-----------|-----------|
| Hg1    | 0.03160 (6) | 0.02915 (6) | 0.02704 (6) | 0.01267 (4) | 0.01398 (4) | 0.01231 (4) |
| Se1    | 0.02882 (13) | 0.02585 (13) | 0.02935 (14) | 0.00876 (10) | 0.01531 (11) | 0.01336 (11) |
| Se2    | 0.02821 (13) | 0.02356 (13) | 0.02013 (13) | 0.00917 (10) | 0.00767 (10) | 0.00348 (10) |
| Se3    | 0.02908 (13) | 0.02367 (12) | 0.02107 (13) | 0.00690 (10) | 0.00785 (10) | 0.00730 (10) |
| Co1    | 0.02233 (16) | 0.01826 (16) | 0.02694 (18) | 0.00221 (12) | 0.00697 (14) | 0.01050 (14) |
| Co2    | 0.02932 (18) | 0.01654 (16) | 0.01857 (17) | 0.00271 (13) | 0.00503 (14) | 0.00182 (13) |
| Co3    | 0.02007 (16) | 0.01581 (15) | 0.02571 (18) | 0.00371 (12) | 0.00727 (14) | 0.00689 (13) |
| C1     | 0.0466 (18)  | 0.0297 (15)  | 0.071 (2)   | −0.0005 (13) | 0.0282 (17)  | 0.0274 (16)  |
| C2     | 0.0366 (16)  | 0.0237 (14)  | 0.064 (2)   | 0.0061 (12)  | 0.0136 (15)  | 0.0233 (14)  |
| C3     | 0.057 (2)    | 0.0213 (14)  | 0.054 (2)   | 0.0030 (13)  | 0.0219 (17)  | 0.0022 (14)  |
| C4     | 0.059 (2)    | 0.0277 (16)  | 0.047 (2)   | −0.0104 (15) | −0.0151 (18) | 0.0080 (15)  |
| C5     | 0.0243 (15)  | 0.0290 (16)  | 0.090 (3)   | −0.0009 (12) | 0.0104 (17)  | 0.0234 (17)  |
| C6     | 0.0413 (15)  | 0.0252 (13)  | 0.0229 (13) | 0.0037 (11)  | 0.0104 (12)  | 0.0079 (11)  |
| C7     | 0.0294 (14)  | 0.0290 (14)  | 0.0305 (15) | −0.0014 (11) | −0.0020 (12) | 0.0132 (12)  |
| C8     | 0.0223 (13)  | 0.0301 (14)  | 0.0419 (16) | 0.0020 (10)  | 0.0085 (12)  | 0.0202 (13)  |
| C9     | 0.0259 (13)  | 0.0285 (13)  | 0.0318 (14) | 0.0039 (10)  | 0.0129 (11)  | 0.0180 (11)  |
| C10    | 0.0254 (12)  | 0.0158 (11)  | 0.0250 (13) | 0.0033 (9)   | 0.0073 (10)  | 0.0072 (10)  |
| C11    | 0.0577 (19)  | 0.0170 (13)  | 0.0280 (15) | −0.0002 (12) | 0.0064 (14)  | 0.0039 (11)  |
| C12    | 0.0337 (15)  | 0.0198 (13)  | 0.0475 (19) | 0.0063 (11)  | 0.0087 (14)  | −0.0024 (12) |
| C13    | 0.0564 (19)  | 0.0258 (14)  | 0.0254 (15) | 0.0006 (13)  | 0.0142 (14)  | −0.0041 (12) |
| C14    | 0.0368 (16)  | 0.0258 (14)  | 0.0384 (18) | 0.0021 (12)  | −0.0049 (14) | −0.0017 (13) |
| C15    | 0.0432 (17)  | 0.0223 (14)  | 0.052 (2)   | −0.0044 (12) | 0.0247 (15)  | −0.0040 (13) |
| C16    | 0.0404 (16)  | 0.0215 (13)  | 0.0314 (15) | −0.0066 (11) | 0.0171 (13)  | 0.0015 (11)  |
| C17    | 0.083 (3)    | 0.0272 (15)  | 0.0290 (16) | −0.0053 (15) | 0.0226 (17)  | 0.0083 (13)  |
| C18    | 0.075 (2)    | 0.0218 (14)  | 0.0302 (16) | 0.0126 (15)  | 0.0033 (16)  | 0.0100 (12)  |
| C19    | 0.0404 (15)  | 0.0177 (12)  | 0.0280 (14) | 0.0108 (11)  | 0.0058 (12)  | 0.0030 (11)  |
| C20    | 0.0290 (13)  | 0.0130 (11)  | 0.0209 (12) | −0.0007 (9)  | 0.0072 (10)  | −0.0001 (9)  |
| C21    | 0.0231 (14)  | 0.0267 (15)  | 0.073 (2)   | 0.0011 (11)  | 0.0160 (15)  | 0.0105 (15)  |
| C22    | 0.0359 (15)  | 0.0291 (14)  | 0.0299 (15) | −0.0080 (12) | 0.0041 (12)  | 0.0064 (12)  |
| C23    | 0.0366 (16)  | 0.0152 (13)  | 0.072 (2)   | 0.0037 (11)  | 0.0158 (16)  | 0.0076 (14)  |
| C24    | 0.070 (2)    | 0.042 (2)    | 0.054 (2)   | −0.0220 (18) | −0.0121 (19) | 0.0341 (18)  |
| C25    | 0.079 (3)    | 0.0366 (18)  | 0.053 (2)   | −0.0262 (18) | 0.045 (2)    | −0.0056 (16) |
| C26    | 0.0362 (14)  | 0.0185 (12)  | 0.0326 (15) | 0.0019 (10)  | 0.0189 (12)  | 0.0101 (11)  |
**Data reports**

| Atom | U1  | U2  | U3  | U4  | U5  | U6  |
|------|-----|-----|-----|-----|-----|-----|
| C27  | 0.0395 (16) | 0.0289 (14) | 0.0458 (18) | −0.0005 (12) | 0.0294 (14) | 0.0069 (13) |
| C28  | 0.0216 (14) | 0.0340 (15) | 0.061 (2) | 0.0054 (11) | 0.0183 (14) | −0.0007 (15) |
| C29  | 0.0176 (12) | 0.0309 (14) | 0.0404 (17) | 0.0037 (10) | 0.0027 (12) | 0.0043 (12) |
| C30  | 0.0208 (12) | 0.0166 (11) | 0.0290 (14) | −0.0013 (9) | 0.0090 (10) | 0.0041 (10) |
| P1   | 0.0506 (5) | 0.0761 (6) | 0.0418 (5) | 0.0398 (5) | 0.0252 (4) | 0.0293 (5) |
| F1   | 0.101 (2) | 0.136 (2) | 0.0600 (15) | 0.0695 (18) | 0.0506 (15) | 0.0277 (16) |
| F2   | 0.0968 (18) | 0.132 (2) | 0.0508 (13) | 0.0788 (17) | 0.0438 (13) | 0.0416 (15) |
| F3   | 0.0510 (15) | 0.205 (4) | 0.076 (2) | 0.0419 (19) | 0.0156 (14) | 0.014 (2) |
| F4   | 0.0610 (15) | 0.108 (2) | 0.0796 (18) | 0.0221 (14) | 0.0262 (13) | 0.0368 (16) |
| F5   | 0.134 (2) | 0.0842 (18) | 0.092 (2) | 0.0295 (17) | 0.0632 (19) | 0.0511 (16) |
| F6   | 0.192 (4) | 0.111 (2) | 0.102 (2) | 0.091 (3) | 0.067 (2) | 0.075 (2) |
| P2   | 0.0680 (6) | 0.0642 (6) | 0.0458 (5) | 0.0353 (5) | 0.0347 (5) | 0.0346 (5) |
| F11  | 0.204 (4) | 0.137 (3) | 0.114 (3) | 0.113 (3) | 0.071 (3) | 0.095 (2) |
| F12  | 0.0914 (17) | 0.0751 (15) | 0.0558 (13) | 0.0603 (13) | 0.0336 (13) | 0.0318 (12) |
| N1   | 0.095 (6) | 0.114 (6) | 0.053 (4) | 0.060 (5) | 0.044 (4) | 0.046 (4) |
| C31  | 0.075 (8) | 0.086 (6) | 0.041 (6) | 0.045 (6) | 0.037 (5) | 0.036 (5) |
| C32  | 0.066 (9) | 0.117 (9) | 0.063 (7) | 0.042 (9) | 0.035 (8) | 0.040 (6) |
| N1A  | 0.046 (3) | 0.070 (4) | 0.050 (4) | 0.020 (3) | 0.020 (3) | 0.031 (3) |
| C31A | 0.051 (4) | 0.053 (4) | 0.035 (4) | 0.012 (3) | 0.017 (3) | 0.019 (3) |
| C32A | 0.103 (18) | 0.103 (9) | 0.089 (16) | 0.036 (15) | 0.077 (16) | 0.036 (11) |
| F7   | 0.150 (7) | 0.212 (10) | 0.061 (4) | 0.111 (6) | 0.079 (5) | 0.079 (6) |
| F8   | 0.104 (4) | 0.122 (7) | 0.058 (4) | 0.084 (4) | 0.056 (4) | 0.039 (5) |
| F9   | 0.069 (3) | 0.107 (4) | 0.076 (4) | −0.009 (3) | 0.009 (3) | 0.022 (3) |
| F10  | 0.081 (3) | 0.114 (4) | 0.122 (5) | −0.002 (3) | 0.019 (4) | 0.077 (4) |
| F7A  | 0.134 (12) | 0.122 (11) | 0.199 (17) | 0.046 (9) | 0.120 (13) | 0.114 (14) |
| F8A  | 0.070 (8) | 0.29 (2) | 0.22 (2) | 0.032 (10) | 0.076 (13) | 0.17 (2) |
| F9A  | 0.211 (19) | 0.061 (6) | 0.050 (6) | 0.051 (8) | 0.008 (10) | 0.012 (5) |
| F10A | 0.25 (3) | 0.133 (17) | 0.041 (8) | 0.141 (19) | 0.021 (12) | 0.007 (8) |

**Geometric parameters (Å, °)**

| Bond 1 | Length (Å) | Bond 2 | Length (Å) |
|--------|------------|--------|------------|
| Hg1—Se3 | 2.5451 (3) | C12—H12 | 0.9500 |
| Hg1—Se1 | 2.5476 (3) | C13—C14 | 1.404 (5) |
| Hg1—Se2 | 2.6254 (3) | C13—H13 | 0.9500 |
| Hg1—Se2' | 3.1537 (4) | C14—C15 | 1.413 (5) |
| Se1—C10 | 1.894 (3) | C14—H14 | 0.9500 |
| Se2—C20 | 1.895 (3) | C15—H15 | 0.9500 |
| Se2—Hg1' | 3.1537 (4) | C16—C17 | 1.417 (5) |
| Se3—C30 | 1.886 (3) | C16—C20 | 1.427 (4) |
| Co1—C6 | 2.018 (3) | C16—H16 | 0.9500 |
| Co1—C1 | 2.019 (3) | C17—C18 | 1.411 (5) |
| Co1—C7 | 2.019 (3) | C17—H17 | 0.9500 |
| Co1—C8 | 2.024 (3) | C18—C19 | 1.423 (4) |
| Co1—C5 | 2.029 (3) | C18—H18 | 0.9500 |
| Co1—C2 | 2.030 (3) | C19—C20 | 1.426 (4) |
| Co1—C4 | 2.030 (3) | C19—H19 | 0.9500 |
| Co1—C3 | 2.033 (3) | C21—C25 | 1.380 (5) |
| Co1—C9 | 2.035 (2) | C21—C22 | 1.390 (4) |
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|
| Co1—C10      | 2.056 (2)    | C21—H21      | 0.9500       |
| Co2—C17      | 2.013 (3)    | C22—C23      | 1.395 (4)    |
| Co2—C18      | 2.019 (3)    | C22—H22      | 0.9500       |
| Co2—C13      | 2.023 (3)    | C23—C24      | 1.398 (6)    |
| Co2—C14      | 2.030 (3)    | C23—H23      | 0.9500       |
| Co2—C12      | 2.031 (3)    | C24—C25      | 1.405 (6)    |
| Co2—C16      | 2.034 (3)    | C24—H24      | 0.9500       |
| Co2—C15      | 2.035 (3)    | C25—H25      | 0.9500       |
| Co2—C11      | 2.037 (3)    | C26—C27      | 1.418 (4)    |
| Co2—C19      | 2.041 (3)    | C26—C30      | 1.425 (4)    |
| Co2—C20      | 2.075 (2)    | C26—H26      | 0.9500       |
| Co3—C25      | 2.006 (3)    | C27—C28      | 1.411 (5)    |
| Co3—C28      | 2.008 (3)    | C27—H27      | 0.9500       |
| Co3—C24      | 2.010 (3)    | C28—C29      | 1.422 (4)    |
| Co3—C27      | 2.015 (3)    | C28—H28      | 0.9500       |
| Co3—C29      | 2.021 (3)    | C29—C30      | 1.435 (4)    |
| Co3—C21      | 2.025 (3)    | C29—H29      | 0.9500       |
| Co3—C23      | 2.032 (3)    | P1—F3        | 1.559 (3)    |
| Co3—C26      | 2.039 (2)    | P1—F1        | 1.571 (2)    |
| Co3—C22      | 2.039 (3)    | P1—F4        | 1.583 (3)    |
| Co3—C30      | 2.081 (2)    | P1—F5        | 1.584 (3)    |
| C1—C5        | 1.397 (5)    | P1—F2        | 1.585 (2)    |
| C1—C2        | 1.408 (5)    | P1—F6        | 1.595 (3)    |
| C1—H1        | 0.9500       | P2—F7A       | 1.471 (11)   |
| C2—C3        | 1.399 (5)    | P2—F9        | 1.505 (6)    |
| C2—H2        | 0.9500       | P2—F10A      | 1.54 (2)     |
| C3—C4        | 1.423 (5)    | P2—F8        | 1.553 (8)    |
| C3—H3        | 0.9500       | P2—F11       | 1.566 (3)    |
| C4—C5        | 1.402 (6)    | P2—F7        | 1.570 (5)    |
| C4—H4        | 0.9500       | P2—F12       | 1.585 (2)    |
| C5—H5        | 0.9500       | P2—F9A       | 1.621 (12)   |
| C6—C7        | 1.418 (4)    | P2—F8A       | 1.642 (14)   |
| C6—C10       | 1.432 (4)    | P2—F10       | 1.642 (6)    |
| C6—H6        | 0.9500       | N1—C31       | 1.131 (12)   |
| C7—C8        | 1.406 (4)    | C31—C32      | 1.427 (16)   |
| C7—H7        | 0.9500       | C32—H32A     | 0.9800       |
| C8—C9        | 1.425 (4)    | C32—H32B     | 0.9800       |
| C8—H8        | 0.9500       | C32—H32C     | 0.9800       |
| C9—C10       | 1.422 (4)    | N1A—C31A     | 1.126 (9)    |
| C9—H9        | 0.9500       | N1A—N1Ae     | 1.345 (12)   |
| C11—C12      | 1.400 (5)    | C31A—C32A    | 1.440 (15)   |
| C11—C15      | 1.413 (5)    | C32A—H32D    | 0.9800       |
| C11—H11      | 0.9500       | C32A—H32E    | 0.9800       |
| C12—C13      | 1.407 (5)    | C32A—H32F    | 0.9800       |
| Se3—Hgl1—Se1 | 124.083 (9)  | Co1—C8—H8    | 126.4        |
| Se3—Hgl1—Se2 | 116.198 (10) | C10—C9—C8    | 108.5 (2)    |
| Se1—Hgl1—Se2 | 115.319 (10) | C10—C9—Co1   | 70.43 (14)   |
| Bond/Angle Descriptions          | Bond Length (Å) | Bond Angle (°) |
|---------------------------------|-----------------|----------------|
| Se3—Hg1—Se2i                    | 99.723 (10)     | 69.04 (14)     |
| Se1—Hg1—Se2i                    | 99.201 (9)      | 125.8          |
| Se2—Hg1—Se2i                    | 91.509 (10)     | 125.8          |
| C10—Se1—Hg1                     | 104.54 (8)      | 126.4          |
| C20—Se2—Hg1                     | 106.04 (7)      | 106.6 (2)      |
| C20—Se2—Hg1i                    | 98.79 (7)       | 129.78 (19)    |
| Hg1—Se2—Hg1i                    | 88.491 (10)     | 123.6 (2)      |
| C30—Se3—Hg1                     | 102.46 (8)      | 68.88 (14)     |
| C6—Co1—C1                       | 106.10 (13)     | 68.01 (14)     |
| C6—Co1—C7                       | 41.12 (12)      | 126.55 (12)    |
| C1—Co1—C7                       | 113.44 (14)     | 107.9 (3)      |
| C6—Co1—C8                       | 68.77 (12)      | 69.63 (17)     |
| C1—Co1—C8                       | 146.55 (13)     | 69.62 (17)     |
| C7—Co1—C8                       | 40.69 (12)      | 126.0          |
| C6—Co1—C5                       | 113.78 (14)     | 126.0          |
| C7—Co1—C5                       | 40.39 (14)      | 126.3          |
| C8—Co1—C5                       | 145.45 (15)     | 108.3 (3)      |
| C6—Co1—C2                       | 129.59 (13)     | 70.10 (16)     |
| C1—Co1—C2                       | 40.71 (13)      | 125.8          |
| C7—Co1—C2                       | 107.44 (12)     | 125.8          |
| C8—Co1—C2                       | 115.98 (12)     | 69.38 (17)     |
| C5—Co1—C2                       | 68.15 (12)      | 126.3          |
| C6—Co1—C4                       | 146.87 (15)     | 108.0 (3)      |
| C1—Co1—C4                       | 68.11 (16)      | 69.98 (16)     |
| C7—Co1—C4                       | 171.93 (15)     | 70.02 (16)     |
| C8—Co1—C4                       | 134.13 (16)     | 126.0          |
| C5—Co1—C4                       | 40.42 (16)      | 126.0          |
| C2—Co1—C4                       | 68.22 (14)      | 125.6          |
| C6—Co1—C3                       | 169.18 (13)     | 108.0 (3)      |
| C1—Co1—C3                       | 68.23 (15)      | 69.47 (16)     |
| C7—Co1—C3                       | 131.41 (13)     | 69.88 (16)     |
| C8—Co1—C3                       | 110.49 (13)     | 126.0          |
| C5—Co1—C3                       | 68.37 (14)      | 126.0          |
| C2—Co1—C3                       | 40.27 (14)      | 126.2          |
| C4—Co1—C3                       | 40.99 (15)      | 107.7 (3)      |
| C6—Co1—C9                       | 68.73 (11)      | 69.44 (17)     |
| C1—Co1—C9                       | 169.81 (12)     | 69.78 (16)     |
| C7—Co1—C9                       | 68.91 (11)      | 126.1          |
| C8—Co1—C9                       | 41.10 (10)      | 126.1          |
| C5—Co1—C9                       | 132.51 (13)     | 126.2          |
| C2—Co1—C9                       | 149.25 (12)     | 108.3 (3)      |
| C4—Co1—C9                       | 111.05 (14)     | 68.69 (17)     |
| C3—Co1—C9                       | 118.31 (13)     | 71.22 (14)     |
| C6—Co1—C10                      | 41.14 (10)      | 125.9          |
| C1—Co1—C10                      | 129.79 (12)     | 125.9          |
| C7—Co1—C10                      | 69.29 (10)      | 108.2 (3)      |
| C8—Co1—C10                      | 68.99 (10)      | 69.77 (18)     |

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C5—Co1—C10 108.10 (11) C16—C17—Co2 70.33 (16)
C2—Co1—C10 168.83 (12) C18—C17—H17 125.9
C4—Co1—C10 116.29 (12) C16—C17—H17 125.9
C3—Co1—C10 149.47 (13) C17—Co1—C10 125.6
C9—Co1—C10 40.70 (10) C17—C18—C19 108.2 (3)
C17—Co2—C18 40.97 (15) C17—C18—C20 69.26 (17)
C17—Co2—C13 104.66 (13) C19—C18—Co2 70.27 (16)
C18—Co2—C13 118.79 (13) C17—C18—H18 125.9
C17—Co2—C14 122.20 (14) C19—C18—H18 126.1
C18—Co2—C14 106.12 (13) C18—C19—C20 108.0 (3)
C13—Co2—C14 40.55 (13) C18—C19—Co2 68.68 (16)
C12—Co2—C14 119.40 (14) C18—C19—H18 71.02 (14)
C13—Co2—C12 154.38 (14) C18—C19—H19 126.0
C14—Co2—C12 40.60 (13) C18—C19—H19 126.0
C17—Co2—C16 68.12 (12) C20—C19—H19 125.9
C17—Co2—C16 40.98 (13) C20—C19—H19 125.9
C18—Co2—C16 68.82 (14) C19—C20—C16 107.3 (2)
C13—Co2—C16 122.91 (12) C19—C20—Se2 128.4 (2)
C14—Co2—C16 159.32 (13) C16—C20—Se2 124.3 (2)
C12—Co2—C16 107.28 (12) C19—C20—Co2 68.43 (14)
C17—Co2—C15 160.25 (15) C16—C20—Co2 68.17 (14)
C18—Co2—C15 124.82 (15) C19—C20—Co2 128.02 (12)
C13—Co2—C15 68.31 (13) C25—C21—C22 108.4 (3)
C14—Co2—C15 40.68 (14) C25—C21—Co3 69.25 (19)
C12—Co2—C15 68.04 (12) C22—C21—Co3 70.55 (16)
C16—Co2—C15 158.24 (14) C25—C21—Co3 125.8
C17—Co2—C11 155.77 (15) C22—C21—H21 125.8
C18—Co2—C11 162.92 (15) C22—C21—H21 125.8
C13—Co2—C11 68.18 (13) C21—C22—C23 126.0
C14—Co2—C11 68.27 (13) C21—C22—C23 108.1 (3)
C12—Co2—C11 40.27 (13) C21—C22—Co3 69.44 (17)
C16—Co2—C11 122.15 (13) C23—C22—Co3 69.68 (16)
C15—Co2—C11 40.60 (13) C21—C22—H22 125.9
C17—Co2—C19 69.01 (13) C23—C22—H22 125.9
C18—Co2—C19 41.04 (12) C22—C23—C24 126.5
C13—Co2—C19 155.45 (12) C22—C23—C24 107.8 (3)
C14—Co2—C19 121.50 (12) C22—C23—Co3 70.25 (16)
C12—Co2—C19 163.16 (12) C24—C23—Co3 68.93 (18)
C16—Co2—C19 68.67 (12) C22—C23—H23 126.1
C15—Co2—C19 68.51 (11) C24—C23—H23 126.1
C11—Co2—C19 109.28 (12) C23—C24—C25 126.3
C17—Co2—C20 126.94 (12) C23—C24—C25 107.6 (3)
C18—Co2—C20 68.61 (11) C23—C24—Co3 70.62 (18)
C13—Co2—C20 68.51 (11) C25—C24—Co3 69.38 (18)
C14—Co2—C20 161.03 (12) C23—C24—H24 126.2
C12—Co2—C20 158.00 (12) C25—C24—H24 126.2
C16—Co2—C20 125.96 (11) Co3—C24—H24 125.4
C15—Co2—C20 40.62 (10) C21—C25—C24 108.1 (3)
C12—Co2—C20 123.73 (12) C21—C25—Co3 70.72 (18)
| Bond | Distance (Å) | Standard Deviation (Å) |
|------|-------------|------------------------|
| C11—Co2—C20 | 110.28 (11) | 69.7 (2) |
| C19—Co2—C20 | 40.55 (10) | 125.9 |
| C25—Co3—C28 | 151.76 (18) | 125.9 |
| C25—Co3—C24 | 40.96 (17) | 125.3 |
| C28—Co3—C24 | 117.02 (17) | 108.8 (3) |
| C25—Co3—C27 | 166.20 (17) | 68.63 (15) |
| C28—Co3—C27 | 41.05 (14) | 71.34 (14) |
| C24—Co3—C27 | 151.55 (17) | 125.6 |
| C25—Co3—C29 | 117.88 (15) | 125.6 |
| C28—Co3—C29 | 41.32 (13) | 126.0 |
| C24—Co3—C29 | 106.39 (14) | 108.1 (3) |
| C27—Co3—C29 | 69.23 (13) | 69.21 (17) |
| C25—Co3—C31 | 40.03 (16) | 70.43 (15) |
| C28—Co3—C31 | 165.87 (15) | 125.9 |
| C24—Co3—C31 | 67.94 (15) | 125.9 |
| C27—Co3—C31 | 128.78 (15) | 126.0 |
| C25—Co3—C31 | 152.40 (13) | 108.1 (3) |
| C28—Co3—C31 | 68.09 (14) | 69.74 (16) |
| C24—Co3—C32 | 106.95 (12) | 69.80 (16) |
| C27—Co3—C32 | 40.45 (16) | 126.0 |
| C25—Co3—C32 | 118.42 (13) | 126.0 |
| C28—Co3—C32 | 126.63 (12) | 126.1 |
| C25—Co3—C21 | 67.55 (12) | 108.4 (3) |
| C26—Co3—C21 | 128.18 (14) | 68.88 (16) |
| C28—Co3—C21 | 68.92 (12) | 71.79 (14) |
| C24—Co3—C21 | 165.64 (16) | 125.8 |
| C27—Co3—C21 | 40.94 (11) | 125.8 |
| C25—Co3—C22 | 68.77 (12) | 125.1 |
| C28—Co3—C22 | 68.77 (12) | 106.6 (2) |
| C24—Co3—C22 | 109.67 (12) | 130.28 (19) |
| C25—Co3—C22 | 153.11 (14) | 123.1 (2) |
| C28—Co3—C22 | 67.48 (14) | 68.20 (14) |
| C24—Co3—C22 | 127.60 (13) | 67.29 (14) |
| C27—Co3—C22 | 67.71 (13) | 129.52 (12) |
| C29—Co3—C22 | 108.91 (13) | 90.82 (16) |
| C29—Co3—C22 | 164.94 (12) | 177.97 (19) |
| C21—Co3—C22 | 40.01 (13) | 90.61 (16) |
| C23—Co3—C22 | 40.07 (13) | 94.2 (2) |
| C25—Co3—C30 | 120.28 (12) | 90.20 (16) |
| C28—Co3—C30 | 108.22 (12) | 87.26 (16) |
| C24—Co3—C30 | 68.96 (11) | 88.73 (16) |
| C27—Co3—C30 | 127.29 (14) | 179.55 (15) |
| C29—Co3—C30 | 68.69 (11) | 89.84 (15) |
| C21—Co3—C30 | 40.91 (10) | 89.87 (15) |
| C23—Co3—C30 | 119.73 (11) | 88.3 (2) |
| C25—Co3—C30 | 164.93 (13) | 90.27 (17) |
| C26—Co3—C30 | 40.46 (10) | 90.23 (19) |
| C22—Co3—C30 | 153.56 (11) | 177.5 (2) |
| C5—C1—C2 | 108.3 (3) | F3—P1—F1 | 90.27 (17) |
| Bond               | Distance (Å)  | Torsion (°)  |
|--------------------|--------------|--------------|
| C5—C1—Co1         | 70.19 (18)   | F2—P1—F6    | 89.67 (16)   |
| C2—C1—Co1         | 70.06 (16)   | F7A—P2—F10A | 97.8 (13)    |
| C5—C1—H1          | 125.9        | F9—P2—F8    | 92.2 (5)     |
| C2—C1—H1          | 125.9        | F7A—P2—F11  | 77.8 (6)     |
| C1—C2—Co1         | 69.24 (16)   | F9—P2—F7    | 92.0 (4)     |
| C3—C2—H2          | 125.9        | F8—P2—F7    | 175.3 (5)    |
| C1—C2—H2          | 125.9        | F11—P2—F7   | 90.6 (3)     |
| Co1—C2—H2         | 126.4        | F7A—P2—F12  | 99.1 (6)     |
| C2—C3—C4          | 107.6 (3)    | F9—P2—F12   | 96.2 (3)     |
| C2—C3—Co1         | 69.72 (17)   | F10A—P2—F12 | 95.3 (10)    |
| C4—C3—Co1         | 69.39 (18)   | F8—P2—F12   | 88.6 (4)     |
| C2—C3—H3          | 126.2        | F11—P2—F12  | 176.7 (2)    |
| C4—C3—H3          | 126.2        | F7—P2—F12   | 88.7 (3)     |
| Co1—C3—H3         | 126.3        | F7A—P2—F9A  | 92.5 (9)     |
| C5—C4—C3          | 107.8 (3)    | F10A—P2—F9A | 169.3 (13)   |
| C5—C4—Co1         | 69.73 (19)   | F11—P2—F9A  | 95.3 (5)     |
| C3—C4—Co1         | 69.62 (18)   | F12—P2—F9A  | 85.9 (5)     |
| C5—C4—H4          | 126.1        | F7A—P2—F8A  | 175.2 (11)   |
| C3—C4—H4          | 126.1        | F10A—P2—F8A | 86.6 (13)    |
| Co1—C4—H4         | 126.1        | F11—P2—F8A  | 100.8 (7)    |
| C1—C5—C4          | 108.2 (3)    | F12—P2—F8A  | 82.4 (7)     |
| C1—C5—Co1         | 69.43 (17)   | F9A—P2—F8A  | 83.0 (10)    |
| C4—C5—Co1         | 69.85 (18)   | F9—P2—F10   | 177.7 (3)    |
| C1—C5—H5          | 125.9        | F8—P2—F10   | 87.0 (5)     |
| C4—C5—H5          | 125.9        | F11—P2—F10  | 95.2 (3)     |
| Co1—C5—H5         | 126.4        | F7—P2—F10   | 88.7 (4)     |
| C7—C6—C10         | 108.8 (2)    | F12—P2—F10  | 81.5 (2)     |
| C7—C6—Co1         | 69.48 (16)   | N1—C31—C32  | 176.8 (19)   |
| C10—C6—Co1        | 70.84 (14)   | C31—C32—H32A | 109.5       |
| C7—C6—H6          | 125.6        | C31—C32—H32B | 109.5       |
| C10—C6—H6         | 125.6        | H32A—C32—H32B | 109.5     |
| Co1—C6—H6         | 125.6        | C31—C32—H32C | 109.5     |
| C8—C7—C6          | 107.9 (2)    | H32A—C32—H32C | 109.5   |
| C8—C7—Co1         | 69.85 (15)   | H32B—C32—H32C | 109.5   |
| C6—C7—Co1         | 69.40 (15)   | C31A—N1A—N1A# | 163.0 (9) |
| C8—C7—H7          | 126.0        | N1A—C31A—C32A | 179.9 (11) |
| C6—C7—H7          | 126.0        | C31A—C32A—H32D | 109.5 |
| Co1—C7—H7         | 126.3        | C31A—C32A—H32E | 109.5 |
| C7—C8—C9          | 108.3 (2)    | H32D—C32A—H32E | 109.5 |
| C7—C8—Co1         | 69.46 (15)   | C31A—C32A—H32F | 109.5 |
| C9—C8—Co1         | 69.87 (14)   | H32D—C32A—H32F | 109.5 |
| C7—C8—H8          | 125.9        | H32E—C32A—H32F | 109.5 |
| C9—C8—H8          | 125.9        |                  |             |
| C5—C1—C2—C3       | 0.6 (3)      | C16—C17—C18—Co2 | −60.1 (2) |
| Bond/Angle | Value (deg) | Standard Deviation (deg) |
|------------|-------------|--------------------------|
| Co1—C1—C2—C3 | -59.4 (2) | Co17—C18—C19—C20 | 1.4 (3) |
| C5—C1—C2—Co1 | 60.0 (2) | Co2—C18—C19—C20 | 60.42 (18) |
| C1—C2—C3—C4 | -0.4 (3) | C17—C18—C19—Co2 | -59.1 (2) |
| Co1—C2—C3—C4 | -59.3 (2) | C18—C19—C20—C16 | -1.8 (3) |
| C1—C2—C3—Co1 | 58.9 (2) | C18—C19—C20—Se2 | 57.16 (17) |
| C2—C3—C4—C5 | 0.0 (3) | Co2—C19—C20—Se2 | 178.91 (19) |
| Co1—C3—C4—C5 | -59.5 (2) | Co2—C19—C20—Co2 | -122.13 (19) |
| C2—C1—C5—C4 | -0.6 (3) | C18—C19—C20—Co2 | -58.96 (18) |
| Co1—C1—C5—C4 | 59.5 (2) | C17—C16—C20—C19 | 1.6 (3) |
| C5—C1—C2—Co1 | 60.0 (2) | Co2—C16—C20—C19 | -57.32 (17) |
| Co1—C2—C3—C4 | -59.3 (2) | C17—C16—C20—Se2 | -179.09 (18) |
| C1—C2—C3—Co1 | 58.9 (2) | Co2—C16—C20—Co2 | 122.00 (17) |
| C2—C3—C4—Co1 | 0.4 (3) | C17—C16—C20—Co2 | 58.90 (18) |
| Co1—C4—C5—Co1 | 59.5 (2) | Hg1—Se2—C20—C19 | -33.8 (2) |
| C3—C4—C5—Co1 | 59.5 (2) | Hg1—Se2—C20—C19 | -124.7 (2) |
| Co1—C5—C1—C4 | 59.3 (2) | Hg1—Se2—C20—C16 | 147.06 (19) |
| C2—C1—C5—C4 | -0.6 (3) | Hg1—Se2—C20—C16 | 56.1 (2) |
| Co1—C1—C5—C4 | 59.3 (2) | Hg1—Se2—C20—Co2 | -125.16 (14) |
| C3—C4—C5—C1 | 59.5 (2) | Hg1—Se2—C20—Co2 | 143.88 (14) |
| C4—C5—C1—C2 | 59.5 (2) | C25—C21—C22—C23 | 0.0 (3) |
| Co1—C6—C7—C8 | 59.45 (19) | Co3—C21—C22—C23 | -59.1 (2) |
| C10—C6—C7—Co1 | -60.18 (18) | C25—C21—C22—Co3 | 59.1 (2) |
| Co1—C6—C7—Co1 | 0.1 (3) | C21—C22—C23—C24 | 0.0 (3) |
| C6—C7—C8—C9 | 59.30 (18) | Co3—C22—C23—C24 | -58.9 (2) |
| Co1—C7—C8—C9 | -59.17 (18) | Co3—C22—C23—Co3 | 59.0 (2) |
| C7—C8—C9—Co1 | 59.37 (17) | Co2—C22—C23—Co3 | -59.9 (2) |
| C8—C9—C10—C6 | 57.75 (17) | Co3—C22—C23—Co3 | 59.8 (2) |
| Co1—C9—C10—C6 | -179.32 (18) | Co3—C22—C23—Co3 | 0.0 (3) |
| C8—C9—C10—Co1 | -120.6 (2) | Co3—C22—C23—Co3 | -59.9 (2) |
| Co1—C9—C10—Co1 | -58.71 (17) | Co3—C22—C23—Co3 | 1.0 (4) |
| C7—C6—C10—C9 | 1.0 (3) | Co3—C24—C25—C21 | -60.5 (2) |
| C10—C6—C7—C8 | 59.34 (18) | C23—C24—C25—Co3 | 60.6 (2) |
| C8—C9—C10—Se1 | 8.8 (2) | C23—C24—C25—Co3 | -1.1 (3) |
| C10—C9—C10—Se1 | 173.14 (19) | Co3—C26—C27—C28 | 59.16 (19) |
| C7—C6—C10—Se1 | -100.68 (14) | Co3—C26—C27—C28 | -60.26 (17) |
| C8—C9—C10—Se1 | 179.53 (17) | C26—C27—C28—C29 | -0.4 (3) |
| C7—C6—C10—Se1 | 120.19 (17) | Co3—C27—C28—C29 | 59.5 (2) |
| C7—C6—C10—Co1 | 59.34 (18) | C26—C27—C28—C29 | -59.92 (18) |
| Hg1—Se1—Co1—C9 | -8.8 (2) | C27—C28—C29—C30 | 1.8 (3) |
| Hg1—Se1—Co1—C6 | 173.14 (19) | Co3—C28—C29—C30 | 61.25 (18) |
| Hg1—Se1—Co1—Co1 | -100.68 (14) | C27—C28—C29—Co3 | -59.45 (19) |
| C15—C11—C12—C13 | 0.3 (3) | C27—C28—C29—Co3 | 2.2 (3) |
| Co2—C11—C12—C13 | -59.0 (2) | C27—C28—C29—C30 | -56.42 (17) |
| C15—C11—C12—Co2 | 59.29 (19) | C27—C28—C29—Se3 | -177.39 (18) |
| C11—C12—C13—Co2 | -0.4 (3) | Co3—C26—C30—Se3 | 124.0 (2) |
| C11—C12—C13—Co2 | -59.9 (2) | Co3—C26—C30—Co3 | 58.60 (17) |
| Bond                        | Angle (°) (E) | Bond                        | Angle (°) (E) |
|-----------------------------|--------------|-----------------------------|--------------|
| C12—C11—C15—C14           | 0.0 (3)      | C28—C29—C30—C26           | −2.4 (3)     |
| Co2—C11—C15—C14           | 59.3 (2)     | Co3—C29—C30—C26           | 56.98 (17)   |
| C12—C11—C15—Co2           | −59.30 (19)  | C28—C29—C30—Se3           | 177.18 (18)  |
| C20—C16—C17—C18           | −0.8 (3)     | Co3—C29—C30—Se3           | −123.41 (17) |
| Co2—C16—C17—C18           | 59.7 (2)     | C28—C29—C30—Co3           | −59.42 (19)  |
| C20—C16—C17—Co2           | −60.48 (18)  | Hg1—Se3—C30—C26           | −2.6 (2)     |
| C16—C17—C18—C19           | −0.4 (3)     | Hg1—Se3—C30—C29           | 177.93 (19)  |
| Co2—C17—C18—C19           | 59.7 (2)     | Hg1—Se3—C30—Co3           | 91.34 (16)   |

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