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Dibenzo[2,3:6,7]thiepino[4,5-*d*][1,2,3]selenadiazole

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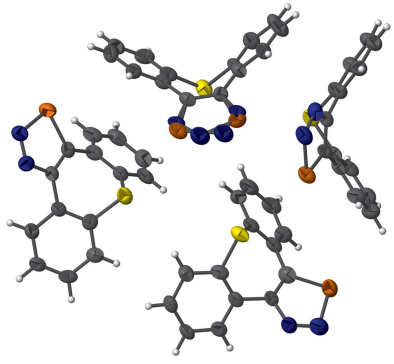
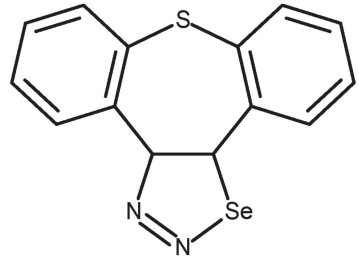
Structural data: full structural data are available from iucrdata.iucr.org

Four tetracyclic molecules of the title compound, $C_{14}H_8N_2SSe$, are present in the asymmetric unit. Their molecular structures are very similar, adopting the shape of a saddle. The selenadiazole moiety of one of the molecules is disordered over two set of sites [occupancy ratio 0.618 (6):0.382 (6)]. In the crystal, layers of molecules with hydrogen surfaces extend parallel to the *ab* plane and are stacked along the *c* axis. The crystal studied was refined as an inversion twin.

3D view



Chemical scheme



Structure description

1,2,3-Selenadiazoles are useful precursors for strained cycloalkynes (Bissinger *et al.*, 1988; Detert & Meier, 1997) and heterocycles (Detert *et al.* 1992), and are precursors for photochemically induced (Jedináková *et al.*, 2016) as well as for strain-accelerated click-reactions (Jewett & Bertozzi, 2010).

Sixteen molecules, *i.e.* four sets of four independent molecules, of the title compound fill the unit cell (Z' = 4). The forms of all four molecules are nearly identical (Fig. 1). Molecule *A* is nearly identical to molecule *B*, and molecule *D* is nearly identical to molecule *C*. However, molecules *A* and *D* are pseudo-mirror images. The selenadiazole moiety of molecule *D* is disordered over two sets of sites, with the ratio *D* (major component):*E* (minor component) being 0.618 (6):0.382 (6). The molecular shape of these tetracycles is that of a saddle, with the sulfur atom being the pommel, the selenadiazole moiety the cantle and the benzene rings the flaps. Representative for the nearly identical parts in molecules *A*–*E*, only details for A are given. The mean planes of the benzene rings are inclined by an angle of 63.7 (7)°. Although the five-membered diphenyl-1,2,3-selenadiazole unit is not symmetrical, the dihedral angles between the mean planes of neighbouring rings are virtually the same: (C1–C6)–selenadiazole: 40.7 (7)° and selenadiazole–(C8–C13): 39.3 (7)°. The C—S—C bond angle at the sulfur atom [99.5 (7)°] is significantly larger than the N—Se—C bond angle of 87.2 (6)°. The

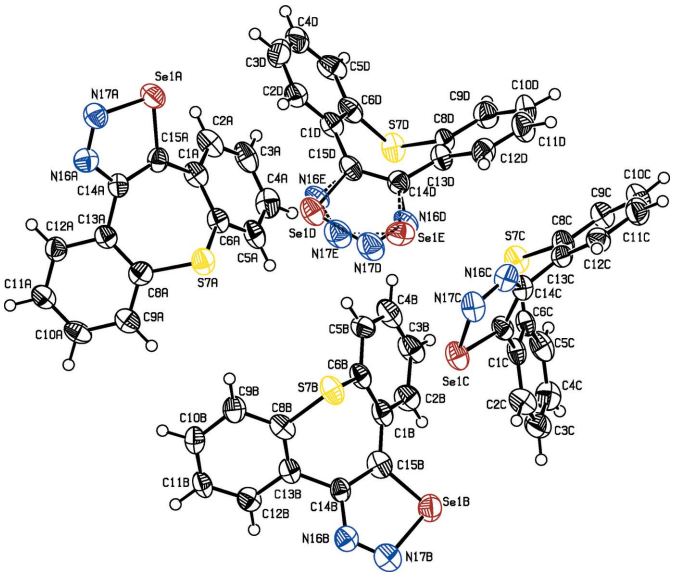


Figure 1
The structures of the four molecules present in the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The minor disorder component is shown with dashed lines.

latter is close to the corresponding angle in a 3-methyl-1,2,3-selenadiazolium salt [89.1 (4)°; Schollmeyer & Detert, 2016].

In the crystal structure (Fig. 2), the molecules are packed according to their molecular shape, forming layers parallel to the *ab* plane. These layers have hydrogen surfaces and are stacked along the *c* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_8N_2SSe$
M_r	315.24
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	193
a, b, c (Å)	20.8533 (8), 9.9698 (3), 23.4151 (8)
V (Å^3)	4868.1 (3)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.24
Crystal size (mm)	0.34 × 0.26 × 0.05
Data collection	
Diffractometer	Stoe *IPDS* 2T
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2006)
T_{min}, T_{max}	0.406, 0.689
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28240, 12118, 8561
R_{int}	0.058
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.674
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.080, 0.189, 1.16
No. of reflections	12118
No. of parameters	666
No. of restraints	33
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, −0.90
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.41 (2)

Computer programs: *X-AREA* (Stoe & Cie, 2006), *X-RED32* (Stoe & Cie, 2006), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009), *publCIF* (Westrip, 2010).

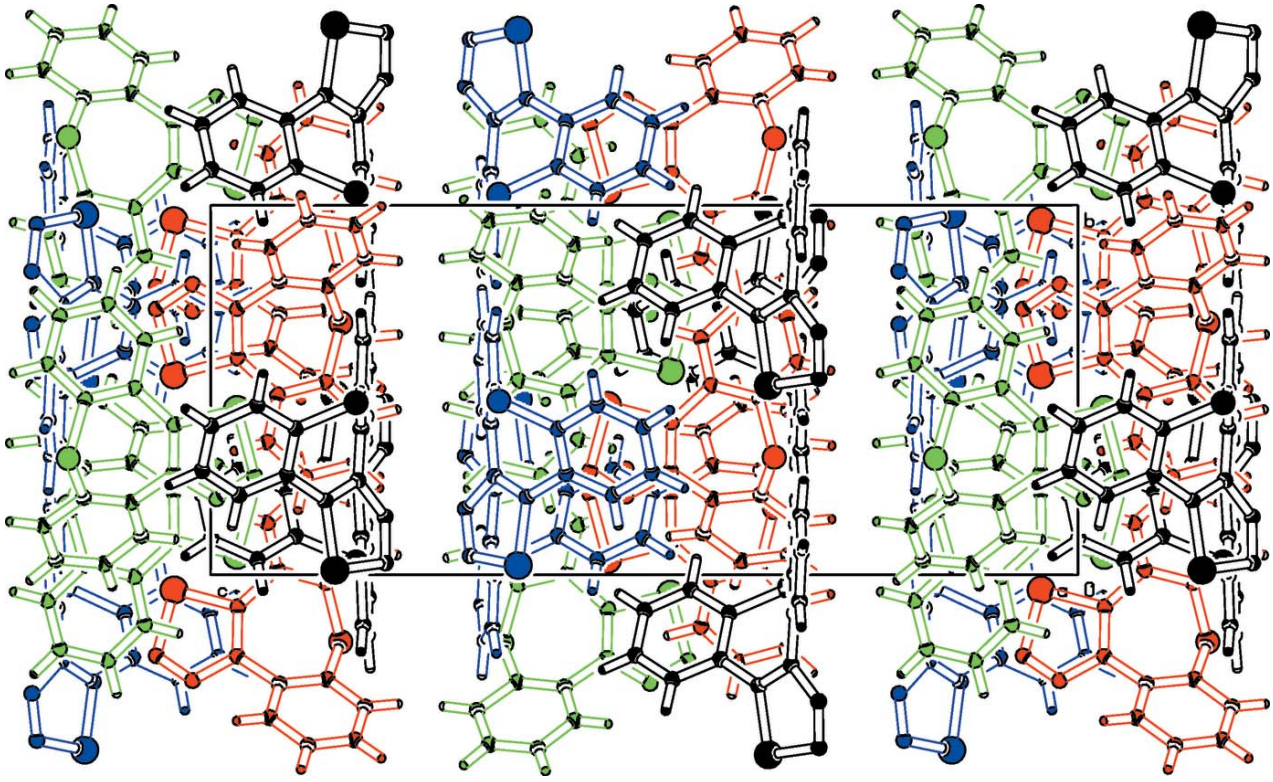


Figure 2
The crystal packing in the title compound in a view along the *a* axis. The four independent molecules are shown in different colours.

Synthesis and crystallization

The title compound was prepared in seven steps from *o*-phenylthiobenzoic acid according to Jílek *et al.* (1965) and Lorch & Meier (1981). ^{1}H NMR ($CDCl_3$, 400 MHz): 8.17 (*dd*, 1 H), 7.71 (m, 2 H), 7.53-7.43 (*m*, 4 H), 7.33 (*ddd*, 1 H); ^{77}Se NMR ($CDCl_3$, 76.3 MHz, δ SeO_2/D_2O) = 0 p.p.m.): δ = 257.3 p.p.m. The title compound was recrystallized from chloroform/2-propanol (1:1, *v*:*v*) to give light-yellow crystals; m.p. = 413 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The two N atoms and the Se atoms of the five membered seleneadiazole ring of molecule *D* are disordered over two sets of sites with a refined occupancy ratio of 0.618 (6)/0.382 (6). The C—N and N—N bond lengths inside the ring were restrained to be equal. RIGU and EADP instructions were used for the corresponding ring atoms. Refinement as a inversion twin with a BASF value of 0.41 (2) improved the final reliability factor by 0.35%.

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full crystallographic data

IUCrData (2018). **3**, x180070 [https://doi.org/10.1107/S2414314618000706]

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Dibenzo[2,3:6,7]thiepino[4,5-*d*][1,2,3]selenadiazole

Crystal data

$C_{14}H_8N_2SSe$
M_r = 315.24
Orthorhombic, $Pna2_1$
a = 20.8533 (8) Å
b = 9.9698 (3) Å
c = 23.4151 (8) Å
V = 4868.1 (3) Å^3
Z = 16
F(000) = 2496
D_x = 1.721 Mg m^{-3}
Melting point: 413 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 38903 reflections
θ = 2.0–28.3°
μ = 3.24 mm^{-1}
T = 193 K
Plate, light yellow
0.34 × 0.26 × 0.05 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2006)
T_{min} = 0.406, T_{max} = 0.689
28240 measured reflections
12118 independent reflections
8561 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.6°, θ_{min} = 2.0°
h = −27→26
k = −11→13
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.189
S = 1.16
12118 reflections
666 parameters
33 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 36.2917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.41 (2)

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.

Refinement. Refined as a 2-component inversion twin

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Se1A	0.05143 (8)	0.45875 (16)	0.54238 (7)	0.0493 (4)	
C1A	0.0215 (7)	0.5129 (13)	0.4230 (7)	0.039 (3)	
C2A	−0.0007 (7)	0.6410 (15)	0.4345 (8)	0.047 (4)	
H2A	−0.012930	0.664452	0.472250	0.056*	
C3A	−0.0051 (7)	0.7355 (16)	0.3911 (8)	0.050 (4)	
H3A	−0.020032	0.823479	0.399162	0.061*	
C4A	0.0123 (8)	0.7008 (18)	0.3357 (8)	0.051 (4)	
H4A	0.008540	0.764993	0.305914	0.061*	
C5A	0.0347 (8)	0.5754 (16)	0.3237 (8)	0.050 (4)	
H5A	0.047064	0.553217	0.285857	0.060*	
C6A	0.0394 (7)	0.4790 (14)	0.3672 (7)	0.041 (3)	
S7A	0.07130 (19)	0.3183 (4)	0.3501 (2)	0.0475 (9)	
C8A	0.0029 (7)	0.2171 (14)	0.3656 (7)	0.042 (3)	
C9A	−0.0228 (7)	0.1421 (14)	0.3223 (7)	0.043 (3)	
H9A	−0.006455	0.150252	0.284574	0.051*	
C10A	−0.0736 (7)	0.0529 (15)	0.3338 (7)	0.044 (4)	
H10A	−0.092918	0.003662	0.303604	0.052*	
C11A	−0.0945 (7)	0.0377 (15)	0.3879 (7)	0.042 (3)	
H11A	−0.126862	−0.026769	0.395763	0.051*	
C12A	−0.0701 (7)	0.1132 (15)	0.4320 (7)	0.042 (3)	
H12A	−0.087109	0.104390	0.469415	0.050*	
C13A	−0.0195 (7)	0.2044 (14)	0.4210 (6)	0.037 (3)	
C14A	0.0083 (6)	0.2796 (14)	0.4697 (6)	0.037 (3)	
C15A	0.0260 (6)	0.4132 (13)	0.4687 (7)	0.039 (3)	
N16A	0.0135 (6)	0.2135 (13)	0.5210 (6)	0.044 (3)	
N17A	0.0339 (7)	0.2808 (13)	0.5628 (6)	0.047 (3)	
Se1B	0.17948 (8)	0.44736 (17)	−0.03038 (8)	0.0527 (4)	
C1B	0.1465 (7)	0.5053 (15)	0.0877 (8)	0.045 (4)	
C2B	0.1273 (7)	0.6349 (16)	0.0762 (8)	0.049 (4)	
H2B	0.116688	0.658540	0.038027	0.058*	
C3B	0.1230 (8)	0.7319 (16)	0.1185 (9)	0.053 (4)	
H3B	0.110984	0.820843	0.108665	0.064*	
C4B	0.1360 (8)	0.7010 (18)	0.1742 (10)	0.057 (5)	
H4B	0.132583	0.767475	0.203078	0.068*	
C5B	0.1544 (8)	0.5700 (16)	0.1880 (7)	0.047 (4)	
H5B	0.162552	0.546371	0.226639	0.056*	
C6B	0.1607 (7)	0.4747 (14)	0.1451 (8)	0.043 (3)	
S7B	0.19277 (19)	0.3150 (4)	0.1643 (2)	0.0484 (10)	
C8B	0.1270 (6)	0.2093 (13)	0.1468 (7)	0.040 (3)	
C9B	0.1004 (7)	0.1329 (16)	0.1929 (8)	0.045 (4)	
H9B	0.114887	0.143828	0.231084	0.054*	
C10B	0.0516 (7)	0.0406 (15)	0.1788 (7)	0.044 (3)	
H10B	0.033834	−0.014707	0.207743	0.053*	
C11B	0.0290 (7)	0.0293 (14)	0.1226 (7)	0.041 (3)	
H11B	−0.004845	−0.030958	0.113904	0.050*	

C12B	0.0560 (7)	0.1054 (15)	0.0804 (7)	0.042 (3)	
H12B	0.040790	0.096279	0.042379	0.050*	
C13B	0.1053 (6)	0.1963 (14)	0.0918 (7)	0.038 (3)	
C14B	0.1346 (6)	0.2741 (13)	0.0429 (7)	0.037 (3)	
C15B	0.1516 (7)	0.4067 (14)	0.0420 (7)	0.044 (3)	
N16B	0.1405 (6)	0.2060 (13)	−0.0067 (6)	0.043 (3)	
N17B	0.1618 (7)	0.2679 (14)	−0.0504 (7)	0.054 (3)	
Se1C	0.33561 (7)	0.52544 (15)	0.14539 (8)	0.0476 (4)	
C1C	0.2971 (6)	0.7737 (14)	0.0899 (6)	0.037 (3)	
C2C	0.2950 (7)	0.7166 (16)	0.0362 (8)	0.049 (4)	
H2C	0.316441	0.633824	0.029887	0.059*	
C3C	0.2626 (9)	0.7764 (18)	−0.0090 (8)	0.057 (5)	
H3C	0.260555	0.734853	−0.045433	0.069*	
C4C	0.2329 (8)	0.9006 (19)	0.0013 (8)	0.052 (4)	
H4C	0.211897	0.945020	−0.029326	0.063*	
C5C	0.2333 (7)	0.9595 (17)	0.0539 (8)	0.052 (4)	
H5C	0.211990	1.042628	0.059847	0.062*	
C6C	0.2659 (6)	0.8952 (14)	0.0997 (7)	0.038 (3)	
S7C	0.26504 (17)	0.9701 (4)	0.16780 (19)	0.0461 (9)	
C8C	0.3469 (7)	1.0082 (14)	0.1729 (7)	0.042 (3)	
C9C	0.3650 (8)	1.1445 (16)	0.1751 (7)	0.049 (4)	
H9C	0.333483	1.212573	0.170622	0.058*	
C10C	0.4289 (9)	1.1796 (18)	0.1838 (8)	0.058 (5)	
H10C	0.440448	1.271461	0.187192	0.069*	
C11C	0.4759 (8)	1.0817 (18)	0.1874 (7)	0.052 (4)	
H11C	0.519689	1.105663	0.191688	0.063*	
C12C	0.4575 (8)	0.9463 (16)	0.1848 (7)	0.046 (4)	
H12C	0.489243	0.878414	0.188238	0.055*	
C13C	0.3940 (7)	0.9097 (16)	0.1772 (6)	0.039 (3)	
C14C	0.3768 (6)	0.7672 (14)	0.1725 (7)	0.035 (3)	
C15C	0.3342 (6)	0.7100 (14)	0.1355 (7)	0.040 (3)	
N16C	0.4114 (6)	0.6782 (13)	0.2063 (6)	0.046 (3)	
N17C	0.3994 (6)	0.5515 (12)	0.2006 (6)	0.047 (3)	
Se1D	0.20970 (16)	0.5125 (3)	0.35682 (17)	0.0487 (10)	0.618 (6)
Se1E	0.2824 (5)	0.6295 (9)	0.2903 (4)	0.051 (2)	0.382 (6)
C1D	0.1705 (7)	0.7708 (14)	0.4123 (7)	0.040 (3)	
C2D	0.1656 (8)	0.7163 (15)	0.4674 (7)	0.048 (4)	
H2D	0.185103	0.632270	0.475315	0.057*	
C3D	0.1331 (9)	0.782 (2)	0.5103 (8)	0.057 (5)	
H3D	0.130491	0.743195	0.547290	0.069*	
C4D	0.1045 (8)	0.9034 (18)	0.4994 (8)	0.054 (4)	
H4D	0.081816	0.948653	0.528863	0.065*	
C5D	0.1085 (7)	0.9587 (17)	0.4466 (8)	0.052 (4)	
H5D	0.088427	1.042690	0.439787	0.062*	
C6D	0.1414 (7)	0.8961 (16)	0.4020 (7)	0.046 (4)	
S7D	0.14250 (18)	0.9657 (4)	0.33250 (19)	0.0480 (9)	
C8D	0.2262 (7)	1.0023 (15)	0.3266 (7)	0.041 (3)	
C9D	0.2462 (8)	1.1366 (18)	0.3245 (8)	0.051 (4)	

H9D	0.215960	1.207576	0.326746	0.061*	
C10D	0.3109 (9)	1.1633 (19)	0.3193 (8)	0.061 (5)	
H10D	0.325387	1.253317	0.316121	0.073*	
C11D	0.3537 (8)	1.0609 (18)	0.3185 (8)	0.058 (5)	
H11D	0.398042	1.082280	0.316193	0.070*	
C12D	0.3366 (7)	0.9281 (18)	0.3210 (7)	0.048 (4)	
H12D	0.368128	0.859450	0.318923	0.057*	
C13D	0.2701 (7)	0.8959 (15)	0.3268 (7)	0.042 (3)	
C14D	0.2510 (8)	0.7555 (15)	0.3305 (6)	0.040 (3)	
C15D	0.2079 (7)	0.7001 (13)	0.3679 (7)	0.040 (3)	
N16D	0.288 (2)	0.657 (4)	0.299 (2)	0.038 (5)	0.618 (6)
N17D	0.2742 (13)	0.532 (3)	0.2986 (12)	0.059 (5)	0.618 (6)
N16E	0.204 (2)	0.558 (3)	0.365 (2)	0.038 (5)	0.382 (6)
N17E	0.239 (2)	0.508 (4)	0.325 (2)	0.059 (5)	0.382 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1A	0.0528 (9)	0.0437 (8)	0.0515 (9)	−0.0091 (7)	−0.0088 (8)	−0.0013 (8)
C1A	0.036 (7)	0.025 (6)	0.057 (9)	0.010 (5)	−0.005 (6)	0.002 (6)
C2A	0.034 (7)	0.035 (8)	0.072 (12)	0.005 (6)	−0.013 (7)	−0.002 (7)
C3A	0.037 (8)	0.033 (8)	0.082 (13)	−0.001 (6)	−0.009 (8)	0.007 (8)
C4A	0.046 (9)	0.052 (9)	0.055 (11)	0.000 (7)	−0.012 (8)	0.020 (8)
C5A	0.034 (8)	0.045 (9)	0.071 (12)	−0.011 (7)	−0.001 (8)	0.000 (8)
C6A	0.035 (7)	0.036 (7)	0.050 (9)	−0.002 (6)	−0.001 (6)	0.001 (7)
S7A	0.040 (2)	0.042 (2)	0.061 (3)	0.0016 (16)	0.0106 (19)	−0.0024 (19)
C8A	0.044 (8)	0.037 (7)	0.046 (8)	0.007 (6)	0.002 (7)	0.000 (7)
C9A	0.044 (8)	0.032 (7)	0.051 (9)	0.006 (6)	−0.008 (7)	0.001 (6)
C10A	0.037 (7)	0.040 (8)	0.054 (9)	0.004 (6)	−0.014 (7)	−0.011 (7)
C11A	0.031 (7)	0.038 (7)	0.058 (9)	0.001 (6)	0.001 (6)	−0.011 (7)
C12A	0.039 (8)	0.037 (8)	0.049 (9)	−0.001 (6)	0.007 (7)	−0.001 (7)
C13A	0.034 (7)	0.030 (7)	0.048 (9)	0.004 (5)	0.002 (6)	−0.003 (6)
C14A	0.034 (7)	0.038 (7)	0.040 (7)	−0.003 (5)	0.000 (6)	0.005 (7)
C15A	0.036 (7)	0.036 (7)	0.045 (8)	0.002 (5)	0.006 (6)	0.004 (7)
N16A	0.040 (7)	0.048 (7)	0.045 (7)	0.002 (6)	−0.003 (6)	−0.001 (6)
N17A	0.043 (7)	0.047 (7)	0.051 (8)	−0.004 (6)	−0.005 (6)	0.001 (6)
Se1B	0.0546 (9)	0.0460 (8)	0.0576 (10)	−0.0042 (7)	0.0079 (8)	0.0039 (8)
C1B	0.032 (7)	0.040 (8)	0.062 (10)	−0.007 (6)	0.001 (7)	0.000 (7)
C2B	0.047 (9)	0.041 (8)	0.058 (11)	0.005 (7)	−0.001 (8)	−0.002 (7)
C3B	0.042 (9)	0.030 (7)	0.088 (13)	0.006 (6)	0.007 (9)	−0.015 (8)
C4B	0.043 (9)	0.042 (9)	0.086 (14)	−0.007 (7)	0.005 (9)	−0.013 (9)
C5B	0.049 (9)	0.044 (8)	0.048 (9)	−0.006 (7)	0.003 (7)	−0.011 (7)
C6B	0.031 (6)	0.041 (7)	0.057 (9)	−0.008 (6)	−0.002 (7)	−0.002 (8)
S7B	0.0357 (18)	0.041 (2)	0.068 (3)	−0.0033 (15)	−0.0106 (18)	0.0054 (18)
C8B	0.028 (6)	0.032 (6)	0.061 (9)	0.009 (5)	−0.009 (7)	−0.005 (7)
C9B	0.032 (7)	0.049 (9)	0.054 (10)	0.000 (6)	0.001 (7)	0.003 (7)
C10B	0.037 (8)	0.039 (8)	0.056 (10)	−0.003 (6)	0.008 (7)	0.007 (7)
C11B	0.030 (7)	0.030 (7)	0.064 (10)	−0.004 (5)	0.008 (7)	−0.003 (7)

C12B	0.029 (7)	0.045 (8)	0.052 (9)	0.002 (6)	−0.001 (6)	−0.005 (7)
C13B	0.030 (7)	0.030 (7)	0.055 (9)	0.003 (5)	0.003 (6)	0.000 (6)
C14B	0.028 (6)	0.034 (7)	0.048 (8)	0.000 (5)	0.004 (6)	0.001 (7)
C15B	0.041 (8)	0.032 (7)	0.058 (9)	0.011 (6)	−0.007 (7)	0.008 (7)
N16B	0.030 (6)	0.047 (7)	0.053 (8)	0.003 (5)	0.001 (6)	−0.001 (6)
N17B	0.045 (7)	0.049 (8)	0.068 (9)	0.005 (6)	−0.002 (7)	−0.004 (7)
Se1C	0.0406 (8)	0.0325 (6)	0.0695 (10)	0.0016 (6)	−0.0008 (8)	0.0042 (8)
C1C	0.023 (6)	0.036 (7)	0.052 (9)	−0.004 (5)	−0.004 (6)	0.009 (6)
C2C	0.040 (8)	0.043 (8)	0.064 (11)	0.006 (6)	−0.009 (7)	−0.006 (8)
C3C	0.066 (12)	0.054 (10)	0.052 (10)	−0.011 (9)	−0.009 (9)	0.000 (8)
C4C	0.036 (8)	0.066 (11)	0.055 (10)	−0.003 (7)	−0.012 (7)	0.011 (9)
C5C	0.025 (7)	0.054 (10)	0.078 (13)	−0.006 (6)	−0.009 (7)	0.001 (9)
C6C	0.025 (7)	0.037 (7)	0.051 (9)	−0.006 (5)	−0.005 (6)	0.006 (6)
S7C	0.0301 (17)	0.042 (2)	0.066 (3)	0.0062 (14)	0.0034 (16)	−0.0021 (18)
C8C	0.039 (7)	0.030 (7)	0.059 (9)	0.002 (6)	0.000 (7)	0.005 (6)
C9C	0.045 (9)	0.044 (9)	0.057 (10)	−0.006 (7)	−0.002 (7)	−0.001 (7)
C10C	0.055 (10)	0.047 (9)	0.071 (12)	−0.015 (8)	−0.008 (9)	0.004 (9)
C11C	0.046 (9)	0.055 (10)	0.057 (10)	−0.011 (7)	−0.001 (8)	0.003 (8)
C12C	0.041 (8)	0.048 (9)	0.049 (9)	−0.002 (7)	−0.002 (7)	−0.002 (7)
C13C	0.034 (7)	0.048 (8)	0.037 (8)	−0.008 (6)	0.002 (6)	−0.003 (7)
C14C	0.022 (6)	0.036 (7)	0.047 (8)	0.005 (5)	0.001 (6)	0.004 (6)
C15C	0.026 (6)	0.042 (7)	0.051 (9)	−0.004 (5)	−0.001 (6)	−0.004 (7)
N16C	0.043 (7)	0.046 (7)	0.050 (8)	0.007 (6)	0.005 (6)	0.009 (6)
N17C	0.033 (6)	0.038 (7)	0.070 (9)	0.009 (5)	0.003 (6)	0.009 (6)
Se1D	0.0419 (17)	0.0320 (14)	0.072 (2)	0.0013 (13)	−0.0030 (14)	−0.0002 (15)
Se1E	0.038 (3)	0.060 (6)	0.054 (4)	0.008 (3)	0.001 (3)	−0.015 (3)
C1D	0.034 (7)	0.032 (7)	0.055 (9)	0.003 (5)	−0.002 (7)	−0.002 (6)
C2D	0.056 (10)	0.040 (8)	0.047 (9)	−0.007 (7)	0.000 (8)	0.001 (7)
C3D	0.053 (11)	0.070 (12)	0.049 (10)	−0.013 (9)	0.002 (8)	0.010 (9)
C4D	0.034 (8)	0.060 (11)	0.067 (12)	−0.014 (7)	0.008 (8)	−0.013 (9)
C5D	0.039 (8)	0.044 (9)	0.072 (11)	0.009 (7)	−0.003 (8)	−0.020 (8)
C6D	0.030 (7)	0.042 (8)	0.065 (11)	−0.002 (6)	−0.005 (7)	−0.007 (7)
S7D	0.0354 (19)	0.046 (2)	0.063 (3)	0.0019 (16)	−0.0041 (17)	0.0098 (19)
C8D	0.043 (8)	0.041 (8)	0.040 (8)	−0.016 (6)	0.000 (6)	0.000 (6)
C9D	0.049 (9)	0.046 (9)	0.059 (10)	0.001 (7)	0.002 (8)	0.001 (8)
C10D	0.057 (11)	0.056 (11)	0.070 (12)	−0.024 (9)	0.010 (9)	0.004 (9)
C11D	0.040 (9)	0.059 (11)	0.076 (12)	−0.014 (8)	0.004 (8)	−0.001 (9)
C12D	0.030 (7)	0.063 (10)	0.050 (9)	−0.004 (7)	0.000 (7)	0.001 (8)
C13D	0.035 (7)	0.039 (8)	0.052 (9)	−0.003 (6)	−0.002 (7)	0.004 (7)
C14D	0.043 (8)	0.035 (7)	0.041 (8)	0.000 (6)	−0.002 (6)	0.004 (6)
C15D	0.036 (7)	0.029 (6)	0.054 (9)	0.000 (5)	−0.008 (6)	0.002 (6)
N16D	0.029 (10)	0.034 (8)	0.050 (13)	0.000 (7)	−0.013 (8)	−0.005 (9)
N17D	0.059 (13)	0.039 (8)	0.078 (14)	0.002 (8)	0.006 (8)	−0.009 (8)
N16E	0.029 (10)	0.034 (8)	0.050 (13)	0.000 (7)	−0.013 (8)	−0.005 (9)
N17E	0.059 (13)	0.039 (8)	0.078 (14)	0.002 (8)	0.006 (8)	−0.009 (8)

Geometric parameters (Å, º)

Se1A—C15A	1.862 (16)	C1C—C2C	1.38 (2)
Se1A—N17A	1.874 (13)	C1C—C6C	1.39 (2)
C1A—C2A	1.384 (19)	C1C—C15C	1.462 (19)
C1A—C6A	1.40 (2)	C2C—C3C	1.39 (2)
C1A—C15A	1.46 (2)	C2C—H2C	0.9500
C2A—C3A	1.39 (2)	C3C—C4C	1.41 (2)
C2A—H2A	0.9500	C3C—H3C	0.9500
C3A—C4A	1.39 (2)	C4C—C5C	1.36 (3)
C3A—H3A	0.9500	C4C—H4C	0.9500
C4A—C5A	1.36 (2)	C5C—C6C	1.42 (2)
C4A—H4A	0.9500	C5C—H5C	0.9500
C5A—C6A	1.40 (2)	C6C—S7C	1.760 (16)
C5A—H5A	0.9500	S7C—C8C	1.753 (15)
C6A—S7A	1.779 (15)	C8C—C13C	1.39 (2)
S7A—C8A	1.785 (16)	C8C—C9C	1.41 (2)
C8A—C9A	1.37 (2)	C9C—C10C	1.39 (2)
C8A—C13A	1.38 (2)	C9C—H9C	0.9500
C9A—C10A	1.41 (2)	C10C—C11C	1.38 (2)
C9A—H9A	0.9500	C10C—H10C	0.9500
C10A—C11A	1.35 (2)	C11C—C12C	1.40 (2)
C10A—H10A	0.9500	C11C—H11C	0.9500
C11A—C12A	1.37 (2)	C12C—C13C	1.39 (2)
C11A—H11A	0.9500	C12C—H12C	0.9500
C12A—C13A	1.42 (2)	C13C—C14C	1.47 (2)
C12A—H12A	0.9500	C14C—C15C	1.366 (19)
C13A—C14A	1.48 (2)	C14C—N16C	1.390 (18)
C14A—N16A	1.373 (18)	N16C—N17C	1.294 (17)
C14A—C15A	1.383 (18)	Se1D—C15D	1.889 (14)
N16A—N17A	1.262 (18)	Se1D—N17D	1.93 (3)
Se1B—C15B	1.836 (17)	Se1E—C14D	1.700 (17)
Se1B—N17B	1.885 (14)	Se1E—N17E	1.72 (5)
C1B—C2B	1.38 (2)	C1D—C2D	1.40 (2)
C1B—C6B	1.41 (2)	C1D—C6D	1.41 (2)
C1B—C15B	1.46 (2)	C1D—C15D	1.48 (2)
C2B—C3B	1.39 (2)	C2D—C3D	1.37 (2)
C2B—H2B	0.9500	C2D—H2D	0.9500
C3B—C4B	1.37 (3)	C3D—C4D	1.38 (3)
C3B—H3B	0.9500	C3D—H3D	0.9500
C4B—C5B	1.40 (2)	C4D—C5D	1.36 (2)
C4B—H4B	0.9500	C4D—H4D	0.9500
C5B—C6B	1.39 (2)	C5D—C6D	1.40 (2)
C5B—H5B	0.9500	C5D—H5D	0.9500
C6B—S7B	1.783 (16)	C6D—S7D	1.770 (17)
S7B—C8B	1.777 (14)	S7D—C8D	1.787 (15)
C8B—C13B	1.37 (2)	C8D—C13D	1.40 (2)
C8B—C9B	1.43 (2)	C8D—C9D	1.40 (2)

C9B—C10B	1.41 (2)	C9D—C10D	1.38 (2)
C9B—H9B	0.9500	C9D—H9D	0.9500
C10B—C11B	1.40 (2)	C10D—C11D	1.36 (3)
C10B—H10B	0.9500	C10D—H10D	0.9500
C11B—C12B	1.37 (2)	C11D—C12D	1.37 (2)
C11B—H11B	0.9500	C11D—H11D	0.9500
C12B—C13B	1.40 (2)	C12D—C13D	1.43 (2)
C12B—H12B	0.9500	C12D—H12D	0.9500
C13B—C14B	1.51 (2)	C13D—C14D	1.46 (2)
C14B—N16B	1.35 (2)	C14D—C15D	1.37 (2)
C14B—C15B	1.369 (19)	C14D—N16D	1.45 (4)
N16B—N17B	1.273 (19)	C15D—N16E	1.42 (3)
Se1C—C15C	1.855 (15)	N16D—N17D	1.28 (4)
Se1C—N17C	1.874 (14)	N16E—N17E	1.28 (4)

C15A—Se1A—N17A	87.2 (6)	C1C—C2C—C3C	122.1 (15)
C2A—C1A—C6A	119.5 (14)	C1C—C2C—H2C	118.9
C2A—C1A—C15A	120.5 (15)	C3C—C2C—H2C	118.9
C6A—C1A—C15A	120.0 (12)	C2C—C3C—C4C	117.5 (17)
C1A—C2A—C3A	120.4 (17)	C2C—C3C—H3C	121.2
C1A—C2A—H2A	119.8	C4C—C3C—H3C	121.2
C3A—C2A—H2A	119.8	C5C—C4C—C3C	122.1 (17)
C2A—C3A—C4A	119.8 (16)	C5C—C4C—H4C	118.9
C2A—C3A—H3A	120.1	C3C—C4C—H4C	118.9
C4A—C3A—H3A	120.1	C4C—C5C—C6C	119.3 (16)
C5A—C4A—C3A	120.6 (16)	C4C—C5C—H5C	120.3
C5A—C4A—H4A	119.7	C6C—C5C—H5C	120.3
C3A—C4A—H4A	119.7	C1C—C6C—C5C	119.4 (15)
C4A—C5A—C6A	120.2 (17)	C1C—C6C—S7C	121.5 (11)
C4A—C5A—H5A	119.9	C5C—C6C—S7C	119.1 (12)
C6A—C5A—H5A	119.9	C8C—S7C—C6C	98.3 (7)
C1A—C6A—C5A	119.5 (14)	C13C—C8C—C9C	119.2 (14)
C1A—C6A—S7A	121.7 (11)	C13C—C8C—S7C	122.6 (11)
C5A—C6A—S7A	118.8 (13)	C9C—C8C—S7C	118.1 (11)
C6A—S7A—C8A	99.5 (7)	C10C—C9C—C8C	120.2 (16)
C9A—C8A—C13A	120.9 (15)	C10C—C9C—H9C	119.9
C9A—C8A—S7A	118.1 (12)	C8C—C9C—H9C	119.9
C13A—C8A—S7A	120.8 (12)	C11C—C10C—C9C	120.5 (16)
C8A—C9A—C10A	119.8 (15)	C11C—C10C—H10C	119.7
C8A—C9A—H9A	120.1	C9C—C10C—H10C	119.7
C10A—C9A—H9A	120.1	C10C—C11C—C12C	118.8 (15)
C11A—C10A—C9A	119.6 (14)	C10C—C11C—H11C	120.6
C11A—C10A—H10A	120.2	C12C—C11C—H11C	120.6
C9A—C10A—H10A	120.2	C13C—C12C—C11C	121.3 (16)
C10A—C11A—C12A	121.6 (14)	C13C—C12C—H12C	119.4
C10A—C11A—H11A	119.2	C11C—C12C—H12C	119.4
C12A—C11A—H11A	119.2	C12C—C13C—C8C	119.9 (14)
C11A—C12A—C13A	119.4 (14)	C12C—C13C—C14C	119.7 (14)

C11A—C12A—H12A	120.3	C8C—C13C—C14C	120.3 (13)
C13A—C12A—H12A	120.3	C15C—C14C—N16C	115.6 (13)
C8A—C13A—C12A	118.7 (14)	C15C—C14C—C13C	127.6 (14)
C8A—C13A—C14A	123.0 (13)	N16C—C14C—C13C	116.7 (13)
C12A—C13A—C14A	118.4 (13)	C14C—C15C—C1C	128.7 (14)
N16A—C14A—C15A	117.2 (14)	C14C—C15C—Se1C	108.9 (11)
N16A—C14A—C13A	117.5 (12)	C1C—C15C—Se1C	122.1 (10)
C15A—C14A—C13A	125.3 (14)	N17C—N16C—C14C	117.7 (13)
C14A—C15A—C1A	130.6 (15)	N16C—N17C—Se1C	110.0 (10)
C14A—C15A—Se1A	107.1 (11)	C15D—Se1D—N17D	90.6 (9)
C1A—C15A—Se1A	122.0 (10)	C14D—Se1E—N17E	92.9 (15)
N17A—N16A—C14A	116.8 (13)	C2D—C1D—C6D	117.9 (14)
N16A—N17A—Se1A	111.8 (11)	C2D—C1D—C15D	120.0 (13)
C15B—Se1B—N17B	87.6 (7)	C6D—C1D—C15D	122.0 (14)
C2B—C1B—C6B	116.8 (15)	C3D—C2D—C1D	121.5 (16)
C2B—C1B—C15B	120.6 (15)	C3D—C2D—H2D	119.2
C6B—C1B—C15B	122.6 (14)	C1D—C2D—H2D	119.2
C1B—C2B—C3B	122.1 (17)	C2D—C3D—C4D	119.8 (17)
C1B—C2B—H2B	119.0	C2D—C3D—H3D	120.1
C3B—C2B—H2B	119.0	C4D—C3D—H3D	120.1
C4B—C3B—C2B	120.8 (16)	C5D—C4D—C3D	120.0 (17)
C4B—C3B—H3B	119.6	C5D—C4D—H4D	120.0
C2B—C3B—H3B	119.6	C3D—C4D—H4D	120.0
C3B—C4B—C5B	119.1 (17)	C4D—C5D—C6D	122.0 (16)
C3B—C4B—H4B	120.5	C4D—C5D—H5D	119.0
C5B—C4B—H4B	120.5	C6D—C5D—H5D	119.0
C6B—C5B—C4B	119.8 (17)	C5D—C6D—C1D	118.7 (16)
C6B—C5B—H5B	120.1	C5D—C6D—S7D	121.2 (13)
C4B—C5B—H5B	120.1	C1D—C6D—S7D	119.9 (12)
C5B—C6B—C1B	121.4 (15)	C6D—S7D—C8D	99.4 (7)
C5B—C6B—S7B	117.7 (14)	C13D—C8D—C9D	121.8 (14)
C1B—C6B—S7B	120.8 (12)	C13D—C8D—S7D	118.9 (11)
C8B—S7B—C6B	100.5 (6)	C9D—C8D—S7D	119.2 (13)
C13B—C8B—C9B	122.0 (13)	C10D—C9D—C8D	118.6 (16)
C13B—C8B—S7B	121.7 (12)	C10D—C9D—H9D	120.7
C9B—C8B—S7B	116.2 (12)	C8D—C9D—H9D	120.7
C10B—C9B—C8B	116.7 (15)	C11D—C10D—C9D	119.9 (17)
C10B—C9B—H9B	121.7	C11D—C10D—H10D	120.0
C8B—C9B—H9B	121.7	C9D—C10D—H10D	120.0
C11B—C10B—C9B	121.0 (14)	C10D—C11D—C12D	123.7 (16)
C11B—C10B—H10B	119.5	C10D—C11D—H11D	118.2
C9B—C10B—H10B	119.5	C12D—C11D—H11D	118.2
C12B—C11B—C10B	119.7 (13)	C11D—C12D—C13D	118.2 (16)
C12B—C11B—H11B	120.1	C11D—C12D—H12D	120.9
C10B—C11B—H11B	120.1	C13D—C12D—H12D	120.9
C11B—C12B—C13B	121.7 (15)	C8D—C13D—C12D	117.6 (14)
C11B—C12B—H12B	119.2	C8D—C13D—C14D	123.3 (13)
C13B—C12B—H12B	119.2	C12D—C13D—C14D	119.1 (14)

C8B—C13B—C12B	118.9 (14)	C15D—C14D—N16D	114 (2)
C8B—C13B—C14B	122.0 (13)	C15D—C14D—C13D	127.1 (14)
C12B—C13B—C14B	119.1 (14)	N16D—C14D—C13D	118 (2)
N16B—C14B—C15B	116.6 (15)	C15D—C14D—Se1E	108.0 (11)
N16B—C14B—C13B	115.5 (12)	C13D—C14D—Se1E	124.9 (12)
C15B—C14B—C13B	127.7 (15)	C14D—C15D—N16E	115 (2)
C14B—C15B—C1B	128.4 (16)	C14D—C15D—C1D	127.1 (13)
C14B—C15B—Se1B	108.0 (12)	N16E—C15D—C1D	118 (2)
C1B—C15B—Se1B	123.5 (11)	C14D—C15D—Se1D	107.3 (11)
N17B—N16B—C14B	118.6 (13)	C1D—C15D—Se1D	125.4 (11)
N16B—N17B—Se1B	109.2 (11)	N17D—N16D—C14D	123 (4)
C15C—Se1C—N17C	87.7 (6)	N16D—N17D—Se1D	104 (3)
C2C—C1C—C6C	119.5 (13)	N17E—N16E—C15D	112 (3)
C2C—C1C—C15C	120.1 (13)	N16E—N17E—Se1E	112 (3)
C6C—C1C—C15C	120.3 (14)		

C6A—C1A—C2A—C3A	0 (2)	C15C—C1C—C6C—C5C	176.2 (13)
C15A—C1A—C2A—C3A	−179.8 (14)	C2C—C1C—C6C—S7C	178.2 (11)
C1A—C2A—C3A—C4A	1 (2)	C15C—C1C—C6C—S7C	−4.6 (18)
C2A—C3A—C4A—C5A	−1 (2)	C4C—C5C—C6C—C1C	0 (2)
C3A—C4A—C5A—C6A	1 (3)	C4C—C5C—C6C—S7C	−178.9 (12)
C2A—C1A—C6A—C5A	0 (2)	C1C—C6C—S7C—C8C	67.0 (12)
C15A—C1A—C6A—C5A	179.7 (14)	C5C—C6C—S7C—C8C	−113.8 (12)
C2A—C1A—C6A—S7A	177.5 (11)	C6C—S7C—C8C—C13C	−67.5 (15)
C15A—C1A—C6A—S7A	−3 (2)	C6C—S7C—C8C—C9C	115.2 (14)
C4A—C5A—C6A—C1A	0 (2)	C13C—C8C—C9C—C10C	−3 (3)
C4A—C5A—C6A—S7A	−178.0 (12)	S7C—C8C—C9C—C10C	174.8 (14)
C1A—C6A—S7A—C8A	65.1 (14)	C8C—C9C—C10C—C11C	3 (3)
C5A—C6A—S7A—C8A	−117.4 (13)	C9C—C10C—C11C—C12C	−3 (3)
C6A—S7A—C8A—C9A	119.9 (12)	C10C—C11C—C12C—C13C	2 (3)
C6A—S7A—C8A—C13A	−66.5 (13)	C11C—C12C—C13C—C8C	−1 (2)
C13A—C8A—C9A—C10A	1 (2)	C11C—C12C—C13C—C14C	177.8 (15)
S7A—C8A—C9A—C10A	175.0 (11)	C9C—C8C—C13C—C12C	1 (2)
C8A—C9A—C10A—C11A	−3 (2)	S7C—C8C—C13C—C12C	−175.8 (13)
C9A—C10A—C11A—C12A	4 (2)	C9C—C8C—C13C—C14C	−177.3 (15)
C10A—C11A—C12A—C13A	−3 (2)	S7C—C8C—C13C—C14C	5 (2)
C9A—C8A—C13A—C12A	−1 (2)	C12C—C13C—C14C—C15C	−138.0 (16)
S7A—C8A—C13A—C12A	−174.2 (11)	C8C—C13C—C14C—C15C	41 (2)
C9A—C8A—C13A—C14A	177.7 (13)	C12C—C13C—C14C—N16C	37 (2)
S7A—C8A—C13A—C14A	4.3 (19)	C8C—C13C—C14C—N16C	−144.7 (14)
C11A—C12A—C13A—C8A	2 (2)	N16C—C14C—C15C—C1C	−171.6 (14)
C11A—C12A—C13A—C14A	−176.9 (13)	C13C—C14C—C15C—C1C	3 (3)
C8A—C13A—C14A—N16A	−141.8 (14)	N16C—C14C—C15C—Se1C	1.8 (16)
C12A—C13A—C14A—N16A	36.7 (19)	C13C—C14C—C15C—Se1C	176.4 (12)
C8A—C13A—C14A—C15A	42 (2)	C2C—C1C—C15C—C14C	132.5 (17)
C12A—C13A—C14A—C15A	−139.5 (15)	C6C—C1C—C15C—C14C	−45 (2)
N16A—C14A—C15A—C1A	−174.6 (14)	C2C—C1C—C15C—Se1C	−40.2 (18)
C13A—C14A—C15A—C1A	2 (2)	C6C—C1C—C15C—Se1C	142.6 (12)

N16A—C14A—C15A—Se1A	−0.6 (16)
C13A—C14A—C15A—Se1A	175.5 (11)
C2A—C1A—C15A—C14A	135.4 (16)
C6A—C1A—C15A—C14A	−44 (2)
C2A—C1A—C15A—Se1A	−37.8 (19)
C6A—C1A—C15A—Se1A	142.5 (12)
N17A—Se1A—C15A—C14A	0.6 (10)
N17A—Se1A—C15A—C1A	175.3 (12)
C15A—C14A—N16A—N17A	0 (2)
C13A—C14A—N16A—N17A	−176.3 (13)
C14A—N16A—N17A—Se1A	0.4 (17)
C15A—Se1A—N17A—N16A	−0.6 (11)
C6B—C1B—C2B—C3B	1 (2)
C15B—C1B—C2B—C3B	−178.8 (15)
C1B—C2B—C3B—C4B	−2 (3)
C2B—C3B—C4B—C5B	1 (3)
C3B—C4B—C5B—C6B	2 (2)
C4B—C5B—C6B—C1B	−3 (2)
C4B—C5B—C6B—S7B	173.2 (12)
C2B—C1B—C6B—C5B	1 (2)
C15B—C1B—C6B—C5B	−179.0 (14)
C2B—C1B—C6B—S7B	−174.3 (11)
C15B—C1B—C6B—S7B	5 (2)
C5B—C6B—S7B—C8B	118.4 (12)
C1B—C6B—S7B—C8B	−65.9 (14)
C6B—S7B—C8B—C13B	63.7 (13)
C6B—S7B—C8B—C9B	−119.8 (12)
C13B—C8B—C9B—C10B	1 (2)
S7B—C8B—C9B—C10B	−175.0 (11)
C8B—C9B—C10B—C11B	−2 (2)
C9B—C10B—C11B—C12B	2 (2)
C10B—C11B—C12B—C13B	−1 (2)
C9B—C8B—C13B—C12B	0 (2)
S7B—C8B—C13B—C12B	176.1 (10)
C9B—C8B—C13B—C14B	−178.2 (13)
S7B—C8B—C13B—C14B	−1.9 (18)
C11B—C12B—C13B—C8B	0 (2)
C11B—C12B—C13B—C14B	177.9 (13)
C8B—C13B—C14B—N16B	141.3 (13)
C12B—C13B—C14B—N16B	−36.7 (18)
C8B—C13B—C14B—C15B	−44 (2)
C12B—C13B—C14B—C15B	138.5 (16)
N16B—C14B—C15B—C1B	175.8 (14)
C13B—C14B—C15B—C1B	1 (3)
N16B—C14B—C15B—Se1B	−1.0 (16)
C13B—C14B—C15B—Se1B	−176.1 (11)
C2B—C1B—C15B—C14B	−139.9 (16)
C6B—C1B—C15B—C14B	40 (2)
N17C—Se1C—C15C—C14C	−1.4 (11)
N17C—Se1C—C15C—C1C	172.5 (12)
C15C—C14C—N16C—N17C	−1 (2)
C13C—C14C—N16C—N17C	−176.5 (13)
C14C—N16C—N17C—Se1C	0.1 (16)
C15C—Se1C—N17C—N16C	0.8 (11)
C6D—C1D—C2D—C3D	1 (2)
C15D—C1D—C2D—C3D	177.6 (15)
C1D—C2D—C3D—C4D	0 (3)
C2D—C3D—C4D—C5D	0 (3)
C3D—C4D—C5D—C6D	0 (3)
C4D—C5D—C6D—C1D	1 (2)
C4D—C5D—C6D—S7D	176.6 (13)
C2D—C1D—C6D—C5D	−1 (2)
C15D—C1D—C6D—C5D	−178.0 (13)
C2D—C1D—C6D—S7D	−176.8 (11)
C15D—C1D—C6D—S7D	6 (2)
C5D—C6D—S7D—C8D	115.3 (13)
C1D—C6D—S7D—C8D	−69.0 (13)
C6D—S7D—C8D—C13D	64.6 (14)
C6D—S7D—C8D—C9D	−112.5 (14)
C13D—C8D—C9D—C10D	4 (3)
S7D—C8D—C9D—C10D	−179.2 (14)
C8D—C9D—C10D—C11D	−3 (3)
C9D—C10D—C11D—C12D	2 (3)
C10D—C11D—C12D—C13D	−2 (3)
C9D—C8D—C13D—C12D	−4 (2)
S7D—C8D—C13D—C12D	178.9 (12)
C9D—C8D—C13D—C14D	178.3 (15)
S7D—C8D—C13D—C14D	1 (2)
C11D—C12D—C13D—C8D	3 (2)
C11D—C12D—C13D—C14D	−179.0 (16)
C8D—C13D—C14D—C15D	−47 (2)
C12D—C13D—C14D—C15D	135.1 (17)
C8D—C13D—C14D—N16D	144 (3)
C12D—C13D—C14D—N16D	−33 (3)
C8D—C13D—C14D—Se1E	136.2 (15)
C12D—C13D—C14D—Se1E	−41 (2)
N17E—Se1E—C14D—C15D	−1.0 (19)
N17E—Se1E—C14D—C13D	176.0 (19)
C13D—C14D—C15D—N16E	−174 (2)
Se1E—C14D—C15D—N16E	3 (3)
N16D—C14D—C15D—C1D	170 (3)
C13D—C14D—C15D—C1D	1 (3)
Se1E—C14D—C15D—C1D	178.0 (13)
N16D—C14D—C15D—Se1D	−5 (3)
C13D—C14D—C15D—Se1D	−174.3 (13)
C2D—C1D—C15D—C14D	−135.1 (17)

C2B—C1B—C15B—Se1B	36 (2)	C6D—C1D—C15D—C14D	42 (2)
C6B—C1B—C15B—Se1B	−143.4 (12)	C2D—C1D—C15D—N16E	40 (3)
N17B—Se1B—C15B—C14B	0.7 (11)	C6D—C1D—C15D—N16E	−143 (2)
N17B—Se1B—C15B—C1B	−176.2 (13)	C2D—C1D—C15D—Se1D	39 (2)
C15B—C14B—N16B—N17B	1 (2)	C6D—C1D—C15D—Se1D	−143.6 (13)
C13B—C14B—N16B—N17B	176.5 (13)	N17D—Se1D—C15D—C14D	0.5 (13)
C14B—N16B—N17B—Se1B	0.0 (16)	N17D—Se1D—C15D—C1D	−175.0 (14)
C15B—Se1B—N17B—N16B	−0.4 (11)	C15D—C14D—N16D—N17D	12 (6)
C6C—C1C—C2C—C3C	0 (2)	C13D—C14D—N16D—N17D	−179 (4)
C15C—C1C—C2C—C3C	−177.3 (15)	C14D—N16D—N17D—Se1D	−10 (5)
C1C—C2C—C3C—C4C	2 (3)	C14D—C15D—N16E—N17E	−4 (5)
C2C—C3C—C4C—C5C	−2 (3)	C1D—C15D—N16E—N17E	−179 (3)
C3C—C4C—C5C—C6C	1 (2)	C15D—N16E—N17E—Se1E	3 (5)
C2C—C1C—C6C—C5C	−1 (2)	C14D—Se1E—N17E—N16E	−1 (4)