IUCrData

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3-Methyl-4,5,6,7,8,9-hexahydrocycloocteno-1,2,3-selenadiazolium iodide–trichloromethane (4/1)

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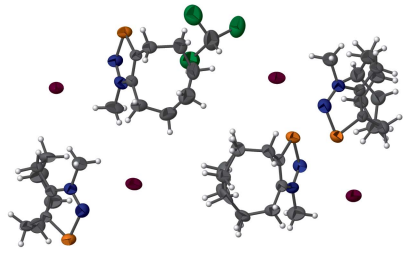
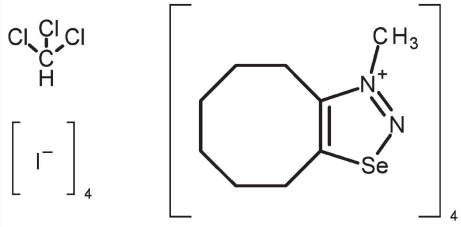
Structural data: full structural data are available from iucrdata.iucr.org

The title solvated salt, $4C_9H_{15}N_2Se^+\cdot 4I^-\cdot CHCl_3$, co-crystallizes with chloroform. The asymmetric unit contains four very similar ion pairs and one solvent molecule. In the crystal, layers of parallel chloroform-filled channels formed by two different ion pairs alternate with layers formed by the other two ion pairs. Disorder is observed for some C and H atoms in two of the cations with occupancy ratios of 0.68:0.32 and 0.62:0.38.

3D view



Chemical scheme



Structure description

1,2,3-Selenadiazoles are useful precursors for strained cycloalkynes (Bissinger *et al.*, 1988; Detert & Meier, 1997). Cycloocteno-1,2,3-selenadiazole, first prepared by Meier & Voigt (1972), reacts with iodomethane to yield the 3-methyl-substituted selenadiazolium iodide. Crystals with this cation have been obtained with a 2/1 mixture of iodide and triiodide anions (Schollmeyer & Detert, 2016). Here, the only anion is iodide, but the compound co-crystallizes with 1/4 chloroform molecules per ion pair. The molecular geometries of the cations reported here and in the previous article are nearly identical.

The asymmetric unit (Fig. 1) is composed of four slightly different ion pairs of the title compound and one chloroform molecule. The cations *A*, *B*, and *C* are very similar, differing from cation *D*. All cations adopt an L-type shape, but the conformation at C6—C7 of the hexamethylene tether is inverted in *D*. All heterocyclic rings are identical, with a maximum deviation of 0.02 Å at N2(*A*) from the mean plane.

In all ion pairs, the shortest distance between the iodide and the cation is to atom N2 of the selenadiazolium ring: N2*A*···I2 = 3.869 (9) Å, N2*B* ···I1= 3.287 (9) Å, N2*C*···I3 = 3.754 (8) Å and N2*D*···I4 = 3.768 (9) Å. Only N1*C* has a comparable distance to the next iodide: N1*C*···I3 = 3.784 (9) Å. The shortest spacing between iodide ions are I1···I4 = 6.042 (1) Å and I4···I4 = 5.940 (2) Å.

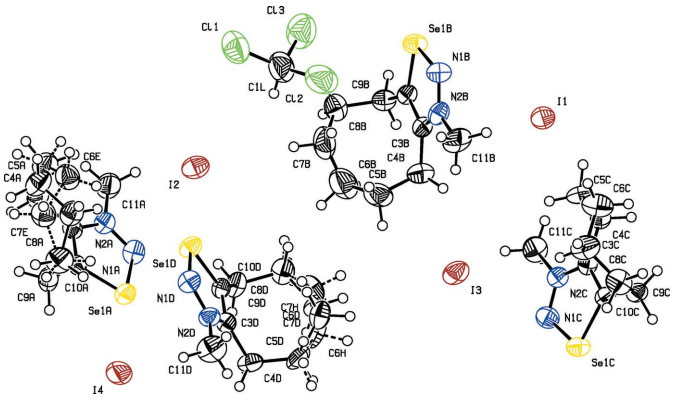


Figure 1
Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level.

The packing of the molecules is quite complex (Fig. 2). A channel along the *a*-axis direction is composed of two molecules each of *B* and *D*, connected *via* a center of symmetry. The channel is filled with chloroform molecules forming the spindle of a spiral stair. The steps are represented by alternating cations and iodide ions. These channels are arranged in layers parallel to the *b* axis. Along the *c* axis, layers of the channels alternate with layers of 'inverted' channels formed from two *A* and two *B* molecules.

Synthesis and crystallization

The title compound was prepared from cycloocteno-1,2,3-selenadiazole (Meier & Voigt, 1972) and methyl iodide as reported by us (Schollmeyer & Detert, 2016). Chromatographic purification followed by recrystallization from chloroform yielded brownish crystals with m.p. 471 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The s.o.f. for the disordered carbon atoms in molecules *A* and *D* were kept fixed, while the anisotropic displacement parameters were restrained using the RIGU instruction.

Table 1
Experimental details.

Crystal data	
Chemical formula	$4C_9H_{15}N_2Se^+\cdot 4I^-\cdot CHCl_3$
M_r	1547.73
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	295
a, b, c (Å)	10.5250 (9), 13.4368 (9), 20.112 (2)
α, β, γ (°)	71.141 (8), 89.472 (9), 76.460 (6)
V (Å^3)	2609.9 (4)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	23.62
Crystal size (mm)	0.56 × 0.32 × 0.12
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	Numerical (*PLATON*; Spek, 2009)
T_{min}, T_{max}	0.006, 0.202
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11193, 10589, 7331
R_{int}	0.067
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.623
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.067, 0.197, 1.05
No. of reflections	10589
No. of parameters	542
No. of restraints	75
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.84, −1.19

Computer programs: *CAD-4 Software* (Enraf–Nonius, 1989), *CORINC* (Dräger & Gattow, 1971), *SIR2004* (Burla *et al.*, 2005), *SHELXL2014* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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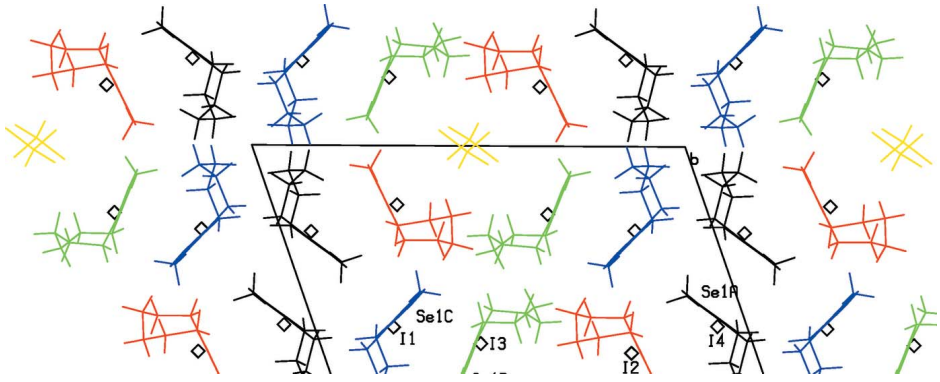

Figure 2
Partial packing diagram. View along (100). The symmetry-independent entities are drawn with different colours.

full crystallographic data

IUCrData (2017). **2**, x170167 [https://doi.org/10.1107/S2414314617001675]

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Crystal data

$4C_9H_{15}N_2Se^+·4I^-·CHCl_3$
M_r = 1547.73
Triclinic, $P\overline{1}$
a = 10.5250 (9) Å
b = 13.4368 (9) Å
c = 20.112 (2) Å
α = 71.141 (8)°
β = 89.472 (9)°
γ = 76.460 (6)°
V = 2609.9 (4) Å^3
Z = 2
F(000) = 1476
D_x = 1.969 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 25 reflections
θ = 24–38°
μ = 23.62 mm^{-1}
T = 295 K
Plate, yellow
0.56 × 0.32 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: Rotating anode
$\omega/2\theta$ scan
Absorption correction: numerical (PLATON; Spek, 2009)
T_{min} = 0.006, T_{max} = 0.202
11193 measured reflections
10589 independent reflections
7331 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 74.0°, θ_{min} = 2.3°
h = −13→0
k = −16→16
l = −25→25
3 standard reflections every 60 min

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.197
S = 1.05
10589 reflections
542 parameters
75 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1024P)^2 + 1.7825P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.84 e Å^{-3}
$\Delta\rho_{min}$ = −1.19 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00067 (6)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Se1A	0.54844 (11)	0.41276 (9)	0.09780 (5)	0.0497 (3)	
N1A	0.3841 (9)	0.4588 (7)	0.1214 (4)	0.0498 (19)	
N2A	0.3060 (8)	0.4144 (6)	0.0971 (4)	0.0413 (16)	
C3A	0.3520 (9)	0.3509 (8)	0.0564 (4)	0.041 (2)	
C4A	0.2640 (10)	0.3023 (9)	0.0257 (5)	0.049 (2)	
H4A1	0.2911	0.3032	−0.0207	0.059*	
H4A2	0.1756	0.3476	0.0197	0.059*	
C5A	0.2616 (13)	0.1887 (10)	0.0683 (6)	0.064 (3)	
H5A1	0.1849	0.1724	0.0521	0.077*	0.68
H5A2	0.2523	0.1847	0.1171	0.077*	0.68
H5A3	0.1943	0.1935	0.1012	0.077*	0.32
H5A4	0.2325	0.1565	0.0363	0.077*	0.32
C6A	0.3899 (19)	0.0961 (15)	0.0651 (11)	0.066 (4)	0.68
H6A1	0.3706	0.0258	0.0852	0.079*	0.68
H6A2	0.4059	0.1062	0.0160	0.079*	0.68
C7A	0.5121 (18)	0.0950 (15)	0.1022 (9)	0.059 (3)	0.68
H7A1	0.5565	0.0202	0.1276	0.070*	0.68
H7A2	0.4882	0.1310	0.1369	0.070*	0.68
C6E	0.380 (4)	0.111 (3)	0.1092 (19)	0.063 (7)	0.32
H6E1	0.3594	0.0423	0.1336	0.075*	0.32
H6E2	0.4082	0.1382	0.1443	0.075*	0.32
C7E	0.496 (4)	0.092 (3)	0.060 (2)	0.063 (6)	0.32
H7E1	0.5348	0.0150	0.0754	0.075*	0.32
H7E2	0.4565	0.1127	0.0130	0.075*	0.32
C8A	0.6081 (13)	0.1486 (10)	0.0553 (7)	0.066 (3)	
H8A1	0.6366	0.1084	0.0233	0.079*	0.68
H8A2	0.6846	0.1403	0.0850	0.079*	0.68
H8A3	0.6803	0.1138	0.0338	0.079*	0.32
H8A4	0.6393	0.1418	0.1022	0.079*	0.32
C9A	0.5614 (11)	0.2692 (10)	0.0110 (5)	0.055 (2)	
H9A1	0.6373	0.2972	−0.0050	0.066*	
H9A2	0.5089	0.2758	−0.0303	0.066*	
C10A	0.4826 (9)	0.3370 (8)	0.0500 (4)	0.0400 (19)	
C11A	0.1701 (12)	0.4392 (11)	0.1149 (6)	0.068 (3)	
H11A	0.1204	0.4031	0.0948	0.102*	
H11B	0.1668	0.4147	0.1652	0.102*	
H11C	0.1337	0.5161	0.0964	0.102*	
Se1B	0.17468 (11)	0.16520 (9)	0.68091 (5)	0.0477 (3)	
N1B	0.3405 (9)	0.0958 (7)	0.7154 (4)	0.051 (2)	

N2B	0.4185 (8)	0.1591 (7)	0.6874 (4)	0.0462 (18)
C3B	0.3660 (10)	0.2609 (8)	0.6410 (4)	0.043 (2)
C4B	0.4498 (12)	0.3365 (10)	0.6062 (6)	0.059 (3)
H4B1	0.5291	0.3182	0.6363	0.070*
H4B2	0.4032	0.4098	0.6022	0.070*
C5B	0.4881 (13)	0.3346 (13)	0.5336 (7)	0.078 (4)
H5B1	0.5613	0.3679	0.5213	0.093*
H5B2	0.5173	0.2598	0.5351	0.093*
C6B	0.3785 (16)	0.3924 (16)	0.4771 (8)	0.101 (5)
H6B1	0.3359	0.4608	0.4834	0.121*
H6B2	0.4162	0.4093	0.4318	0.121*
C7B	0.2812 (15)	0.3357 (16)	0.4748 (7)	0.093 (4)
H7B1	0.3170	0.2599	0.5017	0.112*
H7B2	0.2667	0.3401	0.4263	0.112*
C8B	0.1477 (12)	0.3714 (9)	0.5016 (5)	0.059 (3)
H8B1	0.0968	0.3196	0.5021	0.071*
H8B2	0.1020	0.4410	0.4686	0.071*
C9B	0.1529 (10)	0.3816 (8)	0.5757 (5)	0.047 (2)
H9B1	0.1888	0.4427	0.5736	0.057*
H9B2	0.0645	0.3960	0.5907	0.057*
C10B	0.2340 (9)	0.2818 (7)	0.6286 (4)	0.0366 (18)
C11B	0.5560 (11)	0.1129 (10)	0.7106 (7)	0.068 (3)
H11D	0.6057	0.1643	0.6876	0.102*
H11E	0.5671	0.0958	0.7607	0.102*
H11F	0.5862	0.0480	0.6987	0.102*
Se1C	1.06674 (11)	0.40224 (9)	0.75799 (5)	0.0477 (3)
N1C	0.9037 (9)	0.4587 (7)	0.7156 (4)	0.051 (2)
N2C	0.8211 (8)	0.4127 (6)	0.7556 (4)	0.0405 (16)
C3C	0.8670 (9)	0.3333 (7)	0.8188 (4)	0.0398 (19)
C4C	0.7769 (10)	0.2783 (9)	0.8665 (5)	0.049 (2)
H4C1	0.6886	0.3243	0.8548	0.059*
H4C2	0.8020	0.2705	0.9146	0.059*
C5C	0.7763 (11)	0.1681 (10)	0.8627 (6)	0.062 (3)
H5C1	0.7685	0.1739	0.8135	0.074*
H5C2	0.6990	0.1479	0.8840	0.074*
C6C	0.9014 (14)	0.0730 (10)	0.9001 (7)	0.074 (4)
H6C1	0.9179	0.0754	0.9469	0.089*
H6C2	0.8805	0.0043	0.9057	0.089*
C7C	1.0242 (13)	0.0753 (10)	0.8632 (7)	0.068 (3)
H7C1	1.0012	0.1186	0.8140	0.082*
H7C2	1.0661	0.0020	0.8649	0.082*
C8C	1.1226 (12)	0.1195 (9)	0.8919 (6)	0.060 (3)
H8C1	1.1966	0.1184	0.8629	0.072*
H8C2	1.1543	0.0699	0.9389	0.072*
C9C	1.0774 (9)	0.2327 (8)	0.8965 (5)	0.044 (2)
H9C1	1.0258	0.2293	0.9370	0.052*
H9C2	1.1539	0.2572	0.9043	0.052*
C10C	0.9986 (9)	0.3137 (7)	0.8333 (4)	0.0361 (17)

C11C	0.6841 (11)	0.4514 (10)	0.7276 (6)	0.061 (3)	
H11G	0.6312	0.4131	0.7605	0.091*	
H11H	0.6549	0.5277	0.7204	0.091*	
H11I	0.6764	0.4391	0.6836	0.091*	
Se1D	0.66986 (10)	0.14268 (8)	0.25878 (5)	0.0452 (2)	
N1D	0.8346 (8)	0.0743 (6)	0.2528 (4)	0.0435 (17)	
N2D	0.9146 (8)	0.1331 (7)	0.2587 (4)	0.0432 (17)	
C3D	0.8657 (9)	0.2298 (7)	0.2662 (4)	0.0384 (18)	
C4D	0.9528 (11)	0.3008 (9)	0.2740 (6)	0.052 (2)	
H4D1	0.9076	0.3763	0.2519	0.062*	
H4D2	1.0317	0.2864	0.2498	0.062*	
C5D	0.9904 (12)	0.2806 (12)	0.3512 (7)	0.067 (3)	
H5D1	1.0236	0.3410	0.3535	0.081*	0.62
H5D2	1.0624	0.2163	0.3670	0.081*	0.62
H5D3	1.0703	0.3030	0.3555	0.081*	0.38
H5D4	1.0045	0.2042	0.3782	0.081*	0.38
C6D	0.883 (2)	0.2653 (18)	0.4049 (9)	0.062 (5)	0.62
H6D1	0.9210	0.2512	0.4518	0.075*	0.62
H6D2	0.8509	0.2032	0.4052	0.075*	0.62
C7D	0.7664 (18)	0.3690 (15)	0.3851 (9)	0.047 (4)	0.62
H7D1	0.7456	0.3883	0.4271	0.057*	0.62
H7D2	0.7943	0.4285	0.3515	0.057*	0.62
C6H	0.869 (4)	0.352 (3)	0.3793 (16)	0.065 (9)	0.38
H6H1	0.9011	0.3678	0.4189	0.079*	0.38
H6H2	0.8340	0.4202	0.3422	0.079*	0.38
C7H	0.768 (3)	0.297 (3)	0.4005 (13)	0.054 (7)	0.38
H7H1	0.7507	0.2921	0.4488	0.065*	0.38
H7H2	0.7962	0.2241	0.3987	0.065*	0.38
C8D	0.6420 (12)	0.3557 (10)	0.3536 (6)	0.057 (3)	
H8D1	0.5691	0.4140	0.3556	0.069*	0.62
H8D2	0.6240	0.2879	0.3826	0.069*	0.62
H8D3	0.6182	0.4302	0.3530	0.069*	0.38
H8D4	0.5726	0.3221	0.3745	0.069*	0.38
C9D	0.6486 (10)	0.3562 (8)	0.2772 (5)	0.047 (2)	
H9D1	0.5604	0.3675	0.2577	0.056*	
H9D2	0.6826	0.4170	0.2499	0.056*	
C10D	0.7316 (9)	0.2549 (7)	0.2693 (4)	0.0355 (17)	
C11D	1.0563 (12)	0.0861 (11)	0.2558 (8)	0.070 (3)	
H11J	1.1058	0.1353	0.2606	0.105*	
H11K	1.0838	0.0182	0.2934	0.105*	
H11L	1.0708	0.0743	0.2115	0.105*	
I1	0.38141 (7)	0.31708 (7)	0.81714 (4)	0.0639 (2)	
I2	0.35417 (7)	0.22279 (7)	0.28803 (4)	0.0632 (2)	
I3	0.85843 (7)	0.25666 (7)	0.62885 (4)	0.0628 (2)	
I4	0.86700 (8)	0.32453 (9)	0.06828 (4)	0.0809 (3)	
C1L	0.2649 (18)	0.0221 (13)	0.4924 (7)	0.089 (5)	
H1L	0.2917	0.0844	0.4598	0.107*	
Cl1	0.2328 (5)	−0.0580 (3)	0.44457 (19)	0.0949 (12)	

Cl2	0.3942 (5)	−0.0512 (5)	0.5587 (2)	0.1172 (17)
Cl3	0.1264 (5)	0.0702 (4)	0.5302 (3)	0.1084 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1A	0.0442 (6)	0.0586 (6)	0.0464 (5)	−0.0179 (5)	−0.0026 (4)	−0.0135 (4)
N1A	0.049 (5)	0.045 (4)	0.053 (4)	−0.003 (4)	−0.002 (4)	−0.019 (3)
N2A	0.034 (4)	0.039 (4)	0.049 (4)	−0.001 (3)	−0.001 (3)	−0.017 (3)
C3A	0.036 (5)	0.048 (5)	0.035 (3)	−0.007 (4)	0.001 (3)	−0.008 (3)
C4A	0.031 (5)	0.063 (5)	0.056 (5)	−0.007 (4)	−0.001 (4)	−0.025 (4)
C5A	0.051 (6)	0.072 (6)	0.072 (6)	−0.012 (4)	0.004 (4)	−0.028 (5)
C6A	0.054 (7)	0.068 (8)	0.088 (10)	−0.013 (6)	0.000 (6)	−0.043 (7)
C7A	0.048 (7)	0.064 (8)	0.065 (7)	−0.007 (6)	0.000 (5)	−0.029 (6)
C6E	0.054 (9)	0.074 (12)	0.059 (10)	−0.008 (7)	0.008 (7)	−0.025 (8)
C7E	0.056 (9)	0.069 (11)	0.064 (14)	−0.009 (8)	0.009 (9)	−0.028 (10)
C8A	0.047 (6)	0.068 (6)	0.084 (6)	−0.001 (5)	0.010 (5)	−0.036 (5)
C9A	0.042 (6)	0.078 (6)	0.050 (4)	−0.008 (5)	0.001 (4)	−0.033 (4)
C10A	0.034 (5)	0.052 (5)	0.034 (3)	−0.008 (4)	0.004 (3)	−0.017 (3)
C11A	0.045 (7)	0.095 (9)	0.072 (7)	−0.012 (6)	0.006 (5)	−0.041 (7)
Se1B	0.0339 (6)	0.0460 (6)	0.0570 (5)	−0.0073 (4)	0.0049 (4)	−0.0105 (4)
N1B	0.044 (5)	0.048 (5)	0.060 (4)	−0.015 (4)	0.008 (4)	−0.014 (4)
N2B	0.039 (5)	0.047 (4)	0.052 (4)	−0.004 (4)	−0.008 (3)	−0.019 (3)
C3B	0.039 (5)	0.048 (5)	0.043 (4)	−0.012 (4)	0.000 (3)	−0.016 (4)
C4B	0.043 (6)	0.058 (6)	0.073 (5)	−0.018 (5)	0.007 (4)	−0.016 (5)
C5B	0.044 (6)	0.106 (10)	0.073 (5)	−0.016 (6)	0.012 (4)	−0.016 (6)
C6B	0.062 (7)	0.153 (12)	0.070 (6)	−0.010 (7)	0.006 (5)	−0.026 (7)
C7B	0.067 (7)	0.158 (13)	0.068 (6)	−0.011 (7)	0.009 (5)	−0.066 (8)
C8B	0.057 (6)	0.056 (6)	0.049 (4)	0.002 (5)	−0.006 (4)	−0.009 (4)
C9B	0.038 (5)	0.043 (5)	0.057 (4)	−0.005 (4)	0.004 (4)	−0.014 (4)
C10B	0.028 (4)	0.037 (4)	0.044 (4)	−0.002 (4)	0.000 (3)	−0.016 (3)
C11B	0.031 (6)	0.072 (8)	0.083 (7)	−0.002 (5)	−0.016 (5)	−0.010 (6)
Se1C	0.0382 (6)	0.0469 (6)	0.0551 (5)	−0.0129 (5)	0.0058 (4)	−0.0111 (4)
N1C	0.055 (6)	0.043 (4)	0.050 (4)	−0.013 (4)	0.006 (4)	−0.010 (3)
N2C	0.033 (4)	0.039 (4)	0.047 (3)	−0.003 (3)	0.001 (3)	−0.015 (3)
C3C	0.030 (5)	0.045 (5)	0.044 (4)	0.001 (4)	−0.001 (3)	−0.020 (4)
C4C	0.028 (5)	0.073 (7)	0.049 (4)	−0.010 (5)	0.005 (4)	−0.027 (5)
C5C	0.040 (6)	0.081 (8)	0.073 (6)	−0.033 (6)	0.011 (5)	−0.025 (6)
C6C	0.068 (9)	0.061 (7)	0.088 (8)	−0.020 (7)	0.020 (7)	−0.015 (6)
C7C	0.054 (8)	0.061 (7)	0.095 (8)	−0.012 (6)	0.014 (6)	−0.036 (6)
C8C	0.049 (7)	0.053 (6)	0.059 (5)	0.004 (5)	−0.004 (5)	−0.004 (5)
C9C	0.028 (5)	0.053 (5)	0.047 (4)	−0.009 (4)	−0.001 (3)	−0.012 (4)
C10C	0.031 (5)	0.038 (4)	0.043 (4)	−0.008 (4)	0.004 (3)	−0.020 (3)
C11C	0.035 (6)	0.074 (7)	0.061 (5)	0.005 (5)	−0.006 (4)	−0.018 (5)
Se1D	0.0334 (5)	0.0458 (5)	0.0609 (5)	−0.0070 (4)	0.0001 (4)	−0.0252 (4)
N1D	0.043 (5)	0.032 (4)	0.057 (4)	−0.003 (3)	0.003 (3)	−0.021 (3)
N2D	0.033 (4)	0.050 (4)	0.051 (4)	−0.011 (4)	0.008 (3)	−0.022 (3)
C3D	0.037 (5)	0.037 (4)	0.041 (4)	−0.006 (4)	0.004 (3)	−0.016 (3)

C4D	0.044 (6)	0.049 (6)	0.071 (6)	−0.021 (5)	0.014 (5)	−0.026 (5)
C5D	0.048 (7)	0.100 (10)	0.085 (7)	−0.036 (7)	0.008 (6)	−0.060 (7)
C6D	0.061 (13)	0.068 (13)	0.055 (9)	−0.006 (10)	−0.016 (8)	−0.023 (9)
C7D	0.044 (11)	0.042 (10)	0.070 (9)	−0.014 (8)	0.007 (7)	−0.034 (8)
C6H	0.07 (2)	0.08 (2)	0.063 (16)	−0.022 (19)	−0.026 (16)	−0.039 (17)
C7H	0.07 (2)	0.039 (15)	0.047 (12)	0.003 (15)	0.019 (13)	−0.022 (11)
C8D	0.045 (6)	0.063 (7)	0.065 (6)	0.003 (5)	0.004 (5)	−0.034 (5)
C9D	0.035 (5)	0.047 (5)	0.056 (5)	0.008 (4)	−0.010 (4)	−0.025 (4)
C10D	0.038 (5)	0.032 (4)	0.038 (3)	−0.006 (4)	0.001 (3)	−0.015 (3)
C11D	0.046 (7)	0.066 (8)	0.100 (9)	0.002 (6)	0.011 (6)	−0.041 (7)
I1	0.0370 (4)	0.0961 (6)	0.0605 (4)	−0.0179 (4)	0.0050 (3)	−0.0273 (4)
I2	0.0343 (4)	0.0734 (5)	0.0798 (4)	−0.0090 (3)	0.0032 (3)	−0.0255 (4)
I3	0.0353 (4)	0.0766 (5)	0.0836 (5)	−0.0098 (3)	0.0041 (3)	−0.0386 (4)
I4	0.0440 (5)	0.1349 (9)	0.0612 (4)	−0.0310 (5)	0.0053 (3)	−0.0222 (5)
C1L	0.122 (15)	0.086 (10)	0.058 (6)	−0.036 (10)	0.003 (7)	−0.013 (6)
Cl1	0.128 (4)	0.088 (2)	0.0743 (18)	−0.027 (2)	0.020 (2)	−0.0343 (18)
Cl2	0.091 (3)	0.159 (4)	0.079 (2)	−0.044 (3)	−0.001 (2)	0.002 (2)
Cl3	0.107 (4)	0.124 (4)	0.112 (3)	−0.021 (3)	0.008 (3)	−0.067 (3)

Geometric parameters (Å, º)

Se1A—N1A	1.809 (10)	N1C—N2C	1.305 (11)
Se1A—C10A	1.849 (9)	N2C—C3C	1.371 (11)
N1A—N2A	1.302 (11)	N2C—C11C	1.463 (12)
N2A—C3A	1.372 (12)	C3C—C10C	1.363 (12)
N2A—C11A	1.459 (14)	C3C—C4C	1.490 (13)
C3A—C10A	1.354 (13)	C4C—C5C	1.509 (16)
C3A—C4A	1.489 (13)	C4C—H4C1	0.9700
C4A—C5A	1.496 (16)	C4C—H4C2	0.9700
C4A—H4A1	0.9700	C5C—C6C	1.594 (18)
C4A—H4A2	0.9700	C5C—H5C1	0.9700
C5A—C6E	1.47 (4)	C5C—H5C2	0.9700
C5A—C6A	1.62 (2)	C6C—C7C	1.486 (18)
C5A—H5A1	0.9700	C6C—H6C1	0.9700
C5A—H5A2	0.9700	C6C—H6C2	0.9700
C5A—H5A3	0.9700	C7C—C8C	1.510 (17)
C5A—H5A4	0.9700	C7C—H7C1	0.9700
C6A—C7A	1.49 (2)	C7C—H7C2	0.9700
C6A—H6A1	0.9700	C8C—C9C	1.517 (15)
C6A—H6A2	0.9700	C8C—H8C1	0.9700
C7A—C8A	1.52 (2)	C8C—H8C2	0.9700
C7A—H7A1	0.9700	C9C—C10C	1.480 (11)
C7A—H7A2	0.9700	C9C—H9C1	0.9700
C6E—C7E	1.58 (5)	C9C—H9C2	0.9700
C6E—H6E1	0.9700	C11C—H11G	0.9600
C6E—H6E2	0.9700	C11C—H11H	0.9600
C7E—C8A	1.53 (4)	C11C—H11I	0.9600
C7E—H7E1	0.9700	Se1D—N1D	1.785 (8)

C7E—H7E2	0.9700	Se1D—C10D	1.846 (8)
C8A—C9A	1.537 (16)	N1D—N2D	1.313 (11)
C8A—H8A1	0.9700	N2D—C3D	1.337 (12)
C8A—H8A2	0.9700	N2D—C11D	1.485 (14)
C8A—H8A3	0.9700	C3D—C10D	1.378 (13)
C8A—H8A4	0.9700	C3D—C4D	1.511 (13)
C9A—C10A	1.492 (13)	C4D—C5D	1.527 (15)
C9A—H9A1	0.9700	C4D—H4D1	0.9700
C9A—H9A2	0.9700	C4D—H4D2	0.9700
C11A—H11A	0.9600	C5D—C6D	1.56 (2)
C11A—H11B	0.9600	C5D—C6H	1.62 (4)
C11A—H11C	0.9600	C5D—H5D1	0.9700
Se1B—N1B	1.799 (9)	C5D—H5D2	0.9700
Se1B—C10B	1.826 (9)	C5D—H5D3	0.9700
N1B—N2B	1.312 (12)	C5D—H5D4	0.9700
N2B—C3B	1.370 (12)	C6D—C7D	1.57 (3)
N2B—C11B	1.450 (12)	C6D—H6D1	0.9700
C3B—C10B	1.360 (13)	C6D—H6D2	0.9700
C3B—C4B	1.500 (14)	C7D—C8D	1.53 (2)
C4B—C5B	1.518 (17)	C7D—H7D1	0.9700
C4B—H4B1	0.9700	C7D—H7D2	0.9700
C4B—H4B2	0.9700	C6H—C7H	1.42 (5)
C5B—C6B	1.502 (19)	C6H—H6H1	0.9700
C5B—H5B1	0.9700	C6H—H6H2	0.9700
C5B—H5B2	0.9700	C7H—C8D	1.52 (3)
C6B—C7B	1.42 (2)	C7H—H7H1	0.9700
C6B—H6B1	0.9700	C7H—H7H2	0.9700
C6B—H6B2	0.9700	C8D—C9D	1.535 (13)
C7B—C8B	1.527 (18)	C8D—H8D1	0.9700
C7B—H7B1	0.9700	C8D—H8D2	0.9700
C7B—H7B2	0.9700	C8D—H8D3	0.9700
C8B—C9B	1.544 (14)	C8D—H8D4	0.9700
C8B—H8B1	0.9700	C9D—C10D	1.491 (12)
C8B—H8B2	0.9700	C9D—H9D1	0.9700
C9B—C10B	1.489 (12)	C9D—H9D2	0.9700
C9B—H9B1	0.9700	C11D—H11J	0.9600
C9B—H9B2	0.9700	C11D—H11K	0.9600
C11B—H11D	0.9600	C11D—H11L	0.9600
C11B—H11E	0.9600	C1L—Cl3	1.726 (18)
C11B—H11F	0.9600	C1L—Cl1	1.744 (16)
Se1C—N1C	1.802 (9)	C1L—Cl2	1.777 (16)
Se1C—C10C	1.854 (9)	C1L—H1L	0.9800

N1A—Se1A—C10A	88.5 (4)	N1C—N2C—C11C	115.5 (8)
N2A—N1A—Se1A	108.8 (7)	C3C—N2C—C11C	125.3 (8)
N1A—N2A—C3A	120.4 (8)	C10C—C3C—N2C	113.8 (8)
N1A—N2A—C11A	115.5 (9)	C10C—C3C—C4C	124.9 (8)
C3A—N2A—C11A	124.0 (9)	N2C—C3C—C4C	121.3 (8)

C10A—C3A—N2A	112.4 (8)	C3C—C4C—C5C	114.0 (9)
C10A—C3A—C4A	125.9 (9)	C3C—C4C—H4C1	108.7
N2A—C3A—C4A	121.7 (9)	C5C—C4C—H4C1	108.7
C3A—C4A—C5A	115.0 (8)	C3C—C4C—H4C2	108.7
C3A—C4A—H4A1	108.5	C5C—C4C—H4C2	108.7
C5A—C4A—H4A1	108.5	H4C1—C4C—H4C2	107.6
C3A—C4A—H4A2	108.5	C4C—C5C—C6C	115.7 (10)
C5A—C4A—H4A2	108.5	C4C—C5C—H5C1	108.4
H4A1—C4A—H4A2	107.5	C6C—C5C—H5C1	108.4
C6E—C5A—C4A	121 (2)	C4C—C5C—H5C2	108.4
C4A—C5A—C6A	115.1 (12)	C6C—C5C—H5C2	108.4
C4A—C5A—H5A1	108.5	H5C1—C5C—H5C2	107.4
C6A—C5A—H5A1	108.5	C7C—C6C—C5C	116.1 (11)
C4A—C5A—H5A2	108.5	C7C—C6C—H6C1	108.3
C6A—C5A—H5A2	108.5	C5C—C6C—H6C1	108.3
H5A1—C5A—H5A2	107.5	C7C—C6C—H6C2	108.3
C6E—C5A—H5A3	107.0	C5C—C6C—H6C2	108.3
C4A—C5A—H5A3	107.0	H6C1—C6C—H6C2	107.4
C6E—C5A—H5A4	107.0	C6C—C7C—C8C	115.8 (12)
C4A—C5A—H5A4	107.0	C6C—C7C—H7C1	108.3
H5A3—C5A—H5A4	106.8	C8C—C7C—H7C1	108.3
C7A—C6A—C5A	115.4 (14)	C6C—C7C—H7C2	108.3
C7A—C6A—H6A1	108.4	C8C—C7C—H7C2	108.3
C5A—C6A—H6A1	108.4	H7C1—C7C—H7C2	107.4
C7A—C6A—H6A2	108.4	C7C—C8C—C9C	117.8 (10)
C5A—C6A—H6A2	108.4	C7C—C8C—H8C1	107.9
H6A1—C6A—H6A2	107.5	C9C—C8C—H8C1	107.9
C6A—C7A—C8A	115.4 (16)	C7C—C8C—H8C2	107.9
C6A—C7A—H7A1	108.4	C9C—C8C—H8C2	107.9
C8A—C7A—H7A1	108.4	H8C1—C8C—H8C2	107.2
C6A—C7A—H7A2	108.4	C10C—C9C—C8C	114.4 (8)
C8A—C7A—H7A2	108.4	C10C—C9C—H9C1	108.7
H7A1—C7A—H7A2	107.5	C8C—C9C—H9C1	108.7
C5A—C6E—C7E	112 (3)	C10C—C9C—H9C2	108.7
C5A—C6E—H6E1	109.3	C8C—C9C—H9C2	108.7
C7E—C6E—H6E1	109.3	H9C1—C9C—H9C2	107.6
C5A—C6E—H6E2	109.3	C3C—C10C—C9C	126.8 (8)
C7E—C6E—H6E2	109.3	C3C—C10C—Se1C	108.5 (6)
H6E1—C6E—H6E2	107.9	C9C—C10C—Se1C	124.6 (7)
C8A—C7E—C6E	121 (3)	N2C—C11C—H11G	109.5
C8A—C7E—H7E1	107.0	N2C—C11C—H11H	109.5
C6E—C7E—H7E1	107.0	H11G—C11C—H11H	109.5
C8A—C7E—H7E2	107.0	N2C—C11C—H11I	109.5
C6E—C7E—H7E2	107.0	H11G—C11C—H11I	109.5
H7E1—C7E—H7E2	106.8	H11H—C11C—H11I	109.5
C7A—C8A—C9A	118.2 (11)	N1D—Se1D—C10D	88.8 (4)
C7E—C8A—C9A	110.3 (18)	N2D—N1D—Se1D	109.8 (6)
C7A—C8A—H8A1	107.8	N1D—N2D—C3D	119.3 (8)

C9A—C8A—H8A1	107.8	N1D—N2D—C11D	116.3 (9)
C7A—C8A—H8A2	107.8	C3D—N2D—C11D	124.4 (9)
C9A—C8A—H8A2	107.8	N2D—C3D—C10D	113.9 (8)
H8A1—C8A—H8A2	107.1	N2D—C3D—C4D	121.8 (9)
C7E—C8A—H8A3	109.6	C10D—C3D—C4D	124.2 (9)
C9A—C8A—H8A3	109.6	C3D—C4D—C5D	111.7 (9)
C7E—C8A—H8A4	109.6	C3D—C4D—H4D1	109.3
C9A—C8A—H8A4	109.6	C5D—C4D—H4D1	109.3
H8A3—C8A—H8A4	108.1	C3D—C4D—H4D2	109.3
C10A—C9A—C8A	113.6 (9)	C5D—C4D—H4D2	109.3
C10A—C9A—H9A1	108.8	H4D1—C4D—H4D2	107.9
C8A—C9A—H9A1	108.8	C4D—C5D—C6D	118.3 (11)
C10A—C9A—H9A2	108.8	C4D—C5D—C6H	106.4 (13)
C8A—C9A—H9A2	108.8	C4D—C5D—H5D1	107.7
H9A1—C9A—H9A2	107.7	C6D—C5D—H5D1	107.7
C3A—C10A—C9A	124.9 (9)	C4D—C5D—H5D2	107.7
C3A—C10A—Se1A	109.8 (7)	C6D—C5D—H5D2	107.7
C9A—C10A—Se1A	125.3 (7)	H5D1—C5D—H5D2	107.1
N2A—C11A—H11A	109.5	C4D—C5D—H5D3	110.5
N2A—C11A—H11B	109.5	C6H—C5D—H5D3	110.5
H11A—C11A—H11B	109.5	C4D—C5D—H5D4	110.5
N2A—C11A—H11C	109.5	C6H—C5D—H5D4	110.5
H11A—C11A—H11C	109.5	H5D3—C5D—H5D4	108.6
H11B—C11A—H11C	109.5	C5D—C6D—C7D	110.8 (16)
N1B—Se1B—C10B	89.0 (4)	C5D—C6D—H6D1	109.5
N2B—N1B—Se1B	109.2 (6)	C7D—C6D—H6D1	109.5
N1B—N2B—C3B	119.2 (9)	C5D—C6D—H6D2	109.5
N1B—N2B—C11B	115.0 (9)	C7D—C6D—H6D2	109.5
C3B—N2B—C11B	125.8 (9)	H6D1—C6D—H6D2	108.1
C10B—C3B—N2B	112.8 (8)	C8D—C7D—C6D	114.3 (14)
C10B—C3B—C4B	125.2 (9)	C8D—C7D—H7D1	108.7
N2B—C3B—C4B	121.9 (9)	C6D—C7D—H7D1	108.7
C3B—C4B—C5B	114.9 (11)	C8D—C7D—H7D2	108.7
C3B—C4B—H4B1	108.6	C6D—C7D—H7D2	108.7
C5B—C4B—H4B1	108.6	H7D1—C7D—H7D2	107.6
C3B—C4B—H4B2	108.6	C7H—C6H—C5D	112 (3)
C5B—C4B—H4B2	108.6	C7H—C6H—H6H1	109.2
H4B1—C4B—H4B2	107.5	C5D—C6H—H6H1	109.2
C6B—C5B—C4B	113.4 (12)	C7H—C6H—H6H2	109.2
C6B—C5B—H5B1	108.9	C5D—C6H—H6H2	109.2
C4B—C5B—H5B1	108.9	H6H1—C6H—H6H2	107.9
C6B—C5B—H5B2	108.9	C6H—C7H—C8D	112 (3)
C4B—C5B—H5B2	108.9	C6H—C7H—H7H1	109.3
H5B1—C5B—H5B2	107.7	C8D—C7H—H7H1	109.3
C7B—C6B—C5B	116.1 (16)	C6H—C7H—H7H2	109.3
C7B—C6B—H6B1	108.3	C8D—C7H—H7H2	109.3
C5B—C6B—H6B1	108.3	H7H1—C7H—H7H2	107.9
C7B—C6B—H6B2	108.3	C7H—C8D—C9D	115.3 (12)

C5B—C6B—H6B2	108.3	C7D—C8D—C9D	114.7 (11)
H6B1—C6B—H6B2	107.4	C7D—C8D—H8D1	108.6
C6B—C7B—C8B	118.6 (14)	C9D—C8D—H8D1	108.6
C6B—C7B—H7B1	107.7	C7D—C8D—H8D2	108.6
C8B—C7B—H7B1	107.7	C9D—C8D—H8D2	108.6
C6B—C7B—H7B2	107.7	H8D1—C8D—H8D2	107.6
C8B—C7B—H7B2	107.7	C7H—C8D—H8D3	108.5
H7B1—C7B—H7B2	107.1	C9D—C8D—H8D3	108.5
C7B—C8B—C9B	114.8 (10)	C7H—C8D—H8D4	108.5
C7B—C8B—H8B1	108.6	C9D—C8D—H8D4	108.4
C9B—C8B—H8B1	108.6	H8D3—C8D—H8D4	107.5
C7B—C8B—H8B2	108.6	C10D—C9D—C8D	114.2 (8)
C9B—C8B—H8B2	108.6	C10D—C9D—H9D1	108.7
H8B1—C8B—H8B2	107.5	C8D—C9D—H9D1	108.7
C10B—C9B—C8B	112.3 (8)	C10D—C9D—H9D2	108.7
C10B—C9B—H9B1	109.1	C8D—C9D—H9D2	108.7
C8B—C9B—H9B1	109.1	H9D1—C9D—H9D2	107.6
C10B—C9B—H9B2	109.1	C3D—C10D—C9D	126.6 (8)
C8B—C9B—H9B2	109.1	C3D—C10D—Se1D	108.1 (6)
H9B1—C9B—H9B2	107.9	C9D—C10D—Se1D	125.2 (7)
C3B—C10B—C9B	124.5 (9)	N2D—C11D—H11J	109.5
C3B—C10B—Se1B	109.8 (6)	N2D—C11D—H11K	109.5
C9B—C10B—Se1B	125.5 (7)	H11J—C11D—H11K	109.5
N2B—C11B—H11D	109.5	N2D—C11D—H11L	109.5
N2B—C11B—H11E	109.5	H11J—C11D—H11L	109.5
H11D—C11B—H11E	109.5	H11K—C11D—H11L	109.5
N2B—C11B—H11F	109.5	Cl3—C1L—Cl1	110.9 (10)
H11D—C11B—H11F	109.5	Cl3—C1L—Cl2	109.7 (8)
H11E—C11B—H11F	109.5	Cl1—C1L—Cl2	111.2 (9)
N1C—Se1C—C10C	88.8 (4)	Cl3—C1L—H1L	108.3
N2C—N1C—Se1C	109.7 (6)	Cl1—C1L—H1L	108.3
N1C—N2C—C3C	119.2 (8)	Cl2—C1L—H1L	108.3

C10A—Se1A—N1A—N2A	2.7 (6)	C10C—Se1C—N1C—N2C	−0.3 (7)
Se1A—N1A—N2A—C3A	−4.3 (10)	Se1C—N1C—N2C—C3C	−0.7 (10)
Se1A—N1A—N2A—C11A	177.0 (7)	Se1C—N1C—N2C—C11C	179.7 (7)
N1A—N2A—C3A—C10A	3.8 (11)	N1C—N2C—C3C—C10C	1.7 (12)
C11A—N2A—C3A—C10A	−177.6 (9)	C11C—N2C—C3C—C10C	−178.7 (9)
N1A—N2A—C3A—C4A	−177.8 (8)	N1C—N2C—C3C—C4C	179.8 (9)
C11A—N2A—C3A—C4A	0.9 (13)	C11C—N2C—C3C—C4C	−0.6 (14)
C10A—C3A—C4A—C5A	83.2 (12)	C10C—C3C—C4C—C5C	−81.6 (12)
N2A—C3A—C4A—C5A	−95.0 (11)	N2C—C3C—C4C—C5C	100.4 (11)
C3A—C4A—C5A—C6E	−34 (2)	C3C—C4C—C5C—C6C	74.6 (12)
C3A—C4A—C5A—C6A	−75.0 (14)	C4C—C5C—C6C—C7C	−73.4 (15)
C4A—C5A—C6A—C7A	70.9 (19)	C5C—C6C—C7C—C8C	101.0 (14)
C5A—C6A—C7A—C8A	−100.3 (19)	C6C—C7C—C8C—C9C	−56.3 (15)
C4A—C5A—C6E—C7E	−60 (4)	C7C—C8C—C9C—C10C	−44.3 (14)
C5A—C6E—C7E—C8A	101 (4)	N2C—C3C—C10C—C9C	−179.3 (8)

C6A—C7A—C8A—C9A	59.8 (19)	C4C—C3C—C10C—C9C	2.6 (15)
C6E—C7E—C8A—C9A	−74 (3)	N2C—C3C—C10C—Se1C	−1.7 (10)
C7A—C8A—C9A—C10A	42.3 (16)	C4C—C3C—C10C—Se1C	−179.8 (8)
C7E—C8A—C9A—C10A	77.8 (19)	C8C—C9C—C10C—C3C	84.7 (12)
N2A—C3A—C10A—C9A	177.9 (8)	C8C—C9C—C10C—Se1C	−92.5 (10)
C4A—C3A—C10A—C9A	−0.4 (14)	N1C—Se1C—C10C—C3C	1.1 (7)
N2A—C3A—C10A—Se1A	−1.2 (9)	N1C—Se1C—C10C—C9C	178.8 (8)
C4A—C3A—C10A—Se1A	−179.6 (7)	C10D—Se1D—N1D—N2D	0.3 (6)
C8A—C9A—C10A—C3A	−85.2 (12)	Se1D—N1D—N2D—C3D	−1.5 (10)
C8A—C9A—C10A—Se1A	93.8 (11)	Se1D—N1D—N2D—C11D	179.1 (8)
N1A—Se1A—C10A—C3A	−0.8 (6)	N1D—N2D—C3D—C10D	2.2 (11)
N1A—Se1A—C10A—C9A	−180.0 (8)	C11D—N2D—C3D—C10D	−178.4 (9)
C10B—Se1B—N1B—N2B	−0.3 (7)	N1D—N2D—C3D—C4D	179.5 (8)
Se1B—N1B—N2B—C3B	1.2 (11)	C11D—N2D—C3D—C4D	−1.2 (14)
Se1B—N1B—N2B—C11B	−179.8 (8)	N2D—C3D—C4D—C5D	−92.3 (12)
N1B—N2B—C3B—C10B	−1.7 (12)	C10D—C3D—C4D—C5D	84.7 (12)
C11B—N2B—C3B—C10B	179.4 (10)	C3D—C4D—C5D—C6D	−41.4 (17)
N1B—N2B—C3B—C4B	−178.8 (9)	C3D—C4D—C5D—C6H	−82.7 (17)
C11B—N2B—C3B—C4B	2.3 (15)	C4D—C5D—C6D—C7D	−60.7 (19)
C10B—C3B—C4B—C5B	−81.8 (14)	C5D—C6D—C7D—C8D	106.2 (17)
N2B—C3B—C4B—C5B	95.0 (12)	C4D—C5D—C6H—C7H	84 (2)
C3B—C4B—C5B—C6B	75.4 (17)	C5D—C6H—C7H—C8D	−115 (2)
C4B—C5B—C6B—C7B	−77.2 (19)	C6H—C7H—C8D—C9D	67 (3)
C5B—C6B—C7B—C8B	105.5 (18)	C6D—C7D—C8D—C9D	−74.5 (18)
C6B—C7B—C8B—C9B	−51.1 (18)	C7H—C8D—C9D—C10D	36 (2)
C7B—C8B—C9B—C10B	−52.1 (15)	C7D—C8D—C9D—C10D	73.9 (14)
N2B—C3B—C10B—C9B	−174.1 (8)	N2D—C3D—C10D—C9D	−179.8 (8)
C4B—C3B—C10B—C9B	2.9 (15)	C4D—C3D—C10D—C9D	3.1 (14)
N2B—C3B—C10B—Se1B	1.3 (10)	N2D—C3D—C10D—Se1D	−1.8 (9)
C4B—C3B—C10B—Se1B	178.3 (8)	C4D—C3D—C10D—Se1D	−178.9 (7)
C8B—C9B—C10B—C3B	86.2 (12)	C8D—C9D—C10D—C3D	−83.3 (12)
C8B—C9B—C10B—Se1B	−88.4 (10)	C8D—C9D—C10D—Se1D	99.0 (9)
N1B—Se1B—C10B—C3B	−0.6 (7)	N1D—Se1D—C10D—C3D	0.8 (6)
N1B—Se1B—C10B—C9B	174.7 (8)	N1D—Se1D—C10D—C9D	178.8 (7)