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Structural investigations of halide and polyhalide salts of 1-methyl-2,1,3-benzoselenadiazol-1-ium

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To examine the effect of counteranion identity on chalcogen bonding (ChB), three new crystal structures were obtained by mixing *N*-methyl-2,1,3-benzoselenadiazolium chloride ($C_7H_7N_2Se^+\cdot Cl^-$) with *N*-bromosuccinimide, affording salts of a polybromide [1-methyl-2,1,3-benzoselenadiazol-1-ium bromide hemi(dibromine), $C_7H_7N_2Se^+\cdot Br^-\cdot 0.5Br_2$, denoted [Se]$Br_2$·Br], a disordered bromide/chloride (1-methyl-2,1,3-benzoselenadiazol-1-ium bromide/chloride(0.33/0.67), $C_7H_7N_2Se^+\cdot Br_{0.33}/Cl_{0.67}^-$, denoted [Se]Br/Cl) and a disordered chloride dichlorobromide/tribromide [1-methyl-2,1,3-benzoselenadiazol-1-ium hemichloride dichlorobromide/tribromide(0.365/0.135), $C_7H_7N_2Se^+\cdot 0.5Cl^-\cdot 0.365BrCl_2^-\cdot 0.135Br_3^-$, denoted [Se]Cl·$BrCl_2$/$Br_3$]. In two of the three structures, the selenium centre forms a short contact to a halide *X* (*X* = Cl, Br), *trans* to the Se—N(methyl) bond, with distances ranging from 2.772 (2) to 2.796 (2) Å. These contacts are substantially shorter than the sum of the respective van der Waals radii, and the σ-hole N—Se···*X* angles are highly directional, ranging from 171.5 (3) to 178.98 (5)°. In [Se]Br_2·Br, the polybromide does not occupy this position. The selenadiazolium rings instead form a symmetric $[Se\cdots N]_2$ motif at 2.594 (1) Å [75% of Σr_{vdW}(Se···N) = 3.45 Å], and the bromide engages the second weaker σ-hole *cis* to the Se—N(methyl) bond at 3.2817 (6) Å. Anion identity therefore decides whether the dimeric synthon forms or is displaced by the counteranion for these selenadiazolium systems.

1. Introduction

Derivatives of 1,2,5-chalcogenadiazoles have become established platforms widely exploited as supramolecular building blocks presenting two well-defined Ch···N (Ch = S, Se, Te) chalcogen-bonding (ChB) interactions enabling self-assembly through the dimeric $[Ch\cdots N]_2$ synthon. Tellurium-based chalcogenadiazoles form the strongest chalcogen bonds; however, they are also susceptible to oxidative breakdown and are sensitive to moisture (Cozzolino & Vargas-Baca, 2007; Lee *et al.*, 2016; Lee *et al.*, 2019; Petrov *et al.*, 2020). Selenium analogues, such as 2,1,3-benzoselenadiazoles, form weaker ChB interactions, although these can be strengthened by fine-tuning methods, including *N*-methylation to give the corresponding benzoselenadiazolium cations, increasing the electron-withdrawing ability of the N atom and, in turn, deepening the σ-hole on the chalcogen (Dutton *et al.*, 2006; Risto *et al.*, 2008; Berionni *et al.*, 2009; Lee *et al.*, 2016; Lee *et al.*, 2019; Rowett *et al.*, 2026; Sysoeva *et al.*, 2024). The *N*-methyl derivatives are particularly interesting compared to other alkylated species, as their synthesis is facile and the minimal steric demand of the methyl group leaves the chalcogen-bond donor site accessible for anion binding and catalysis.

Structurally characterized examples of these cations nevertheless remain scarce. Only seven depositions of *N*-methyl-

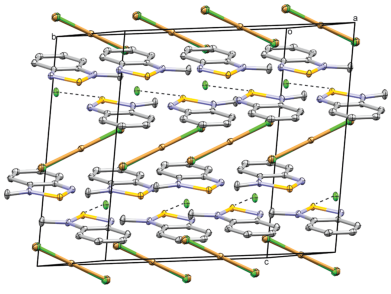

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Table 1
Experimental details.

Experiments were carried out at 100 K with Mo $K\alpha$ radiation. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2016). H-atom parameters were constrained.

	[Se]Br_2·Br	**[Se]Br/Cl**	**[Se]Cl·$BrCl_2$/Br_3**
Crystal data			
Chemical formula	$C_7H_7N_2Se^+\cdot Br^-\cdot 0.5Br_2$	$C_7H_7N_2Se^+\cdot 0.33Br^-/0.67Cl^-$	$C_7H_7N_2Se^+\cdot 0.5Cl^-\cdot 0.365BrCl_2^-\cdot 0.135Br_3^-$
M_r	357.93	248.26	303.30
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$
a, b, c (Å)	7.7284 (18), 7.729 (2), 8.5175 (16)	25.825 (7), 5.8156 (15), 22.219 (7)	11.062 (2), 13.640 (2), 13.498 (2)
α, β, γ (°)	89.276 (6), 70.277 (6), 82.282 (10)	90, 90.018 (11), 90	90, 110.489 (8), 90
V (Å^3)	474.3 (2)	3337.1 (16)	1907.8 (6)
Z	2	16	8
μ (mm^{-1})	12.33	6.23	7.46
Crystal size (mm)	0.1 × 0.1 × 0.05	0.3 × 0.02 × 0.02	0.1 × 0.1 × 0.1
Data collection			
Diffractometer	Bruker Venture	Bruker Venture	Bruker APEXII CCD
T_{min}, T_{max}	0.650, 0.862	0.803, 0.927	0.766, 0.862
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29869, 2879, 2676	141706, 10191, 7304	53658, 3644, 3269
R_{int}	0.048	0.097	0.066
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714	0.715	0.770
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.017, 0.038, 1.09	0.069, 0.160, 1.08	0.024, 0.058, 1.07
No. of reflections	2879	10191	3644
No. of parameters	110	391	116
No. of restraints	0	313	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −0.59	3.61, −1.82	0.86, −1.21

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2016), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2025* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

2,1,3-benzoselenadiazolium cations are so far reported in the Cambridge Structural Database (Groom *et al.*, 2016), containing the tetrafluoroborate (Berionni *et al.*, 2009), iodide (Lee *et al.*, 2016; Sysoeva *et al.*, 2024), and triflate salts (Sysoeva *et al.*, 2024), disordered bromide/chloride and tribromide/chloride salts (Rowett *et al.*, 2026), and a pseudo-trimer structure containing two iodide salts bridged by the neutral 2,1,3-benzoselenaidazole compound (Lee *et al.*, 2016). All of these structures exhibit short Se···anion contacts similar to those observed in the crystals reported here, indicating that the anion is an integral part of the coordination environment of the selenium centre rather than a passive spectator.

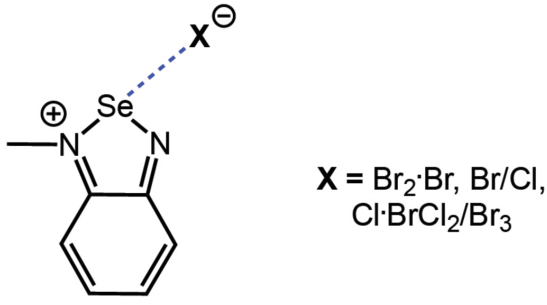

Figure 1
The molecular structure of the *N*-methyl-2,1,3-benzoselenadiazolium cation and counteranions crystallized within the investigated crystal structures. Anion compositions are given per cation and are charge-balanced, except for [Se]Cl·$BrCl_2$/Br_3, which is per two cations. A slash denotes a single crystallographic site shared by two species at partial occupancy, Br/Cl is a halide site with mixed bromide and chloride occupancy [53.1 (4):46.9 (4), 21.3 (7):78.7 (7), 17.8 (7):82.2 (7) and 40.1 (8):59.9 (8)] and Cl·$BrCl_2$/Br_3 is a trihalide site occupied by both $BrCl_2^-$ and Br_3^- [72.9 (2):27.1 (2)]. In [Se]Cl·$BrCl_2$/Br_3, the chloride and the trihalide each lie on an inversion centre and are therefore present at half occupancy.

Strongly coordinating halide counteranions are known to disrupt the supramolecular [Se···N]$_2$ synthon in these salts (Lee *et al.*, 2016; Lee *et al.*, 2019). Such coordination is a limitation in the solid state, but in solution, the counteranion is directly involved in catalysis. We recently showed that benzoselenadiazolium chloride catalyzes aromatic halogenation, the Se···anion ChB and cooperative halogen bonding to chloride together stabilizing the pre-complex and facilitating subsequent bromine and proton transfers (Rowett *et al.*, 2026). The same principle extends to function, Wang and co-workers having recently described a ChB catalysis system in which ChB donation by a selenium-based cation and binding of the $GaCl_4^-$ counteranion operate together in substrate activation (Dong *et al.*, 2026). Together, these results establish the counteranion as a design element rather than an incidental component, and they motivated us to expand the library of structurally characterized benzoselenadiazolium salts so that the accessible anion environments and Se···anion coordination modes can be surveyed systematically.

The present work describes three structurally distinct salts, including polyhalide anions (Fig. 1), showcasing the diversity of supramolecular assemblies accessible from this system.

2. Experimental

2.1. Materials and methods

The 1-methyl-2,1,3-benzoselenadiazol-1-ium chloride salt was prepared according to the procedure of Rowett *et al.* (2026). *N*-Bromosuccinimide (NBS) was purchased from Sigma–Aldrich and used as received. Solvents were obtained commercially and used without further purification.

2.2. Synthesis and crystallization of complexes

Crystals were grown by vapour diffusion of diethyl ether into a solution of the chloride salt and NBS, in a 1:3 molar ratio, in acetonitrile, held at 3 °C to room temperature in the dark. Three crystalline materials formed concomitantly within a single crystallization vial and were separated manually. Yellow and dark-red blocks were hand-picked, mounted on the diffractometer, which identified the yellow crystals as [Se]-Br/Cl and the dark-red crystals as [Se]Br_2·Br and [Se]Cl·$BrCl_2$/Br_3. The latter two crystals were differentiated only after unit-cell determination. Although NBS was present in the crystallization medium, it was not incorporated into any of the products; instead, NBS acted as an *in-situ* bromine source, and halide redistribution afforded cocrystallizing salts of the cation containing chloride, bromide and polybromide anions. Because the three structures crystallize together from the same solution and were isolated only as individual hand-selected species, no yields can be quoted for these materials.

2.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were generated in ideal positions and then updated with each cycle of refinement.

In [Se]Br/Cl and [Se]Cl·$BrCl_2$/Br_3, Br/Cl disorder was modelled at each appropriate site using a free variable, so that the combined occupancies of the two atoms equalled 1, and displacement parameters were constrained to share identical anisotropic displacement parameters. The asymmetric unit in [Se]Br/Cl contained four unique sites featuring Br/Cl disorder, each modelled by a different free variable. The asymmetric unit in [Se]Cl·$BrCl_2$/Br_3 contained a single unique site with Br/Cl disorder (the terminal atom in the X_2Br^- ligand). For [Se]-Cl·$BrCl_2$/Br_3, the occupancies of the free chloride ion and central Br atom were assigned as 0.5 to reflect the presence of half an equivalent of Cl^- and half an equivalent of X_2Br^- (X = Cl or Br) per molecule. For sites where refinement was unstable with respect to the disordered Br and Cl atoms (three of the four Cl/Br sites in [Se]Br/Cl), atom locations were constrained to share identical fractional coordinates. The higher R factors of [Se]Br/Cl ($R1$ = 0.0688 and $wR2$ = 0.1602) compared with the other two structures ($R1$ = 0.0167 and 0.0237) are primary caused by weaker diffraction at high angles, potentially combined with the presence of merohedral twinning.

3. Results and discussion

Vapour diffusion of the chloride salt with NBS, carried out at temperatures from 3 °C to ambient over several days, generated a bromide-rich environment from which three distinct structures were obtained. Decomposition of NBS under these conditions likely liberates Br_2, which combines with residual bromide and chloride to yield the polyhalide species described below.

All structures contain the same *N*-methyl-2,1,3-benzoselenadiazolium monocation, $C_7H_7N_2Se^+$, and differ only in the accompanying bromide or chloride-based counteranions (each crystal will be denoted as [Se]X, where [Se] represents the cation and X the counteranion). The [Se]Br_2·Br salt crystallizes in the triclinic centrosymmetric space group $P\overline{1}$, whereas [Se]Br/Cl and [Se]Cl·$BrCl_2$/Br_3 are monoclinic, in the centrosymmetric space groups $P2_1/c$ and $C2/c$, respectively. The asymmetric units of [Se]Br_2·Br and [Se]Cl·$BrCl_2$/Br_3 contain one cation, while that of [Se]Br/Cl is comprised of four independent cation–anion pairs. Both [Se]Br/Cl and [Se]-

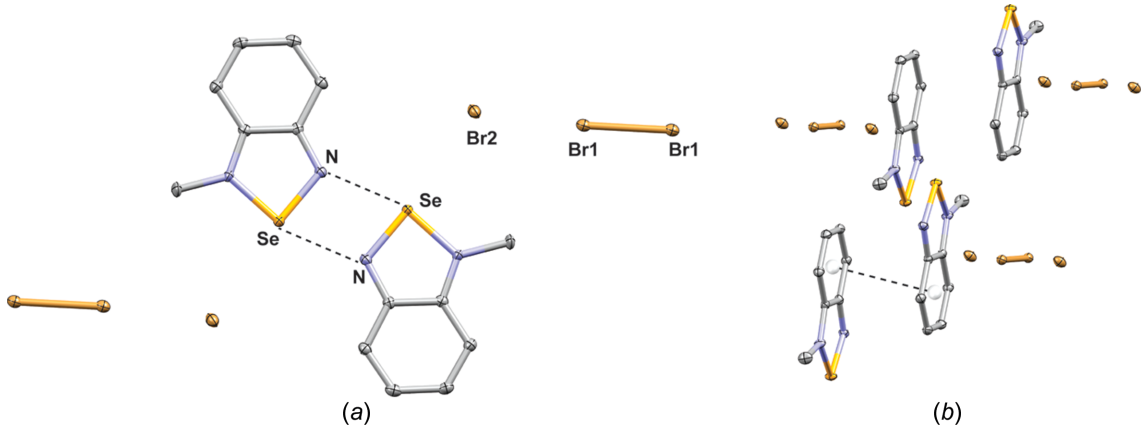

Figure 2
(*a*) The extended structure of [Se]Br_2·Br with Se···N chalcogen-bond and Br···Br halogen-bond interactions. Displacement ellipsoids are drawn at the 50% probability level. All H atoms have been omitted for clarity. (*b*) The packing arrangement, viewed along the *c* axis, showing the π-stacking interactions.

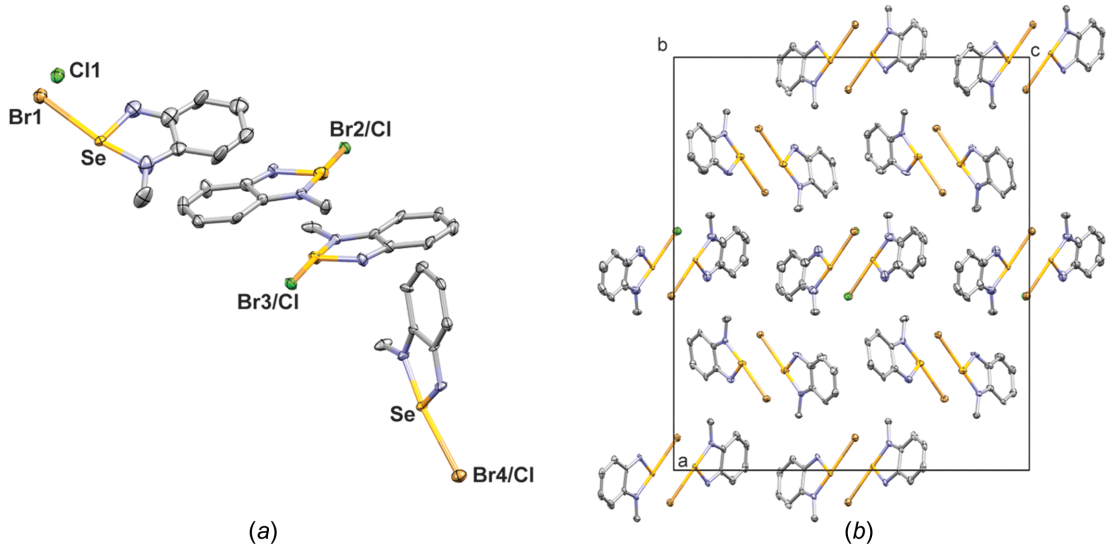

Figure 3
(*a*) The asymmetric unit of [Se]Br/Cl, showing four cation–anion pairs and chalcogen-bond interactions to halide anions (disordered over bromide and chloride). (*b*) The crystal packing arrangement, viewed down the *b* axis, displaying the π-stacking interactions.

Cl·$BrCl_2$/Br_3 contain disordered anion positions over bromide and chloride. Two of the three structures feature nearly planar aromatic benzoselenadiazolium scaffolds in which the dihedral angles between the five-membered C_2N_2Se ring and the fused benzene ring are 0.67 (6)° in [Se]Br_2·Br and 0.09 (7)° in [Se]Cl·$BrCl_2$/Br_3. [Se]Br/Cl exhibits significantly larger dihedral angles ranging from 3.36 (3) to 4.74 (4)° across four cations.

The Se—N1(methyl) and Se—N bond lengths within all cations across the three crystal structures are in the ranges 1.836 (1)–1.911 (1) and 1.758 (8)–1.824 (1) Å, respectively, and the N—CH_3 distances vary over the range 1.453 (1)–1.489 (2) Å. Each of these individual sets of bond distances is very similar to those reported in previous work on benzoselenadiazolium cations, which all feature lengths lying within the above corresponding ranges (Berionni *et al.*, 2009; Lee *et al.*, 2016; Rowett *et al.*, 2026).

The two Se—N bonds in each benzoselenadiazolium cation within the investigated crystal structures are crystallographically distinct, with the bond to the *N*-methylated N atom consistently the longer of the pair, for example, Se1—N1(methyl) = 1.836 (1) Å *versus* Se1—N2 = 1.779 (1) Å in [Se]Br_2·Br [Fig. 2(*a*)]. The shorter Se—N2 bond involves the lone-pair-retaining N atom able to delocalize into the aromatic ring, providing a partial double-bond character. The methylated N atom on the other hand is unable to contribute to delocalization and withdraws electron density away from the chalcogen, resulting in the corresponding Se—N1(methyl) bond being longer, weaker and more polarized. This, in turn, provides a lower-lying more accessible σ^* orbital and enhanced

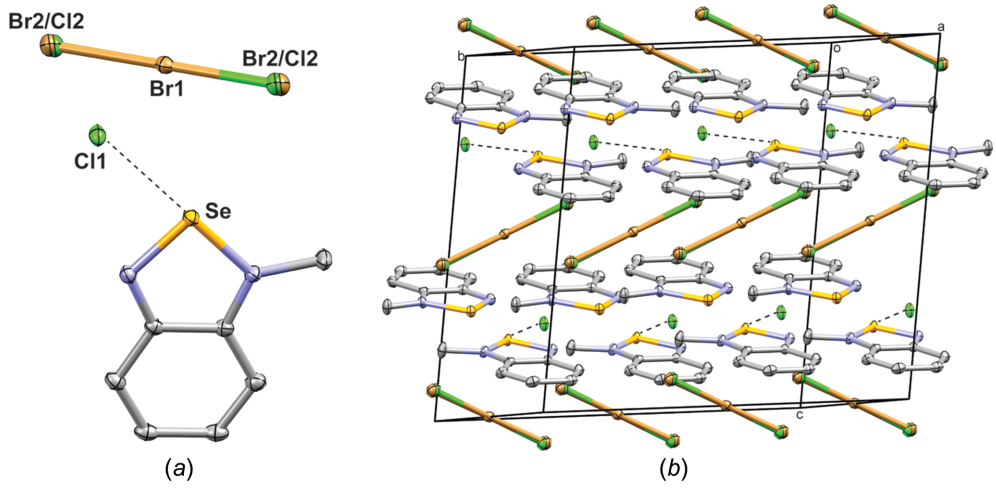

Figure 4
(*a*) The extended structure containing an asymmetric unit and one disordered Br/Cl atom in [Se]Cl·$BrCl_2$/Br_3, showing Se···Cl chalcogen-bond interactions and disordered trihalide. Displacement ellipsoids are drawn at the 50% probability level. All H atoms have been omitted for clarity. (*b*) The packing arrangement projected onto the *bc* plane.

positive electrostatic potential specifically at the extension of this elongated bond, consistent with the partial charge transfer (n→σ^*) component of ChB and reflecting the high directionality of these interactions.

The dimeric motif of [Se]Br_2·Br is shown in Fig. 2(*a*) arranged in the typical antiparallel fashion (Cozzolino & Vargas-Baca, 2007; Cozzolino *et al.*, 2013; Lee *et al.*, 2016) featuring short [2.594 (1) Å] Se···N contacts (75% of the corresponding Σr_{vdW} = 3.45 Å). This supramolecular synthon occupies the position *trans* to the Se—N1(methyl) bond of each cation, displacing the polybromide counteranions further from Se. The polybromide assembly consists of a bromide ion and a dibromine (Br_2) unit; the Br—Br bond length of the Br_2 molecule is 2.407 (4) Å, associating with the bromide ion through a Br···Br contact of 2.996 (5) Å. Each of the benzoselenadiazolium cations also forms contacts with the bromide ion at a distance of 3.282 (6) Å, shorter than the Σr_{vdW}(Se···Br) of 3.75 Å, indicating simultaneous halogen-bond (XB) and ChB interactions from the halide ion, comparable to an occurrence reported in a selenium(IV) polybromide complex featuring pyramidal $[SeBr_5]^-$ anions (Korobeynikov *et al.*, 2022). Another notable structural feature is the π-stacking interaction between the six-membered rings of two selenadiazolium cations [Fig. 2(*b*)], with a centroid-to-centroid distance of 3.527 Å. Due to the relative positioning of the cations and counteranions within [Se]-Br_2·Br, the σ-hole N2—Se1···Br angle of 159.14 (4)° necessarily deviates from linearity as compared to the other investigated structures.

The four selenadiazolium rings within the asymmetric unit of [Se]Br/Cl, shown in Fig. 3(*a*), are each anchored to a disordered halide anion through short charge-assisted Se···*X* ChB interactions (*X* = Cl/Br). From top to bottom, the four halide sites are disordered over Cl/Br in the ratios 46.9 (4)/53.1 (4), 78.7 (7)/21.3 (7), 82.2 (7)/17.8 (7) and 59.9 (8)/40.1 (8)%. The bromide content varies markedly between sites, from 53.1 (4)% at the first site Br1, the only site where bromide is the majority component, down to 17.8 (7)% for Br3. Comparison with the near-isostructural salt reported recently (Rowett *et al.*, 2026) shows that this uneven halide distribution has a substantial effect on the overall symmetry, with the present structure [Se]Br/Cl crystallizing in the monoclinic space group $P2_1/c$ with Z' = 4, whereas the more nearly stoichiometric analogue adopts the higher symmetry orthorhombic space group $Pca2_1$ with Z' = 2. One of the four cations of [Se]Br/Cl is disordered [the C5—C6 distance is short at 1.208 (2) Å], and its geometric parameters are correspondingly less precise than those of the three ordered cations.

The cation–anion units in the crystal packing [Fig. 3(*b*)], viewed down the *b* axis, are arranged in a helical pattern with 2_1 screw axes. In addition, π-stacking interactions occur at centroid-to-centroid distances of 4.861 and 4.900 Å. The Se···*X* distances span the range 2.772 (2)–2.796 (2) Å [Σr_{vdW}(Se···Br) = 3.75 Å and Σr_{vdW}(Se···Cl) = 3.65 Å] and the σ-hole N—Se···*X* angles are highly directional, ranging from 171.5 (3) to 174.9 (2)°.

[Se]Cl·$BrCl_2$/Br_3 contains two crystallographically independent anions, a chloride ion and a trihalide ion disordered over Br_3 and $BrCl_2$ [Fig. 4(*a*)]. Both lie on inversion centres and are therefore present at half occupancy in the asymmetric unit, the trihalide being necessarily linear and centrosymmetric about its central Br1 atom. Unlike said central atom, while the terminal atoms are disordered over Cl [72.9 (2)%] and Br [27.1 (2)%], so that the trihalide is a superposition of dichlorobromide, [Cl—Br—Cl] (major), and tribromide, [Br—Br—Br] (minor) [Br—Cl = 2.402 (11) Å and Br—Br = 2.486 (12) Å; *X*—Br—*X* (*X* = Cl or Br) = 180.0°]. The crystal packing is shown in Fig. 4(*b*), projected onto the *bc* plane, arranged with *C*2 proper rotation axes and 2_1 screw axes. Each selenadiazolium cation forms a Se···Cl ChB interaction to the discrete chloride ion at a distance of 2.785 (6) Å [Σr_{vdW}(Se···Cl) = 3.65 Å], with an almost geometrically ideal σ-hole N—Se···Cl angle of 178.98 (5)°.

4. Conclusions

Three new salts consisting of the *N*-methyl-2,1,3-benzoselenadiazolium cation with Br_2·Br, disordered Br/Cl and disordered Cl·$BrCl_2$/Br_3 anions were synthesized and crystallized from a single reaction mixture of the chloride salt and NBS. Se···*X* contacts span the range from 2.772 (2) to 3.2817 (6) Å, corresponding to 76% of the sum of the van der Waals radii, with N—Se···*X* angles ranging from 159.14 (4) to 178.98 (5)°, consistent with donation into the σ-hole *trans* along the extension of the Se—N1(methyl) bond. Of the three anions, only [Se]Br_2·Br allows formation of the $[Se\cdots N]_2$ supramolecular synthon, the remaining two outcompeting the cation as a ChB acceptor. From a synthetic point of view, the oxidation of bromide by NBS affords a series of accessible bromine-containing anions, offering a route to further members of this family and to the systematic tuning of ChB donor strength in these cationic selenium systems.

Conflict of interest

The authors declare there are no competing interests.

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Structural investigations of halide and polyhalide salts of 1-methyl-2,1,3-benzoselenadiazol-1-ium

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Computing details

1-Methyl-2,1,3-benzoselenadiazol-1-ium bromide hemi(dibromine) (llq1)

Crystal data

$C_7H_7N_2Se^+·Br^-·0.5Br_2$
M_r = 357.93
Triclinic, $P\overline{1}$
a = 7.7284 (18) Å
b = 7.729 (2) Å
c = 8.5175 (16) Å
α = 89.276 (6)°
β = 70.277 (6)°
γ = 82.282 (10)°
V = 474.3 (2) Å^3
Z = 2
$F(000)$ = 334
D_x = 2.506 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9988 reflections
θ = 2.7–30.5°
μ = 12.33 mm^{-1}
T = 100 K
Block, orange
0.1 × 0.1 × 0.05 mm

Data collection

Bruker Venture diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.650, T_{max} = 0.862
29869 measured reflections
2879 independent reflections
2676 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 30.5°, θ_{min} = 2.5°
h = −11→11
k = −11→11
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.038
S = 1.09
2879 reflections
110 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 0.1586P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Special details

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

Refinement. Crystallographic data were obtained from crystals coated in Paratone oil and mounted on a Bruker Dual Source D8 Venture diffractometer using the IμS 3.0 Mo source at 70 W with a HELIOS Mo focusing optic (ELM33) in the McMaster Analytical X-ray (MAX) Diffraction Facility. Raw data were processed using XPREP as part of the APEX (v5/v6 software) and solved by intrinsic phasing (SHELXT) (Sheldrick, 2015*b*). Non-H atoms were refined anisotropically. H atoms were generated in ideal positions and then updated with each cycle of refinement, which was performed with SHELXL (Sheldrick, 2015*a*) in OLEX2-1.5 (Dolomanov *et al.*, 2009).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.07851 (2)	0.55244 (2)	0.86438 (2)	0.01263 (4)
Br2	0.27819 (2)	0.70550 (2)	0.53920 (2)	0.01575 (5)
Se1	0.41327 (2)	0.43826 (2)	0.21096 (2)	0.01129 (4)
N1	0.29073 (18)	0.25661 (17)	0.31033 (16)	0.0114 (2)
N2	0.42818 (17)	0.35004 (17)	0.01413 (15)	0.0108 (2)
C1	0.2218 (2)	0.2356 (2)	0.49200 (19)	0.0158 (3)
H1A	0.278938	0.311770	0.545401	0.024*
H1B	0.253973	0.113715	0.516649	0.024*
H1C	0.086681	0.267282	0.534956	0.024*
C2	0.3474 (2)	0.2067 (2)	0.03058 (18)	0.0104 (3)
C3	0.3358 (2)	0.1088 (2)	−0.10598 (19)	0.0129 (3)
H3	0.388867	0.142957	−0.217683	0.015*
C4	0.2465 (2)	−0.0348 (2)	−0.0714 (2)	0.0140 (3)
H4	0.235405	−0.100197	−0.160432	0.017*
C5	0.1689 (2)	−0.0892 (2)	0.0963 (2)	0.0143 (3)
H5	0.109370	−0.191118	0.114888	0.017*
C6	0.1771 (2)	−0.0003 (2)	0.23052 (19)	0.0127 (3)
H6	0.124642	−0.038399	0.340883	0.015*
C7	0.2670 (2)	0.1511 (2)	0.19861 (18)	0.0108 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01285 (7)	0.01205 (8)	0.01343 (7)	−0.00072 (5)	−0.00531 (5)	−0.00178 (5)
Br2	0.02090 (8)	0.01515 (8)	0.01068 (7)	−0.00086 (6)	−0.00527 (6)	−0.00038 (5)
Se1	0.01401 (8)	0.01232 (8)	0.00815 (7)	−0.00577 (6)	−0.00305 (5)	0.00033 (5)
N1	0.0131 (6)	0.0119 (6)	0.0097 (6)	−0.0054 (5)	−0.0034 (5)	0.0022 (5)
N2	0.0121 (6)	0.0117 (6)	0.0088 (5)	−0.0013 (5)	−0.0038 (5)	−0.0004 (5)
C1	0.0204 (8)	0.0193 (8)	0.0083 (6)	−0.0078 (6)	−0.0039 (6)	0.0045 (6)
C2	0.0096 (6)	0.0107 (7)	0.0105 (6)	0.0000 (5)	−0.0034 (5)	0.0004 (5)
C3	0.0132 (7)	0.0135 (7)	0.0121 (7)	−0.0002 (6)	−0.0053 (5)	−0.0005 (5)
C4	0.0134 (7)	0.0130 (7)	0.0170 (7)	0.0003 (6)	−0.0074 (6)	−0.0034 (6)
C5	0.0134 (7)	0.0119 (7)	0.0191 (7)	−0.0033 (6)	−0.0070 (6)	−0.0001 (6)
C6	0.0124 (7)	0.0119 (7)	0.0136 (7)	−0.0025 (6)	−0.0038 (5)	0.0017 (5)

C7	0.0102 (6)	0.0113 (7)	0.0115 (6)	−0.0003 (5)	−0.0050 (5)	−0.0003 (5)

Geometric parameters (Å, º)

Br1—Br1^{i}	2.4066 (5)	C2—C7	1.441 (2)
Se1—N1	1.8359 (13)	C3—H3	0.9500
Se1—N2	1.7794 (13)	C3—C4	1.362 (2)
N1—C1	1.4714 (19)	C4—H4	0.9500
N1—C7	1.335 (2)	C4—C5	1.433 (2)
N2—C2	1.327 (2)	C5—H5	0.9500
C1—H1A	0.9800	C5—C6	1.365 (2)
C1—H1B	0.9800	C6—H6	0.9500
C1—H1C	0.9800	C6—C7	1.417 (2)
C2—C3	1.430 (2)		
N2—Se1—N1	88.50 (6)	C4—C3—C2	118.14 (14)
C1—N1—Se1	123.41 (10)	C4—C3—H3	120.9
C7—N1—Se1	111.84 (10)	C3—C4—H4	119.3
C7—N1—C1	124.72 (13)	C3—C4—C5	121.35 (14)
C2—N2—Se1	111.62 (10)	C5—C4—H4	119.3
N1—C1—H1A	109.5	C4—C5—H5	118.7
N1—C1—H1B	109.5	C6—C5—C4	122.59 (15)
N1—C1—H1C	109.5	C6—C5—H5	118.7
H1A—C1—H1B	109.5	C5—C6—H6	121.3
H1A—C1—H1C	109.5	C5—C6—C7	117.32 (14)
H1B—C1—H1C	109.5	C7—C6—H6	121.3
N2—C2—C3	124.12 (14)	N1—C7—C2	111.91 (13)
N2—C2—C7	116.12 (13)	N1—C7—C6	127.27 (14)
C3—C2—C7	119.76 (14)	C6—C7—C2	120.82 (14)
C2—C3—H3	120.9		
Se1—N1—C7—C2	1.16 (16)	C1—N1—C7—C2	179.02 (14)
Se1—N1—C7—C6	−179.32 (12)	C1—N1—C7—C6	−1.4 (2)
Se1—N2—C2—C3	179.20 (12)	C2—C3—C4—C5	−1.2 (2)
Se1—N2—C2—C7	−0.44 (16)	C3—C2—C7—N1	179.84 (14)
N1—Se1—N2—C2	0.88 (11)	C3—C2—C7—C6	0.3 (2)
N2—Se1—N1—C1	−179.08 (13)	C3—C4—C5—C6	1.0 (2)
N2—Se1—N1—C7	−1.18 (11)	C4—C5—C6—C7	−0.1 (2)
N2—C2—C3—C4	−179.08 (14)	C5—C6—C7—N1	−179.99 (15)
N2—C2—C7—N1	−0.50 (19)	C5—C6—C7—C2	−0.5 (2)
N2—C2—C7—C6	179.94 (13)	C7—C2—C3—C4	0.6 (2)

Symmetry code: (i) −*x*, −*y*+1, −*z*+2.

1-Methyl-2,1,3-benzoselenadiazol-1-ium bromide/chloride(0.33/0.67) (mo_llq9)

Crystal data

$C_7H_7Br_{0.33}Cl_{0.67}N_2Se^+ \cdot Br0.33/Cl_{0.67}^-$
M_r = 248.26
Monoclinic, $P2_1/c$
a = 25.825 (7) Å
b = 5.8156 (15) Å
c = 22.219 (7) Å
β = 90.018 (11)°
V = 3337.1 (16) Å^3
Z = 16
$F(000)$ = 1919
D_x = 1.977 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9145 reflections
θ = 2.4–29.9°
μ = 6.23 mm^{-1}
T = 100 K
Needle, yellow
0.3 × 0.02 × 0.02 mm

Data collection

Bruker Venture diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.803, T_{max} = 0.927
141706 measured reflections
10191 independent reflections
7304 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 30.5°, θ_{min} = 1.6°
h = −36→36
k = −8→8
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.160
S = 1.08
10191 reflections
391 parameters
313 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 63.2353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 3.61 e Å^{-3}
$\Delta\rho_{min}$ = −1.82 e Å^{-3}

Special details

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

Refinement. Refined as a 2-component twin.

Crystallographic data were obtained from crystals coated in Paratone oil and mounted on a Bruker Dual Source D8 Venture diffractometer using the IμS 3.0 Mo source at 70 W with a HELIOS Mo focusing optic (ELM33) in the McMaster Analytical X-ray (MAX) Diffraction Facility. Raw data were processed using XPREP as part of the APEX (v5/v6 software) and solved by intrinsic phasing (SHELXT) (Sheldrick, 2015*b*). Non-H atoms were refined anisotropically. H atoms were generated in ideal positions and then updated with each cycle of refinement, which was performed with SHELXL (Sheldrick, 2015*a*) in OLEX2-1.5 (Dolomanov *et al.*, 2009).

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Se1	0.50874 (4)	−0.22945 (18)	0.43976 (4)	0.01358 (12)	
N1	0.5644 (4)	−0.1096 (18)	0.3926 (5)	0.036 (2)	
N2	0.4698 (4)	−0.0008 (19)	0.4064 (5)	0.039 (2)	
C1	0.6171 (4)	−0.212 (3)	0.3974 (6)	0.040 (3)	

H1A	0.614039	−0.376975	0.406155	0.060*	
H1B	0.636247	−0.136573	0.429872	0.060*	
H1C	0.635579	−0.191237	0.359287	0.060*	
C2	0.4974 (5)	0.128 (2)	0.3697 (6)	0.039 (2)	
C3	0.4756 (5)	0.300 (3)	0.3358 (6)	0.048 (2)	
H3	0.439047	0.319169	0.334910	0.058*	
C4	0.5077 (6)	0.449 (2)	0.3024 (6)	0.045 (3)	
H4	0.493594	0.579108	0.282267	0.054*	
C5	0.5623 (6)	0.400 (2)	0.2995 (6)	0.045 (3)	
H5	0.584475	0.502329	0.278502	0.054*	
C6	0.5805 (6)	0.231 (3)	0.3230 (6)	0.048 (2)	
H6	0.615992	0.197834	0.315769	0.058*	
C7	0.5514 (5)	0.074 (2)	0.3619 (5)	0.034 (2)	
Br1	0.42181 (8)	−0.3388 (3)	0.50710 (8)	0.0255 (5)	0.531 (4)
Se2	0.75898 (5)	0.72761 (17)	0.31292 (5)	0.0240 (2)	
N3	0.8150 (3)	0.6197 (13)	0.3583 (3)	0.0164 (13)	
N4	0.7200 (3)	0.5150 (14)	0.3474 (4)	0.0226 (16)	
C8	0.8672 (4)	0.7107 (18)	0.3517 (5)	0.0215 (19)	
H8A	0.888596	0.600022	0.329586	0.032*	
H8B	0.882279	0.737372	0.391561	0.032*	
H8C	0.865918	0.856111	0.329426	0.032*	
C9	0.7475 (4)	0.3843 (16)	0.3863 (4)	0.0239 (17)	
C10	0.7264 (4)	0.1902 (19)	0.4171 (5)	0.032 (2)	
H10	0.690645	0.152967	0.413959	0.038*	
C11	0.7589 (5)	0.0607 (17)	0.4512 (4)	0.0289 (19)	
H11	0.745144	−0.064945	0.473351	0.035*	
C12	0.8125 (4)	0.1072 (17)	0.4547 (4)	0.0245 (18)	
H12	0.833953	0.007852	0.477697	0.029*	
C13	0.8342 (4)	0.2884 (17)	0.4262 (4)	0.0204 (16)	
H13	0.870274	0.318564	0.429766	0.024*	
C14	0.8014 (4)	0.4352 (16)	0.3903 (4)	0.0194 (16)	
Br2	0.67206 (8)	0.8358 (3)	0.24344 (8)	0.0191 (5)	0.213 (7)
Se3	0.74109 (5)	0.28193 (16)	0.19257 (5)	0.0206 (2)	
N5	0.6865 (3)	0.3815 (13)	0.1446 (3)	0.0183 (14)	
N6	0.7805 (3)	0.4955 (13)	0.1604 (4)	0.0191 (15)	
C15	0.6338 (4)	0.2895 (19)	0.1489 (5)	0.027 (2)	
H15A	0.634881	0.136456	0.167325	0.041*	
H15B	0.618688	0.278499	0.108574	0.041*	
H15C	0.612646	0.392116	0.173793	0.041*	
C16	0.7538 (4)	0.6230 (15)	0.1210 (4)	0.0215 (16)	
C17	0.7743 (4)	0.8153 (18)	0.0899 (4)	0.0227 (12)	
H17	0.809776	0.854314	0.094613	0.027*	
C18	0.7443 (5)	0.9425 (17)	0.0540 (4)	0.0285 (19)	
H18	0.758685	1.071335	0.033793	0.034*	
C19	0.6900 (4)	0.8872 (18)	0.0454 (4)	0.0250 (18)	
H19	0.669649	0.979423	0.019189	0.030*	
C20	0.6675 (4)	0.7044 (18)	0.0743 (4)	0.0227 (12)	
H20	0.631770	0.670418	0.069362	0.027*	

C21	0.6997 (4)	0.5675 (17)	0.1118 (4)	0.0207 (16)	
Br3	0.82746 (8)	0.1684 (3)	0.26133 (8)	0.0200 (5)	0.178 (7)
Se4	0.99107 (4)	0.26291 (19)	0.05987 (4)	0.01358 (12)	
N7	0.9357 (3)	0.3703 (13)	0.1063 (3)	0.0174 (14)	
N8	1.0308 (3)	0.4747 (13)	0.0952 (3)	0.0178 (14)	
C22	0.8828 (4)	0.286 (2)	0.1036 (5)	0.025 (2)	
H22A	0.862065	0.387473	0.077967	0.038*	
H22B	0.868033	0.282578	0.144193	0.038*	
H22C	0.882603	0.129997	0.086702	0.038*	
C23	1.0029 (4)	0.6032 (15)	0.1328 (4)	0.0151 (15)	
C24	1.0252 (4)	0.7865 (17)	0.1656 (4)	0.0219 (17)	
H24	1.061247	0.818341	0.163202	0.026*	
C25	0.9925 (5)	0.9186 (16)	0.2015 (4)	0.0247 (18)	
H25	1.006023	1.044461	0.223773	0.030*	
C26	0.9401 (4)	0.8659 (18)	0.2046 (4)	0.0273 (19)	
H26	0.918610	0.965092	0.227569	0.033*	
C27	0.9172 (4)	0.6830 (16)	0.1771 (4)	0.0244 (19)	
H27	0.881670	0.647770	0.183033	0.029*	
C28	0.9491 (4)	0.5485 (15)	0.1395 (4)	0.0180 (15)	
Cl1	0.4211 (2)	−0.1778 (9)	0.5112 (2)	0.0255 (5)	0.469 (4)
Cl2	0.67206 (8)	0.8358 (3)	0.24344 (8)	0.0191 (5)	0.787 (7)
Cl3	0.82746 (8)	0.1684 (3)	0.26133 (8)	0.0200 (5)	0.822 (7)
Cl4	0.92138 (6)	0.8306 (3)	0.00993 (7)	0.0243 (5)	0.599 (8)
Br4	0.92138 (6)	0.8306 (3)	0.00993 (7)	0.0243 (5)	0.401 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0129 (2)	0.0158 (2)	0.0121 (2)	0.0000 (2)	0.0006 (3)	−0.0021 (2)
N1	0.030 (4)	0.038 (5)	0.042 (5)	−0.008 (4)	0.002 (4)	0.005 (4)
N2	0.047 (5)	0.041 (5)	0.030 (5)	0.002 (4)	0.003 (4)	−0.001 (4)
C1	0.015 (5)	0.070 (8)	0.036 (7)	−0.003 (5)	−0.001 (4)	0.007 (6)
C2	0.031 (5)	0.048 (6)	0.038 (6)	−0.009 (4)	−0.002 (4)	−0.003 (4)
C3	0.036 (5)	0.078 (6)	0.030 (4)	0.008 (4)	0.018 (4)	0.014 (4)
C4	0.056 (6)	0.041 (6)	0.037 (7)	−0.006 (5)	0.004 (5)	−0.009 (5)
C5	0.061 (6)	0.039 (6)	0.034 (6)	−0.010 (5)	0.024 (5)	−0.008 (4)
C6	0.036 (5)	0.078 (6)	0.030 (4)	0.008 (4)	0.018 (4)	0.014 (4)
C7	0.048 (5)	0.030 (5)	0.024 (5)	−0.002 (4)	0.006 (4)	−0.007 (3)
Br1	0.0281 (10)	0.0262 (9)	0.0223 (8)	−0.0034 (7)	−0.0001 (7)	−0.0005 (7)
Se2	0.0174 (5)	0.0250 (4)	0.0295 (5)	0.0004 (4)	0.0004 (6)	−0.0013 (4)
N3	0.014 (3)	0.020 (3)	0.015 (3)	0.003 (3)	0.001 (2)	0.000 (3)
N4	0.012 (3)	0.022 (4)	0.033 (4)	−0.005 (3)	0.007 (3)	0.005 (3)
C8	0.014 (4)	0.027 (4)	0.023 (5)	−0.001 (3)	0.001 (3)	0.008 (4)
C9	0.018 (4)	0.021 (4)	0.032 (5)	0.000 (3)	0.002 (3)	0.001 (3)
C10	0.027 (5)	0.026 (5)	0.042 (6)	−0.010 (4)	0.002 (4)	0.008 (4)
C11	0.033 (4)	0.027 (4)	0.026 (5)	−0.009 (4)	−0.001 (4)	0.010 (3)
C12	0.031 (4)	0.021 (4)	0.021 (4)	0.004 (3)	−0.001 (4)	0.001 (3)
C13	0.015 (4)	0.030 (4)	0.016 (4)	0.003 (3)	0.008 (3)	0.000 (3)

C14	0.018 (4)	0.018 (4)	0.022 (4)	0.000 (3)	0.004 (3)	−0.002 (3)
Br2	0.0195 (9)	0.0159 (8)	0.0217 (8)	0.0018 (6)	0.0001 (6)	0.0030 (6)
Se3	0.0166 (5)	0.0178 (3)	0.0274 (5)	0.0018 (4)	0.0005 (5)	0.0014 (3)
N5	0.022 (3)	0.018 (3)	0.015 (3)	0.003 (3)	0.002 (3)	−0.004 (3)
N6	0.020 (3)	0.014 (3)	0.024 (4)	−0.004 (3)	0.001 (3)	0.003 (3)
C15	0.018 (4)	0.029 (5)	0.035 (6)	0.002 (4)	−0.004 (4)	−0.017 (4)
C16	0.020 (4)	0.021 (4)	0.023 (4)	0.000 (3)	0.003 (3)	0.001 (3)
C17	0.025 (3)	0.033 (3)	0.010 (3)	0.001 (3)	0.005 (2)	0.005 (2)
C18	0.040 (5)	0.027 (4)	0.019 (4)	−0.004 (4)	0.002 (4)	0.007 (3)
C19	0.033 (4)	0.028 (4)	0.014 (4)	0.003 (4)	0.008 (3)	0.006 (3)
C20	0.025 (3)	0.033 (3)	0.010 (3)	0.001 (3)	0.005 (2)	0.005 (2)
C21	0.020 (4)	0.027 (4)	0.015 (4)	0.003 (3)	0.008 (3)	0.000 (3)
Br3	0.0194 (9)	0.0154 (8)	0.0251 (9)	0.0044 (6)	−0.0003 (7)	0.0036 (6)
Se4	0.0129 (2)	0.0158 (2)	0.0121 (2)	0.0000 (2)	0.0006 (3)	−0.0021 (2)
N7	0.018 (3)	0.020 (3)	0.015 (3)	0.001 (3)	0.005 (3)	−0.003 (3)
N8	0.022 (4)	0.020 (3)	0.011 (3)	0.000 (3)	0.004 (3)	−0.004 (3)
C22	0.018 (4)	0.035 (5)	0.022 (5)	−0.003 (4)	0.002 (4)	−0.014 (4)
C23	0.025 (4)	0.016 (3)	0.005 (3)	0.003 (3)	0.006 (3)	−0.003 (3)
C24	0.029 (5)	0.017 (3)	0.020 (4)	0.001 (3)	0.001 (3)	0.005 (3)
C25	0.049 (5)	0.010 (3)	0.015 (4)	0.003 (3)	−0.001 (4)	0.002 (3)
C26	0.044 (5)	0.025 (4)	0.013 (4)	0.011 (4)	0.007 (4)	0.001 (3)
C27	0.036 (5)	0.015 (4)	0.022 (4)	0.011 (3)	0.007 (4)	−0.003 (3)
C28	0.026 (4)	0.017 (3)	0.011 (3)	0.007 (3)	0.004 (3)	0.003 (3)
Cl1	0.0281 (10)	0.0262 (9)	0.0223 (8)	−0.0034 (7)	−0.0001 (7)	−0.0005 (7)
Cl2	0.0195 (9)	0.0159 (8)	0.0217 (8)	0.0018 (6)	0.0001 (6)	0.0030 (6)
Cl3	0.0194 (9)	0.0154 (8)	0.0251 (9)	0.0044 (6)	−0.0003 (7)	0.0036 (6)
Cl4	0.0254 (9)	0.0273 (9)	0.0202 (8)	0.0010 (6)	0.0007 (5)	−0.0028 (6)
Br4	0.0254 (9)	0.0273 (9)	0.0202 (8)	0.0010 (6)	0.0007 (5)	−0.0028 (6)

Geometric parameters (Å, º)

Se1—N1	1.911 (10)	Se3—N5	1.860 (8)
Se1—N2	1.824 (11)	Se3—N6	1.757 (7)
Se1—Br1	2.772 (2)	Se3—Br3	2.783 (2)
N1—C1	1.489 (15)	N5—C15	1.466 (13)
N1—C7	1.312 (15)	N5—C21	1.347 (12)
N2—C2	1.318 (16)	N6—C16	1.338 (12)
C1—H1A	0.9800	C15—H15A	0.9800
C1—H1B	0.9800	C15—H15B	0.9800
C1—H1C	0.9800	C15—H15C	0.9800
C2—C3	1.374 (19)	C16—C17	1.417 (13)
C2—C7	1.439 (17)	C16—C21	1.448 (13)
C3—H3	0.9500	C17—H17	0.9500
C3—C4	1.409 (19)	C17—C18	1.335 (14)
C4—H4	0.9500	C18—H18	0.9500
C4—C5	1.44 (2)	C18—C19	1.450 (16)
C5—H5	0.9500	C19—H19	0.9500
C5—C6	1.21 (2)	C19—C20	1.371 (13)

C6—H6	0.9500	C20—H20	0.9500
C6—C7	1.465 (17)	C20—C21	1.422 (14)
Se2—N3	1.872 (7)	Se4—N7	1.870 (7)
Se2—N4	1.770 (8)	Se4—N8	1.784 (8)
Se2—Br2	2.796 (2)	Se4—Br4^{i}	2.7957 (19)
N3—C8	1.455 (12)	N7—C22	1.455 (12)
N3—C14	1.335 (11)	N7—C28	1.318 (11)
N4—C9	1.352 (12)	N8—C23	1.333 (10)
C8—H8A	0.9800	C22—H22A	0.9800
C8—H8B	0.9800	C22—H22B	0.9800
C8—H8C	0.9800	C22—H22C	0.9800
C9—C10	1.430 (13)	C23—C24	1.414 (13)
C9—C14	1.425 (13)	C23—C28	1.432 (13)
C10—H10	0.9500	C24—H24	0.9500
C10—C11	1.358 (15)	C24—C25	1.393 (14)
C11—H11	0.9500	C25—H25	0.9500
C11—C12	1.413 (15)	C25—C26	1.390 (16)
C12—H12	0.9500	C26—H26	0.9500
C12—C13	1.351 (13)	C26—C27	1.360 (15)
C13—H13	0.9500	C27—H27	0.9500
C13—C14	1.444 (13)	C27—C28	1.411 (12)

N1—Se1—Br1	171.6 (3)	N5—Se3—Br3	174.9 (3)
N2—Se1—N1	85.7 (5)	N6—Se3—N5	89.2 (4)
N2—Se1—Br1	86.6 (3)	N6—Se3—Br3	85.8 (3)
C1—N1—Se1	120.1 (8)	C15—N5—Se3	123.5 (7)
C7—N1—Se1	112.9 (8)	C21—N5—Se3	111.6 (6)
C7—N1—C1	126.8 (10)	C21—N5—C15	124.4 (9)
C2—N2—Se1	111.7 (9)	C16—N6—Se3	111.1 (6)
N1—C1—H1A	109.5	N5—C15—H15A	109.5
N1—C1—H1B	109.5	N5—C15—H15B	109.5
N1—C1—H1C	109.5	N5—C15—H15C	109.5
H1A—C1—H1B	109.5	H15A—C15—H15B	109.5
H1A—C1—H1C	109.5	H15A—C15—H15C	109.5
H1B—C1—H1C	109.5	H15B—C15—H15C	109.5
N2—C2—C3	122.2 (12)	N6—C16—C17	124.4 (9)
N2—C2—C7	118.3 (12)	N6—C16—C21	117.7 (8)
C3—C2—C7	119.3 (12)	C17—C16—C21	117.8 (9)
C2—C3—H3	120.2	C16—C17—H17	119.6
C2—C3—C4	119.7 (13)	C18—C17—C16	120.8 (10)
C4—C3—H3	120.2	C18—C17—H17	119.6
C3—C4—H4	120.8	C17—C18—H18	119.4
C3—C4—C5	118.5 (13)	C17—C18—C19	121.1 (9)
C5—C4—H4	120.8	C19—C18—H18	119.4
C4—C5—H5	119.2	C18—C19—H19	119.4
C6—C5—C4	121.7 (13)	C20—C19—C18	121.3 (10)
C6—C5—H5	119.2	C20—C19—H19	119.4
C5—C6—H6	118.0	C19—C20—H20	121.3

C5—C6—C7	124.1 (14)	C19—C20—C21	117.4 (10)
C7—C6—H6	118.0	C21—C20—H20	121.3
N1—C7—C2	111.3 (11)	N5—C21—C16	110.3 (8)
N1—C7—C6	133.0 (12)	N5—C21—C20	128.1 (9)
C2—C7—C6	115.7 (12)	C20—C21—C16	121.5 (9)
N3—Se2—Br2	173.4 (2)	N7—Se4—Br4^{i}	171.6 (2)
N4—Se2—N3	88.4 (4)	N8—Se4—N7	88.0 (3)
N4—Se2—Br2	86.5 (3)	N8—Se4—Br4^{i}	85.0 (2)
C8—N3—Se2	122.6 (6)	C22—N7—Se4	125.6 (6)
C14—N3—Se2	110.6 (6)	C28—N7—Se4	111.8 (6)
C14—N3—C8	126.2 (8)	C28—N7—C22	122.4 (8)
C9—N4—Se2	111.7 (6)	C23—N8—Se4	110.6 (6)
N3—C8—H8A	109.5	N7—C22—H22A	109.5
N3—C8—H8B	109.5	N7—C22—H22B	109.5
N3—C8—H8C	109.5	N7—C22—H22C	109.5
H8A—C8—H8B	109.5	H22A—C22—H22B	109.5
H8A—C8—H8C	109.5	H22A—C22—H22C	109.5
H8B—C8—H8C	109.5	H22B—C22—H22C	109.5
N4—C9—C10	123.3 (9)	N8—C23—C24	121.7 (9)
N4—C9—C14	115.9 (8)	N8—C23—C28	117.7 (8)
C14—C9—C10	120.4 (9)	C24—C23—C28	120.6 (8)
C9—C10—H10	121.0	C23—C24—H24	121.2
C11—C10—C9	118.0 (10)	C25—C24—C23	117.6 (9)
C11—C10—H10	121.0	C25—C24—H24	121.2
C10—C11—H11	119.0	C24—C25—H25	120.1
C10—C11—C12	122.0 (9)	C26—C25—C24	119.8 (9)
C12—C11—H11	119.0	C26—C25—H25	120.1
C11—C12—H12	119.0	C25—C26—H26	117.5
C13—C12—C11	122.1 (9)	C27—C26—C25	125.0 (9)
C13—C12—H12	119.0	C27—C26—H26	117.5
C12—C13—H13	120.8	C26—C27—H27	121.8
C12—C13—C14	118.4 (9)	C26—C27—C28	116.4 (10)
C14—C13—H13	120.8	C28—C27—H27	121.8
N3—C14—C9	113.0 (8)	N7—C28—C23	111.8 (7)
N3—C14—C13	127.9 (9)	N7—C28—C27	127.9 (9)
C9—C14—C13	119.1 (8)	C27—C28—C23	120.3 (9)
Se1—N1—C7—C2	−3.3 (12)	Se3—N5—C21—C20	−173.9 (8)
Se1—N1—C7—C6	176.2 (12)	Se3—N6—C16—C17	176.9 (8)
Se1—N2—C2—C3	174.9 (11)	Se3—N6—C16—C21	0.1 (10)
Se1—N2—C2—C7	−0.4 (15)	N5—Se3—N6—C16	1.8 (7)
N1—Se1—N2—C2	−1.1 (9)	N6—Se3—N5—C15	−175.0 (7)
N2—C2—C3—C4	173.1 (13)	N6—Se3—N5—C21	−3.5 (6)
N2—C2—C7—N1	2.6 (16)	N6—C16—C17—C18	−175.8 (9)
N2—C2—C7—C6	−177.0 (12)	N6—C16—C21—N5	−2.8 (12)
C1—N1—C7—C2	−177.6 (11)	N6—C16—C21—C20	175.2 (9)
C1—N1—C7—C6	2 (2)	C15—N5—C21—C16	175.5 (8)
C2—C3—C4—C5	7 (2)	C15—N5—C21—C20	−2.4 (15)

C3—C2—C7—N1	−172.9 (13)	C16—C17—C18—C19	−0.4 (15)
C3—C2—C7—C6	7.5 (18)	C17—C16—C21—N5	−179.8 (8)
C3—C4—C5—C6	3 (2)	C17—C16—C21—C20	−1.8 (13)
C4—C5—C6—C7	−7 (2)	C17—C18—C19—C20	0.8 (15)
C5—C6—C7—N1	−177.4 (14)	C18—C19—C20—C21	−1.6 (14)
C5—C6—C7—C2	2 (2)	C19—C20—C21—N5	179.8 (9)
C7—C2—C3—C4	−12 (2)	C19—C20—C21—C16	2.1 (14)
Br1—Se1—N2—C2	175.3 (9)	C21—C16—C17—C18	0.9 (14)
Se2—N3—C14—C9	−5.8 (10)	Br3—Se3—N6—C16	−177.2 (6)
Se2—N3—C14—C13	173.4 (8)	Se4—N7—C28—C23	−2.7 (9)
Se2—N4—C9—C10	−175.6 (8)	Se4—N7—C28—C27	175.8 (8)
Se2—N4—C9—C14	−2.1 (11)	Se4—N8—C23—C24	−178.8 (7)
N3—Se2—N4—C9	−1.0 (7)	Se4—N8—C23—C28	1.7 (10)
N4—Se2—N3—C8	176.3 (8)	N7—Se4—N8—C23	−2.5 (6)
N4—Se2—N3—C14	4.0 (6)	N8—Se4—N7—C22	177.9 (8)
N4—C9—C10—C11	174.7 (10)	N8—Se4—N7—C28	3.0 (7)
N4—C9—C14—N3	5.4 (12)	N8—C23—C24—C25	176.8 (8)
N4—C9—C14—C13	−173.9 (8)	N8—C23—C28—N7	0.8 (11)
C8—N3—C14—C9	−177.8 (9)	N8—C23—C28—C27	−177.9 (8)
C8—N3—C14—C13	1.4 (15)	C22—N7—C28—C23	−177.8 (8)
C9—C10—C11—C12	−2.6 (17)	C22—N7—C28—C27	0.8 (15)
C10—C9—C14—N3	179.1 (9)	C23—C24—C25—C26	0.8 (14)
C10—C9—C14—C13	−0.2 (14)	C24—C23—C28—N7	−178.8 (8)
C10—C11—C12—C13	2.7 (17)	C24—C23—C28—C27	2.6 (13)
C11—C12—C13—C14	−1.3 (15)	C24—C25—C26—C27	3.7 (15)
C12—C13—C14—N3	−179.1 (9)	C25—C26—C27—C28	−4.7 (15)
C12—C13—C14—C9	0.1 (14)	C26—C27—C28—N7	−176.9 (9)
C14—C9—C10—C11	1.4 (16)	C26—C27—C28—C23	1.5 (13)
Br2—Se2—N4—C9	174.8 (7)	C28—C23—C24—C25	−3.7 (13)
Se3—N5—C21—C16	4.0 (9)	Br4^{i}—Se4—N8—C23	172.7 (6)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.

1-Methyl-2,1,3-benzoselenadiazol-1-ium 0.5-chloride 0.365-dichlorobromate 0.135-tribromide (mo_llq14_0m)

Crystal data

$C_7H_7N_2Se^+·0.5Cl^-·0.365BrCl_2^-·0.135Br_3^-$
M_r = 303.30
Monoclinic, *C*2/*c*
a = 11.062 (2) Å
b = 13.640 (2) Å
c = 13.498 (2) Å
β = 110.489 (8)°
V = 1907.8 (6) Å^3
Z = 8

F(000) = 1159
D_x = 2.112 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9861 reflections
θ = 2.5–32.9°
μ = 7.46 mm^{-1}
T = 100 K
Block, yellow
0.1 × 0.1 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
φ and *ω* scans

Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.766, T_{max} = 0.862

53658 measured reflections
3644 independent reflections
3269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 33.2°$, $\theta_{min} = 2.5°$
$h = -17 \rightarrow 16$
$k = -20 \rightarrow 20$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.058$
$S = 1.07$
3644 reflections
116 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 4.5883P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -1.21$ e Å^{-3}

Special details

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

Refinement. Crystallographic data were obtained from crystals coated in Paratone oil and mounted on a Bruker Dual Source D8 Venture diffractometer using the IμS 3.0 Mo source at 70 W with a HELIOS Mo focusing optic (ELM33) in the McMaster Analytical X-ray (MAX) Diffraction Facility. Raw data were processed using XPREP as part of the APEX (v5/v6 software) and solved by intrinsic phasing (SHELXT) (Sheldrick, 2015*b*). Non-H atoms were refined anisotropically. H atoms were generated in ideal positions and then updated with each cycle of refinement, which was performed with SHELXL (Sheldrick, 2015*a*) in OLEX2-1.5 (Dolomanov *et al.*, 2009).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Se	0.18236 (2)	0.52058 (2)	0.79354 (2)	0.01324 (5)	
Br1	0.000000	0.500000	0.500000	0.01527 (6)	
Cl2	−0.0101 (11)	0.6565 (7)	0.5783 (9)	0.0206 (4)	0.729 (2)
Cl1	0.000000	0.37081 (4)	0.750000	0.01722 (11)	
N1	0.30515 (14)	0.61938 (10)	0.82492 (12)	0.0140 (3)	
N2	0.30759 (14)	0.43259 (11)	0.82653 (12)	0.0144 (3)	
C1	0.27314 (18)	0.72426 (13)	0.81572 (17)	0.0208 (3)	
H1A	0.179278	0.732317	0.792375	0.031*	
H1B	0.305465	0.754527	0.764002	0.031*	
H1C	0.313330	0.755930	0.884654	0.031*	
C7	0.42417 (16)	0.58236 (13)	0.85653 (13)	0.0134 (3)	
C6	0.54255 (17)	0.63534 (13)	0.88755 (14)	0.0165 (3)	
H6	0.544070	0.704976	0.887630	0.020*	
C4	0.65333 (17)	0.47696 (14)	0.91747 (14)	0.0175 (3)	
H4	0.733191	0.442802	0.938469	0.021*	
C3	0.54138 (17)	0.42466 (13)	0.88844 (14)	0.0168 (3)	
H3	0.542597	0.355018	0.889313	0.020*	
C2	0.42242 (16)	0.47704 (13)	0.85672 (13)	0.0134 (3)	
C5	0.65407 (17)	0.58156 (14)	0.91724 (14)	0.0181 (3)	
H5	0.734490	0.614942	0.938362	0.022*	

Br2	−0.0081 (12)	0.6642 (8)	0.5774 (10)	0.0206 (4)	0.271 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se	0.01085 (8)	0.01124 (8)	0.01692 (8)	0.00025 (5)	0.00398 (6)	0.00076 (5)
Br1	0.01204 (10)	0.01718 (11)	0.01554 (11)	0.00019 (8)	0.00349 (8)	0.00201 (8)
Cl2	0.0223 (3)	0.0143 (12)	0.0229 (2)	0.0016 (7)	0.00510 (18)	−0.0003 (6)
Cl1	0.0158 (2)	0.0111 (2)	0.0265 (3)	0.000	0.0095 (2)	0.000
N1	0.0119 (6)	0.0120 (6)	0.0171 (6)	−0.0009 (5)	0.0039 (5)	0.0017 (5)
N2	0.0143 (6)	0.0128 (6)	0.0161 (6)	0.0018 (5)	0.0055 (5)	0.0004 (5)
C1	0.0164 (8)	0.0109 (7)	0.0325 (10)	−0.0007 (6)	0.0054 (7)	0.0018 (6)
C7	0.0123 (7)	0.0155 (7)	0.0124 (7)	−0.0005 (5)	0.0045 (6)	0.0016 (5)
C6	0.0147 (7)	0.0181 (8)	0.0159 (7)	−0.0021 (6)	0.0042 (6)	0.0024 (6)
C4	0.0124 (7)	0.0255 (9)	0.0146 (7)	0.0020 (6)	0.0048 (6)	0.0011 (6)
C3	0.0156 (8)	0.0183 (8)	0.0168 (7)	0.0042 (6)	0.0060 (6)	0.0006 (6)
C2	0.0132 (7)	0.0153 (7)	0.0118 (7)	0.0011 (5)	0.0043 (6)	0.0005 (5)
C5	0.0129 (7)	0.0256 (9)	0.0155 (7)	−0.0010 (6)	0.0045 (6)	0.0020 (6)
Br2	0.0223 (3)	0.0143 (12)	0.0229 (2)	0.0016 (7)	0.00510 (18)	−0.0003 (6)

Geometric parameters (Å, º)

Se—N1	1.8541 (15)	C1—H1C	0.9800
Se—N2	1.7681 (15)	C7—C6	1.424 (2)
Br1—Cl2	2.403 (11)	C7—C2	1.437 (2)
Br1—Cl2^{i}	2.403 (11)	C6—H6	0.9500
Br1—Br2	2.486 (12)	C6—C5	1.369 (3)
Br1—Br2^{i}	2.486 (12)	C4—H4	0.9500
N1—C1	1.469 (2)	C4—C3	1.362 (3)
N1—C7	1.333 (2)	C4—C5	1.427 (3)
N2—C2	1.336 (2)	C3—H3	0.9500
C1—H1A	0.9800	C3—C2	1.425 (2)
C1—H1B	0.9800	C5—H5	0.9500
N2—Se—N1	89.38 (7)	C6—C7—C2	121.23 (15)
Cl2—Br1—Cl2^{i}	180.0	C7—C6—H6	121.4
Cl2^{i}—Br1—Br2^{i}	1.6 (6)	C5—C6—C7	117.11 (17)
Cl2—Br1—Br2^{i}	178.4 (6)	C5—C6—H6	121.4
Br2—Br1—Br2^{i}	180.0	C3—C4—H4	119.1
C1—N1—Se	123.58 (12)	C3—C4—C5	121.89 (17)
C7—N1—Se	111.12 (11)	C5—C4—H4	119.1
C7—N1—C1	125.30 (15)	C4—C3—H3	120.8
C2—N2—Se	110.26 (12)	C4—C3—C2	118.33 (17)
N1—C1—H1A	109.5	C2—C3—H3	120.8
N1—C1—H1B	109.5	N2—C2—C7	117.73 (15)
N1—C1—H1C	109.5	N2—C2—C3	122.92 (16)
H1A—C1—H1B	109.5	C3—C2—C7	119.35 (15)
H1A—C1—H1C	109.5	C6—C5—C4	122.09 (17)

H1B—C1—H1C	109.5	C6—C5—H5	119.0
N1—C7—C6	127.25 (16)	C4—C5—H5	119.0
N1—C7—C2	111.52 (15)		
Se—N1—C7—C6	−179.74 (14)	C1—N1—C7—C6	0.2 (3)
Se—N1—C7—C2	0.17 (17)	C1—N1—C7—C2	−179.93 (16)
Se—N2—C2—C7	−0.36 (18)	C7—C6—C5—C4	0.0 (3)
Se—N2—C2—C3	179.75 (13)	C6—C7—C2—N2	−179.96 (15)
N1—Se—N2—C2	0.37 (12)	C6—C7—C2—C3	−0.1 (2)
N1—C7—C6—C5	−179.99 (17)	C4—C3—C2—N2	179.77 (16)
N1—C7—C2—N2	0.1 (2)	C4—C3—C2—C7	−0.1 (2)
N1—C7—C2—C3	−179.98 (15)	C3—C4—C5—C6	−0.2 (3)
N2—Se—N1—C1	179.79 (15)	C2—C7—C6—C5	0.1 (2)
N2—Se—N1—C7	−0.31 (12)	C5—C4—C3—C2	0.3 (3)

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.