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# (7a*R**,12b*S**)-8,12b-Dihydro-7a*H*-indeno[1′,2′:5,6][1,4]selenazino[2,3,4-*ij*]-quinolin-13-ium hydrogen sulfate

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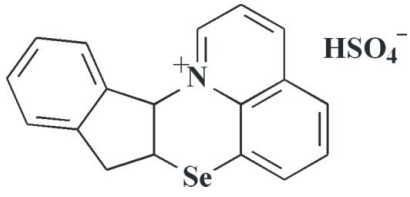
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.044; $wR$ factor = 0.114; data-to-parameter ratio = 17.7.

In the title compound, $C_{18}H_{14}NSe^{+}\cdot HSO_4^{-}$, the cyclopentene ring in the cation has an envelope conformation while the central six-membered 1,4-selenazine ring adopts a sofa conformation. The dihedral angle between the planes of the terminal benzene rings is 68.08 (11)°. In the crystal, the anions form chains along the $c$ axis through O—H···O hydrogen bonds. Weak C—H···O and C—H···$\pi$ hydrogen bonds, as well as attractive Se···Se [3.5608 (8) Å] interactions, further consolidate the crystal structure.

## Related literature

For the synthesis and biological properties of selenium- and nitrogen-containing heterocycles, see: Mugesh *et al.* (2001); Koketsu & Ishihara (2003); Nogueira *et al.* (2004); Bhabak & Mugesh (2007); Mlochowski & Giurg (2009); Back (2009); Mukherjee *et al.* (2010). For related compounds, see: Wright (2001); Garud *et al.* (2007); Sommen *et al.* (2007); Borisov *et al.* (2011).




## Experimental

### Crystal data

$C_{18}H_{14}NSe^{+}\cdot HSO_4^{-}$
$M_r$ = 420.34
Monoclinic, $P2_1/c$
$a$ = 11.1355 (11) Å
$b$ = 19.5653 (19) Å
$c$ = 7.9609 (8) Å
$\beta$ = 107.005 (2)°
$V$ = 1658.6 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.41 mm$^{-1}$
$T$ = 120 K
0.20 × 0.02 × 0.02 mm

### Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min}$ = 0.644, $T_{max}$ = 0.953
14396 measured reflections
4007 independent reflections
2902 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
$S$ = 1.00
4007 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.51 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg* is the centroid of the C3*A*/C4–C6/C6*A*/C13*A* ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4*O*···O3$^{i}$ | 0.96 | 1.59 | 2.548 (3) | 171 |
| C1—H1···O1 | 0.95 | 2.19 | 3.114 (4) | 165 |
| C3—H3···O2$^{ii}$ | 0.95 | 2.28 | 3.154 (4) | 153 |
| C4—H4···O2$^{ii}$ | 0.95 | 2.49 | 3.308 (4) | 144 |
| C5—H5···O4$^{iii}$ | 0.95 | 2.55 | 3.367 (4) | 145 |
| C7*A*—H7*A*···O2$^{iv}$ | 1.00 | 2.49 | 3.367 (4) | 146 |
| C12*B*—H12*B*···O1$^{i}$ | 1.00 | 2.42 | 3.244 (4) | 139 |
| C12*B*—H12*B*···O3$^{i}$ | 1.00 | 2.57 | 3.355 (4) | 135 |
| C11—H11···*Cg*$^{v}$ | 0.95 | 2.78 | 3.679 (4) | 159 |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x, -y+1, -z+1$; (iii) $-x, -y+1, -z$; (iv) $x, y, z-1$; (v) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2313).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o3286-o3287 [ **doi:10.1107/S1600536811047167** ]

# (7a*R**,12b*S**)-8,12b-Dihydro-7a*H*-indeno[1',2':5,6][1,4]selenazino[2,3,4-*ij*]quinolin-13-ium hydrogen sulfate

**G. Z. Mammadova, Z. V. Matsulevich, G. N. Borisova, A. V. Borisov and V. N. Khrustalev**

## Comment

In the last years, the selenium- and nitrogen-containing heterocycles have attracted considerable attention owing to the variety of their pharmacological properties (Mugesh *et al.*, 2001; Wright, 2001; Koketsu & Ishihara, 2003; Nogueira *et al.*, 2004; Bhabak & Mugesh, 2007; Garud *et al.*, 2007; Sommen *et al.*, 2007; Back, 2009; Mlochowski & Giurg, 2009; Mukherjee *et al.*, 2010). This article describes the structure of 8,12*b*-dihydro-7a*H*-indeno[1',2':5,6][1,4]selenazino[2,3,4- *ij*]quinolin-13-ium hydrosulfate, which was obtained by a reaction of 8,12*b*-dihydro-7a*H*-indeno[1',2':5,6][1,4]selenazino[2,3,4-*ij*]quinolin-13-ium chloride (Borisov *et al.*, 2011) with potassium hydrosulfate (Fig. 1).

The title compound of **I**, $[C_{18}H_{14}NSe][HSO_4]$, is a salt consisting of indeno[1',2':5,6][1,4]selenazino[2,3,4-*ij*]quinolin-13-ium cation and hydrosulfate anion. The cation of **I** comprises a fused pentacyclic system containing one five-membered ring (cyclopentene) and four six-membered rings (two benzene, 3,6-dihydro-1,4-selenazine and pyridine) (Fig. 2). The cyclopentene ring has the usual *envelope* conformation (the C7A carbon atom is out of the plane through the other atoms of the ring by 0.549 (5)Å)), and the central six-membered 1,4-selenazine ring adopts a *sofa* conformation (the C7A carbon atom is out of the plane through the other atoms of the ring by 0.677 (4)Å). The dihedral angle between the planes of the terminal benzene rings is 68.08 (11)°.

In the crystal, anions of **I** form chains along the *c* axis through the intermolecular O4—H4O···O3$^{i}$ hydrogen bonding interactions (Table 1, Fig. 3). Weak intermolecular C—H···O (Table 1) and C11—H11···π (C3A$^{v}$–C4$^{v}$) (the H11···C3A$^{v}$ and H11···C4$^{v}$ distances are 2.79Å and 2.86Å, respectively) hydrogen bonds as well as attractive Se···Se$^{vi}$ (3.5608 (8)Å) interactions consolidate further the three-dimensional crystal packing (Fig. 3). Symmetry codes: (i) *x*, -*y*+3/2, *z*-1/2; (v) -*x*+1, -*y*+1, -*z*; (vi) -*x*+1, -*y*+1, -*z*+1.

The cation of **I** possesses two asymmetric centers at the C7A and C12B carbon atoms and can have potentially four diastereomers. The crystal of **I** is racemic and consists of enantiomeric pairs with the following relative configuration of the centers: ***rac***-7a***R*****,12*b****S*****.

## Experimental

A mixture of 8,12*b*-dihydro-7a*H*-indeno[1',2':5,6][1,4]selenazino[2,3,4- *ij*]quinolin-13-ium chloride (0.147 g, 0.4 mmol) with $KHSO_4$ (0.057 g, 0.42 mmol) in $CH_3OH$ (20 ml) was refluxed for 0.5 h to dissolve the starting materials. After that the reaction mixture was concentrated in *vacuo*. Then $CH_2Cl_2$ (20 ml) was added to the solid to give precipitate of KCl which was separated by filtration. The filtrate was concentrated in *vacuo*. The solid was recrystallized from $CH_2Cl_2$ to give **I** as orange needles. Yield is 89%. M.p. = 502–503 K. IR (KBr), ν ($cm^{-1}$): 3481, 2987, 1608, 1552, 1485, 1440, 1294, 1172, 1134, 796, 721, 468, 419. $^1$H NMR (DMSO-$d_6$, 300 MHz, 302 K): δ = 9.72 (dd, 1H, H1, J = 6.0, J = 1.3), 9.45 (dd, 1H, H3, J = 8.4, J = 1.4), 8.37 (dd, 1H, H2, J = 8.3, J = 5.8), 8.28 (dd, 1H, H4, J = 8.1, J = 1.3), 8.23 (dd, 1H, H6, J = 7.5, J = 1.3),

7.83 (t, 1H, H5, J = 7.8), 7.52 (d, 1H, H9, J = 7.5), 7.31 (t, 1H, H10, J = 7.5), 7.14 (t, 1H, H11, J = 7.5), 6.89 (d, 1H, H12*b*, J = 4.7), 6.60 (d, 1H, H12, J = 7.6), 4.87 (t, 1H, H7a, J = 4.7), 3.59 (dd, 1H, H8, J = 16.8, J = 4.7), 3.25 (d, H8, J = 16.8). Anal. Calcd. for $C_{18}H_{15}NO_4SSe$: C, 51.43; H, 3.59; N, 3.33. Found: C, 51.34; H, 3.52; N, 3.29.

### Refinement

The hydroxyl hydrogen atom was localized in the difference-Fourier map and included in the refinement with fixed positional and isotropic displacement parameters [$U_{iso}$(H) = 1.5$U_{eq}$(O)]. The other hydrogen atoms were placed in calculated positions with C—H = 0.95–1.00Å and refined in the riding model with fixed isotropic displacement parameters [$U_{iso}$(H) = 1.2$U_{eq}$(C)].

### Figures

Fig. 1. Reaction of 8,12*b*-dihydro-7a*H*-indeno[1',2':5,6][1,4]selenazino[2,3,4- *ij*]quinolin-13-ium chloride with potassium hydrosulfate.

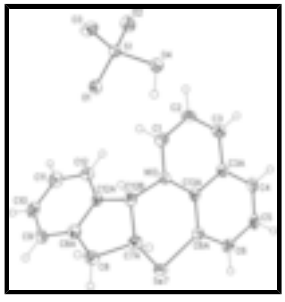

Fig. 2. Molecular structure of **I**. Displacement ellipsoids are shown at the 50% probability level.

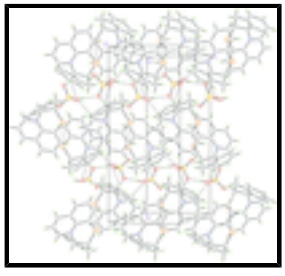

Fig. 3. Crystal packing of **I** demonstrating the anionic chains along the *c* axis. Dashed lines indicate the intermolecular hydrogen bonding and attractive Se···Se interactions.

### (7a*R**,12b*S**)-8,12b-Dihydro-7a*H*- indeno[1',2':5,6][1,4]selenazino[2,3,4-*ij*]quinolin-13-ium hydrogen sulfate

*Crystal data*

| | |
|---|---|
| $C_{18}H_{14}NSe^{+}\cdot HSO_4^{-}$ | $F$(000) = 848 |
| $M_r$ = 420.34 | $D_x$ = 1.683 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point = 502–503 K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $a$ = 11.1355 (11) Å | Cell parameters from 2341 reflections |
| $b$ = 19.5653 (19) Å | θ = 2.2–24.8° |
| $c$ = 7.9609 (8) Å | μ = 2.41 mm$^{-1}$ |
| β = 107.005 (2)° | $T$ = 120 K |
| $V$ = 1658.6 (3) Å$^3$ | Needle, orange |

| | |
|---|---|
| $Z = 4$ | 0.20 × 0.02 × 0.02 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART 1K CCD diffractometer | 4007 independent reflections |
| Radiation source: fine-focus sealed tube | 2902 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.054$ |
| φ and ω scans | $\theta_{max} = 28.0°$, $\theta_{min} = 1.9°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998) | $h = -14 \rightarrow 14$ |
| $T_{min} = 0.644$, $T_{max} = 0.953$ | $k = -24 \rightarrow 25$ |
| 14396 measured reflections | $l = -10 \rightarrow 10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.114$ | H-atom parameters constrained |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 2.36P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4007 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 226 parameters | $\Delta\rho_{max} = 1.00$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.51$ e Å$^{-3}$ |

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1870 (3) | 0.58708 (18) | 0.3376 (5) | 0.0216 (7) |
| H1 | 0.2013 | 0.6277 | 0.4059 | 0.026* |
| C2 | 0.1119 (3) | 0.53643 (18) | 0.3759 (5) | 0.0242 (8) |
| H2 | 0.0772 | 0.5420 | 0.4708 | 0.029* |
| C3 | 0.0884 (3) | 0.47893 (19) | 0.2765 (5) | 0.0236 (7) |
| H3 | 0.0365 | 0.4441 | 0.3010 | 0.028* |

| | | | | |
|---|---|---|---|---|
| C3A | 0.1413 (3) | 0.47090 (17) | 0.1365 (4) | 0.0183 (7) |
| C4 | 0.1189 (3) | 0.40994 (19) | 0.0350 (5) | 0.0227 (7) |
| H4 | 0.0648 | 0.3756 | 0.0564 | 0.027* |
| C5 | 0.1763 (3) | 0.40145 (19) | −0.0938 (5) | 0.0246 (8) |
| H5 | 0.1622 | 0.3608 | −0.1621 | 0.030* |
| C6 | 0.2556 (3) | 0.45222 (19) | −0.1259 (4) | 0.0224 (7) |
| H6 | 0.2938 | 0.4452 | −0.2167 | 0.027* |
| C6A | 0.2801 (3) | 0.51193 (17) | −0.0303 (4) | 0.0192 (7) |
| Se7 | 0.40049 (3) | 0.571862 (19) | −0.07394 (4) | 0.02345 (12) |
| C7A | 0.3453 (3) | 0.65434 (18) | 0.0190 (4) | 0.0218 (7) |
| H7A | 0.2719 | 0.6763 | −0.0679 | 0.026* |
| C8 | 0.4599 (3) | 0.70229 (18) | 0.0743 (4) | 0.0242 (8) |
| H8A | 0.5125 | 0.6978 | −0.0061 | 0.029* |
| H8B | 0.4334 | 0.7505 | 0.0757 | 0.029* |
| C8A | 0.5298 (3) | 0.67800 (17) | 0.2574 (4) | 0.0208 (7) |
| C9 | 0.6519 (3) | 0.69027 (18) | 0.3579 (5) | 0.0237 (7) |
| H9 | 0.7065 | 0.7171 | 0.3129 | 0.028* |
| C10 | 0.6934 (3) | 0.6625 (2) | 0.5264 (5) | 0.0274 (8) |
| H10 | 0.7772 | 0.6704 | 0.5967 | 0.033* |
| C11 | 0.6130 (3) | 0.6235 (2) | 0.5921 (5) | 0.0274 (8) |
| H11 | 0.6426 | 0.6048 | 0.7070 | 0.033* |
| C12 | 0.4901 (3) | 0.61157 (18) | 0.4919 (4) | 0.0215 (7) |
| H12 | 0.4349 | 0.5851 | 0.5369 | 0.026* |
| C12A | 0.4499 (3) | 0.63916 (16) | 0.3249 (4) | 0.0164 (6) |
| C12B | 0.3200 (3) | 0.64029 (17) | 0.1943 (4) | 0.0182 (7) |
| H12B | 0.2770 | 0.6818 | 0.2221 | 0.022* |
| N13 | 0.2398 (2) | 0.58057 (13) | 0.2079 (3) | 0.0155 (5) |
| C13A | 0.2219 (3) | 0.52230 (17) | 0.1038 (4) | 0.0165 (6) |
| S1 | 0.07534 (8) | 0.71231 (4) | 0.61913 (10) | 0.01767 (18) |
| O1 | 0.1979 (2) | 0.70926 (12) | 0.5924 (3) | 0.0217 (5) |
| O2 | 0.0535 (2) | 0.66144 (13) | 0.7377 (3) | 0.0268 (6) |
| O3 | 0.0469 (2) | 0.78149 (12) | 0.6674 (3) | 0.0232 (5) |
| O4 | −0.0231 (2) | 0.69555 (14) | 0.4394 (3) | 0.0290 (6) |
| H4O | 0.0104 | 0.7065 | 0.3440 | 0.043* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0230 (17) | 0.0187 (18) | 0.0244 (17) | 0.0016 (14) | 0.0093 (14) | −0.0044 (13) |
| C2 | 0.0268 (18) | 0.025 (2) | 0.0273 (18) | −0.0002 (15) | 0.0177 (15) | −0.0031 (14) |
| C3 | 0.0234 (17) | 0.0207 (18) | 0.0289 (18) | −0.0007 (14) | 0.0111 (15) | 0.0006 (14) |
| C3A | 0.0149 (15) | 0.0174 (17) | 0.0213 (16) | 0.0016 (13) | 0.0034 (13) | −0.0001 (13) |
| C4 | 0.0169 (16) | 0.0240 (19) | 0.0252 (17) | −0.0037 (14) | 0.0028 (14) | −0.0028 (14) |
| C5 | 0.0223 (18) | 0.0213 (18) | 0.0274 (18) | −0.0050 (14) | 0.0028 (15) | −0.0100 (14) |
| C6 | 0.0197 (17) | 0.0265 (19) | 0.0206 (16) | 0.0021 (15) | 0.0052 (14) | −0.0053 (14) |
| C6A | 0.0184 (16) | 0.0206 (18) | 0.0184 (15) | −0.0026 (13) | 0.0049 (13) | −0.0009 (13) |
| Se7 | 0.0276 (2) | 0.0244 (2) | 0.02247 (19) | −0.00505 (15) | 0.01375 (14) | −0.00375 (14) |
| C7A | 0.0265 (18) | 0.0193 (18) | 0.0191 (16) | 0.0015 (14) | 0.0059 (14) | 0.0041 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.032 (2) | 0.0197 (18) | 0.0226 (17) | −0.0019 (15) | 0.0101 (15) | 0.0031 (14) |
| C8A | 0.0270 (18) | 0.0117 (16) | 0.0262 (17) | 0.0012 (14) | 0.0119 (15) | −0.0013 (13) |
| C9 | 0.0201 (17) | 0.0204 (18) | 0.0335 (19) | −0.0041 (14) | 0.0122 (15) | −0.0062 (15) |
| C10 | 0.0180 (17) | 0.034 (2) | 0.0269 (18) | 0.0022 (15) | 0.0015 (14) | −0.0095 (16) |
| C11 | 0.0248 (19) | 0.029 (2) | 0.0254 (18) | 0.0051 (16) | 0.0026 (15) | 0.0003 (15) |
| C12 | 0.0204 (17) | 0.0222 (18) | 0.0214 (16) | 0.0024 (14) | 0.0055 (13) | 0.0022 (14) |
| C12A | 0.0169 (15) | 0.0141 (16) | 0.0179 (15) | 0.0012 (13) | 0.0046 (12) | −0.0031 (12) |
| C12B | 0.0186 (16) | 0.0150 (16) | 0.0195 (16) | −0.0001 (13) | 0.0034 (13) | 0.0009 (13) |
| N13 | 0.0144 (13) | 0.0135 (14) | 0.0190 (13) | 0.0012 (10) | 0.0056 (10) | 0.0001 (10) |
| C13A | 0.0126 (14) | 0.0155 (16) | 0.0188 (15) | 0.0018 (12) | 0.0007 (12) | −0.0017 (12) |
| S1 | 0.0187 (4) | 0.0188 (4) | 0.0159 (4) | −0.0036 (3) | 0.0057 (3) | −0.0017 (3) |
| O1 | 0.0203 (12) | 0.0209 (13) | 0.0244 (12) | −0.0030 (10) | 0.0074 (10) | −0.0040 (10) |
| O2 | 0.0313 (14) | 0.0236 (14) | 0.0261 (13) | −0.0067 (11) | 0.0095 (11) | 0.0032 (10) |
| O3 | 0.0317 (14) | 0.0212 (13) | 0.0189 (11) | 0.0032 (11) | 0.0107 (10) | 0.0012 (10) |
| O4 | 0.0227 (13) | 0.0483 (17) | 0.0163 (12) | −0.0130 (12) | 0.0064 (10) | −0.0072 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N13 | 1.336 (4) | C8—H8A | 0.9900 |
| C1—C2 | 1.386 (5) | C8—H8B | 0.9900 |
| C1—H1 | 0.9500 | C8A—C9 | 1.382 (5) |
| C2—C3 | 1.356 (5) | C8A—C12A | 1.391 (4) |
| C2—H2 | 0.9500 | C9—C10 | 1.395 (5) |
| C3—C3A | 1.414 (5) | C9—H9 | 0.9500 |
| C3—H3 | 0.9500 | C10—C11 | 1.390 (5) |
| C3A—C4 | 1.421 (5) | C10—H10 | 0.9500 |
| C3A—C13A | 1.422 (5) | C11—C12 | 1.388 (5) |
| C4—C5 | 1.368 (5) | C11—H11 | 0.9500 |
| C4—H4 | 0.9500 | C12—C12A | 1.383 (5) |
| C5—C6 | 1.401 (5) | C12—H12 | 0.9500 |
| C5—H5 | 0.9500 | C12A—C12B | 1.515 (4) |
| C6—C6A | 1.377 (5) | C12B—N13 | 1.494 (4) |
| C6—H6 | 0.9500 | C12B—H12B | 1.0000 |
| C6A—C13A | 1.416 (4) | N13—C13A | 1.389 (4) |
| C6A—Se7 | 1.888 (3) | S1—O2 | 1.441 (2) |
| Se7—C7A | 1.948 (3) | S1—O1 | 1.443 (2) |
| C7A—C12B | 1.527 (4) | S1—O3 | 1.467 (2) |
| C7A—C8 | 1.541 (5) | S1—O4 | 1.562 (2) |
| C7A—H7A | 1.0000 | O4—H4O | 0.9632 |
| C8—C8A | 1.514 (5) | | |
| N13—C1—C2 | 122.1 (3) | C9—C8A—C12A | 120.2 (3) |
| N13—C1—H1 | 118.9 | C9—C8A—C8 | 130.1 (3) |
| C2—C1—H1 | 118.9 | C12A—C8A—C8 | 109.7 (3) |
| C3—C2—C1 | 119.4 (3) | C8A—C9—C10 | 118.8 (3) |
| C3—C2—H2 | 120.3 | C8A—C9—H9 | 120.6 |
| C1—C2—H2 | 120.3 | C10—C9—H9 | 120.6 |
| C2—C3—C3A | 119.9 (3) | C11—C10—C9 | 120.5 (3) |
| C2—C3—H3 | 120.1 | C11—C10—H10 | 119.8 |
| C3A—C3—H3 | 120.1 | C9—C10—H10 | 119.8 |

| | | | |
|---|---|---|---|
| C3—C3A—C4 | 119.8 (3) | C12—C11—C10 | 120.8 (3) |
| C3—C3A—C13A | 119.8 (3) | C12—C11—H11 | 119.6 |
| C4—C3A—C13A | 120.3 (3) | C10—C11—H11 | 119.6 |
| C5—C4—C3A | 119.0 (3) | C12A—C12—C11 | 118.3 (3) |
| C5—C4—H4 | 120.5 | C12A—C12—H12 | 120.8 |
| C3A—C4—H4 | 120.5 | C11—C12—H12 | 120.8 |
| C4—C5—C6 | 120.5 (3) | C12—C12A—C8A | 121.4 (3) |
| C4—C5—H5 | 119.7 | C12—C12A—C12B | 129.9 (3) |
| C6—C5—H5 | 119.7 | C8A—C12A—C12B | 108.5 (3) |
| C6A—C6—C5 | 122.3 (3) | N13—C12B—C12A | 114.2 (3) |
| C6A—C6—H6 | 118.8 | N13—C12B—C7A | 118.7 (3) |
| C5—C6—H6 | 118.8 | C12A—C12B—C7A | 103.6 (3) |
| C6—C6A—C13A | 118.5 (3) | N13—C12B—H12B | 106.5 |
| C6—C6A—Se7 | 117.5 (3) | C12A—C12B—H12B | 106.5 |
| C13A—C6A—Se7 | 123.8 (2) | C7A—C12B—H12B | 106.5 |
| C6A—Se7—C7A | 97.16 (15) | C1—N13—C13A | 121.4 (3) |
| C12B—C7A—C8 | 102.0 (3) | C1—N13—C12B | 112.9 (3) |
| C12B—C7A—Se7 | 111.2 (2) | C13A—N13—C12B | 125.7 (3) |
| C8—C7A—Se7 | 106.6 (2) | N13—C13A—C6A | 123.4 (3) |
| C12B—C7A—H7A | 112.2 | N13—C13A—C3A | 117.3 (3) |
| C8—C7A—H7A | 112.2 | C6A—C13A—C3A | 119.3 (3) |
| Se7—C7A—H7A | 112.2 | O2—S1—O1 | 114.60 (15) |
| C8A—C8—C7A | 103.5 (3) | O2—S1—O3 | 112.03 (15) |
| C8A—C8—H8A | 111.1 | O1—S1—O3 | 111.29 (15) |
| C7A—C8—H8A | 111.1 | O2—S1—O4 | 104.34 (15) |
| C8A—C8—H8B | 111.1 | O1—S1—O4 | 107.28 (14) |
| C7A—C8—H8B | 111.1 | O3—S1—O4 | 106.62 (15) |
| H8A—C8—H8B | 109.0 | S1—O4—H4O | 110.2 |
| N13—C1—C2—C3 | −1.6 (5) | C8—C8A—C12A—C12B | −4.2 (4) |
| C1—C2—C3—C3A | 0.6 (5) | C12—C12A—C12B—N13 | −30.0 (5) |
| C2—C3—C3A—C4 | 178.6 (3) | C8A—C12A—C12B—N13 | 155.7 (3) |
| C2—C3—C3A—C13A | 1.9 (5) | C12—C12A—C12B—C7A | −160.7 (3) |
| C3—C3A—C4—C5 | −176.5 (3) | C8A—C12A—C12B—C7A | 25.1 (3) |
| C13A—C3A—C4—C5 | 0.2 (5) | C8—C7A—C12B—N13 | −162.7 (3) |
| C3A—C4—C5—C6 | −0.3 (5) | Se7—C7A—C12B—N13 | −49.4 (4) |
| C4—C5—C6—C6A | 0.4 (5) | C8—C7A—C12B—C12A | −34.8 (3) |
| C5—C6—C6A—C13A | −0.5 (5) | Se7—C7A—C12B—C12A | 78.5 (3) |
| C5—C6—C6A—Se7 | 174.4 (3) | C2—C1—N13—C13A | 0.1 (5) |
| C6—C6A—Se7—C7A | 159.0 (3) | C2—C1—N13—C12B | −178.1 (3) |
| C13A—C6A—Se7—C7A | −26.4 (3) | C12A—C12B—N13—C1 | 80.4 (3) |
| C6A—Se7—C7A—C12B | 44.9 (3) | C7A—C12B—N13—C1 | −156.9 (3) |
| C6A—Se7—C7A—C8 | 155.2 (2) | C12A—C12B—N13—C13A | −97.7 (4) |
| C12B—C7A—C8—C8A | 32.3 (3) | C7A—C12B—N13—C13A | 25.0 (4) |
| Se7—C7A—C8—C8A | −84.4 (3) | C1—N13—C13A—C6A | −177.3 (3) |
| C7A—C8—C8A—C9 | 163.5 (3) | C12B—N13—C13A—C6A | 0.6 (5) |
| C7A—C8—C8A—C12A | −18.1 (4) | C1—N13—C13A—C3A | 2.3 (4) |
| C12A—C8A—C9—C10 | 0.6 (5) | C12B—N13—C13A—C3A | −179.7 (3) |
| C8—C8A—C9—C10 | 178.8 (3) | C6—C6A—C13A—N13 | −179.9 (3) |
| C8A—C9—C10—C11 | −0.3 (5) | Se7—C6A—C13A—N13 | 5.5 (5) |

| | | | |
|---|---|---|---|
| C9—C10—C11—C12 | −0.2 (6) | C6—C6A—C13A—C3A | 0.5 (5) |
| C10—C11—C12—C12A | 0.3 (5) | Se7—C6A—C13A—C3A | −174.2 (2) |
| C11—C12—C12A—C8A | 0.0 (5) | C3—C3A—C13A—N13 | −3.3 (5) |
| C11—C12—C12A—C12B | −173.6 (3) | C4—C3A—C13A—N13 | −179.9 (3) |
| C9—C8A—C12A—C12 | −0.5 (5) | C3—C3A—C13A—C6A | 176.4 (3) |
| C8—C8A—C12A—C12 | −179.0 (3) | C4—C3A—C13A—C6A | −0.3 (5) |
| C9—C8A—C12A—C12B | 174.4 (3) | | |

*Hydrogen-bond geometry (Å, °)*

Cg is the centroid of the C3A/C4–C6/C6A/C13A ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4O···O3$^{i}$ | 0.96 | 1.59 | 2.548 (3) | 171 |
| C1—H1···O1 | 0.95 | 2.19 | 3.114 (4) | 165 |
| C3—H3···O2$^{ii}$ | 0.95 | 2.28 | 3.154 (4) | 153 |
| C4—H4···O2$^{ii}$ | 0.95 | 2.49 | 3.308 (4) | 144 |
| C5—H5···O4$^{iii}$ | 0.95 | 2.55 | 3.367 (4) | 145 |
| C7A—H7A···O2$^{iv}$ | 1.00 | 2.49 | 3.367 (4) | 146 |
| C12B—H12B···O1$^{i}$ | 1.00 | 2.42 | 3.244 (4) | 139 |
| C12B—H12B···O3$^{i}$ | 1.00 | 2.57 | 3.355 (4) | 135 |
| C11—H11···Cg$^{v}$ | 0.95 | 2.78 | 3.679 (4) | 159 |

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, *y*, *z*−1; (v) −*x*+1, −*y*+1, −*z*+1.

**Fig. 1**

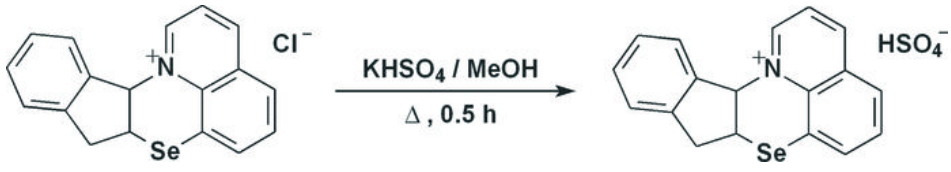

**Fig. 2**

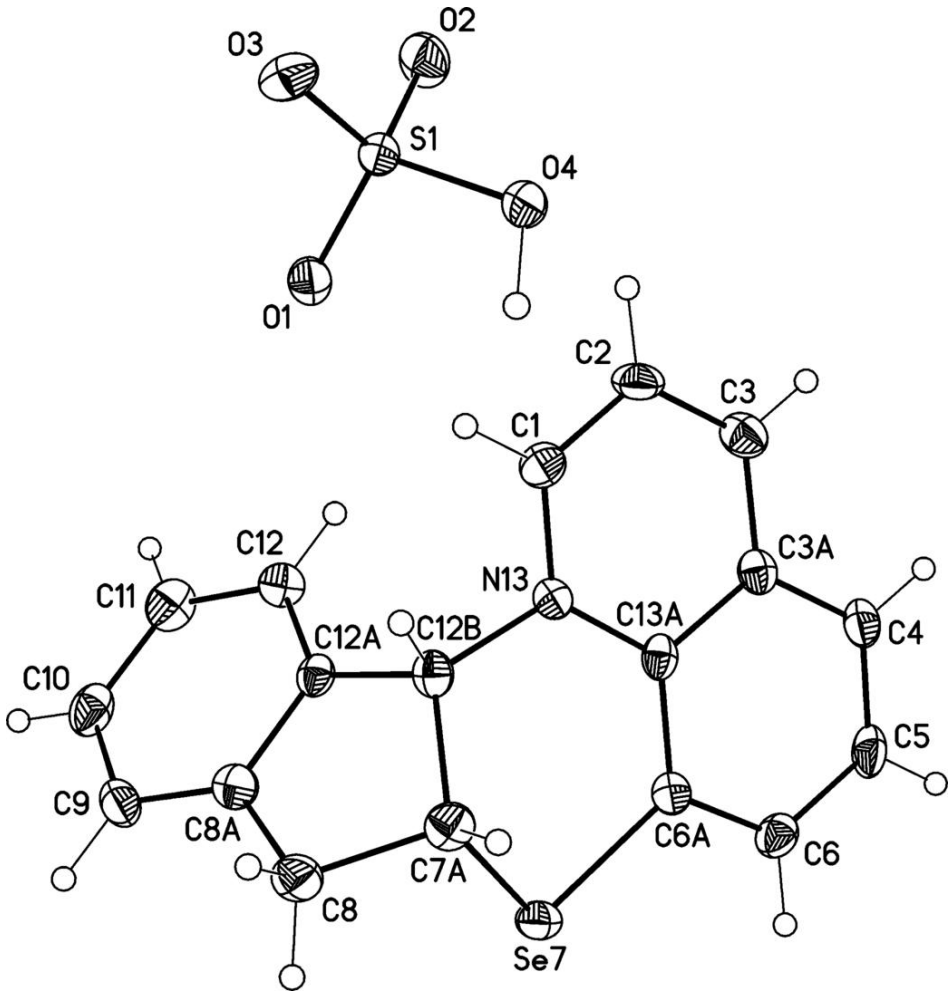
O3
O2
S1
O4
O1
C2
C3
C1
C12
C3A
N13
C11
C13A
C4
C12A
C12B
C10
C5
C9
C8A
C6A
C6
C7A
C8
Se7

**Fig. 3**