Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Methoxyphenyl)-1,3-selenazolo-[2,3-*b*][1,3]benzothiazol-4-ium hydrogen sulfate

Gunay Z. Mammadova,[a]* Zhanna V. Matsulevich,[b] Galina N. Borisova,[b] Alexander V. Borisov[b] and Victor N. Khrustalev[c]

[a]Baku State University, Z. Khalilov St 23, Baku, AZ-1148, Azerbaijan, [b]R.E. Alekseev Nizhny Novgorod State Technical University, 24 Minin St, Nizhny Novgorod, 603950, Russian Federation, and [c]X-Ray Structural Centre, A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov St, B-334, Moscow 119991, Russian Federation
Correspondence e-mail: gunka479@mail.ru

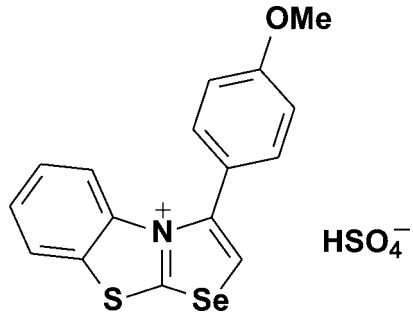
Received 2 April 2013; accepted 5 April 2013

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.085; data-to-parameter ratio = 18.3.

The title compound, $C_{16}H_{12}NOSSe^{+}\cdot HO_4S^{-}$, was obtained from a mixture of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*]-[1,3]benzothiazol-4-ium chloride and potassium hydrogen sulfate. In the cation, the benzene ring is twisted by 71.62 (7)° from the tricycle mean plane. In the crystal, O—H···O hydrogen bonds link the anions into chains along [100]. The anions in adjacent chains are linked *via* weak C—H···O hydrogen bonds. The crystal packing exhibits short intermolecular contacts between the chalcogen unit and the O atoms: Se···O(anion) 2.713 (3), Se···O(cation) 2.987 (3) and S···O(anion) 2.958 (3) Å.

Related literature

For details of the synthesis and the biological properties of selenium- and nitrogen-containing heterocycles, see: Back (2009); Mlochowski & Giurg (2009); Mukherjee *et al.* (2010); Selvakumar *et al.* (2010). For the synthesis of the starting compound, 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]-benzothiazol-4-ium chloride, see: Borisov *et al.* (2012).



Experimental

Crystal data

$C_{16}H_{12}NOSSe^{+}\cdot HO_4S^{-}$
M_r = 442.35
Monoclinic, $P2_1$
a = 4.6408 (8) Å
b = 18.263 (3) Å
c = 9.4482 (16) Å
β = 94.294 (3)°
V = 798.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.64 mm^{-1}
T = 100 K
0.30 × 0.18 × 0.02 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.505, T_{max} = 0.949
8638 measured reflections
4145 independent reflections
3555 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.085
S = 0.97
4145 reflections
227 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
Absolute structure: Flack (1983), 2075 Friedel pairs
Flack parameter: 0.038 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*O*···O4^{i}	0.91	1.80	2.610 (4)	147
C6—H6···O4^{ii}	0.95	2.54	3.494 (5)	178
C8—H8···O2^{iii}	0.95	2.26	3.022 (5)	137

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

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*.

We thank Professor Abel M. Maharramov for fruitful discussions and help in this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5401).

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supporting information

Acta Cryst. (2013). E**69**, o703–o704 [https://doi.org/10.1107/S1600536813009288]

3-(4-Methoxyphenyl)-1,3-selenazolo[2,3-*b*][1,3]benzothiazol-4-ium hydrogen sulfate

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S1. Comment

In the last years, the selenium- and nitrogen-containing heterocycles have attracted considerable attention owing to the variety of their pharmacological properties (Back, 2009; Mlochowski & Giurg, 2009; Mukherjee *et al.*, 2010; Selvakumar *et al.*, 2010). This article describes the structure of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]benzothiazol-4-ium hydrogen sulfate, $[C_{16}H_{12}NOSSe]^{+}.[HSO_4]^{-}$, (**I**), which was obtained by the reaction of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]benzothiazol-4-ium chloride (Borisov *et al.*, 2012) with potassium hydrogen sulfate (Figure 1).

The compound **I** is a salt consisting of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]benzothiazol-4-ium cation and hydrogen sulfate anion (Figure 2). The cation of **I** comprises a fused tricyclic system containing two five-membered rings (1,3-selenazole and 1,3-thiazole) and one six-membered ring (benzene). The tricyclic system is practically planar (r.m.s deviation = 0.020 Å). The methoxy group is almost coplanar to the plane of the phenyl substituent (the C12—C13—O1—C16 torsion angle is 1.7 (5)°). The dihedral angle between the mean planes of the tricyclic system and methoxyphenyl fragment is 71.82 (6)°.

In the crystal, anions form chains along the *a* axis through the intermolecular O—H···O hydrogen bonding interactions (Table 1, Figure 3). Weak intermolecular C—H···O hydrogen bonds (Table 1, Figure 3) as well as non-valent attractive Se···O (Se1···O3^{b} 2.713 (3), Se1···O1^{c} 2.987 (3), Se1···O3 3.366 (3), Se1···O5^{b} 3.423 (3) Å) and S···O [S9···O2^{a} 2.958 (3) and S9···O1^{c} 3.050 (3) Å] interactions consolidate further the three-dimensional-crystal packing (Figure 3) [symmetry codes: (a) *x*, *y*, *z* + 1; (b) *x*–1, *y*, *z*; (c) –*x*, *y* + 0.5, –*z* + 1].

S2. Experimental

A mixture of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]benzothiazol-4-ium chloride (0.19 g, 0.5 mmol) with $KHSO_4$ (0.072 g, 0.53 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 re-crystallized from CH_2Cl_2 to give **I** as colorless crystals. Yield is 93%. *M*.p. = 510–512 K. ^{1}H NMR (DMSO-d_6, 600 MHz, 302 K): δ = 8.42 (1*H*, d, *J* = 8.0, H8), 8.23 (1*H*, s, H2), 7.63 (1*H*, t, *J* = 8.0, H7), 7.59 (2*H*, d, *J* = 8.8, H11, H15), 7.48 (1*H*, t, *J* = 8.0, H6), 7.25 (2*H*, d, *J* = 8.8, H12, H14), 6.81 (1*H*, d, *J* = 8.1, H5), 3.87 (3*H*, s, O*Me*). Anal. Calcd. for $C_{16}H_{13}NO_5S_2Se$: C, 43.45; H, 2.96; N, 3.17. Found: C, 43.37; H, 2.93; N, 3.12.

S3. 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) = 1.5U_{eq}(O)]. The other hydrogen atoms were placed in

calculated positions with C—H = 0.95 Å (CH) and 0.98 Å (CH_3) and refined in the riding model with fixed isotropic displacement parameters [U_{iso}(H) = 1.5U_{eq}(C) for the CH_3 group and 1.2U_{eq}(C) for the CH groups].

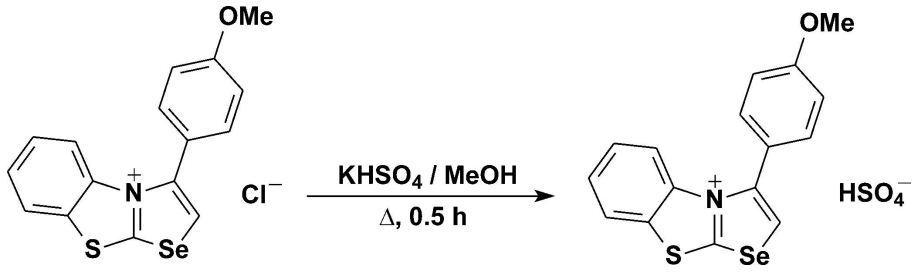

Figure 1

Reaction of 3-(4-methoxyphenyl)[1,3]selenazolo[2,3-*b*][1,3]benzothiazol-4-ium chloride with potassium hydrogen sulfate.

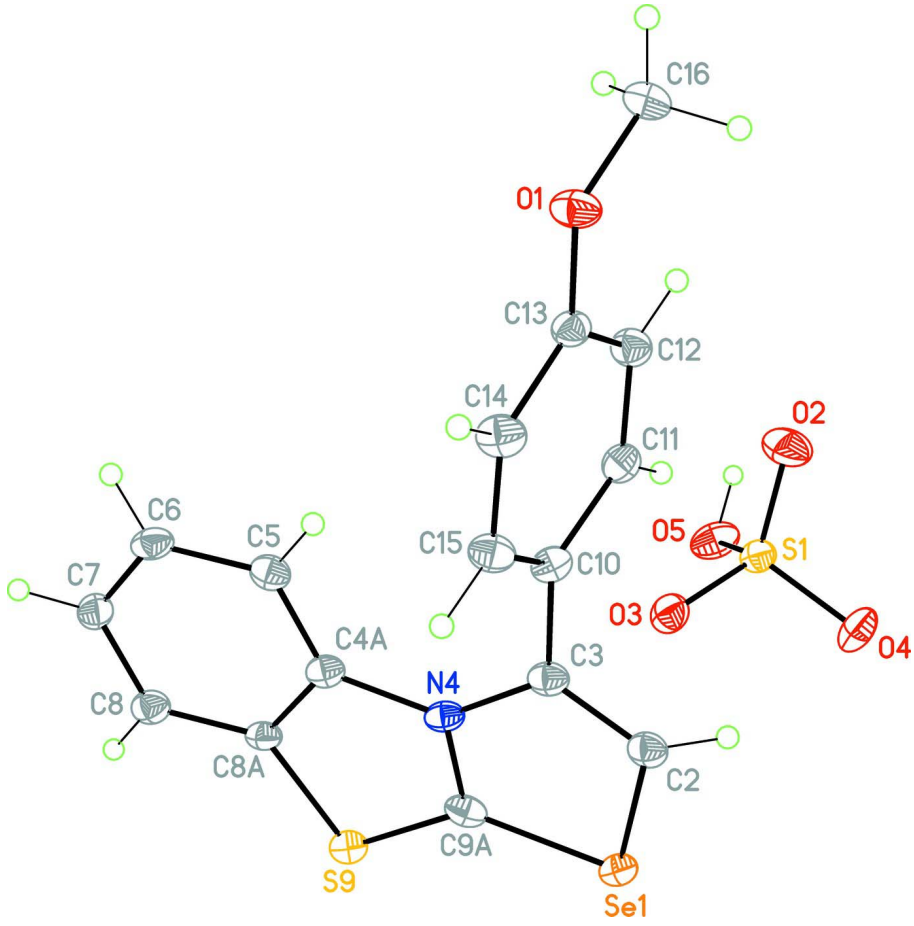

Figure 2

Molecular structure of **I**. Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

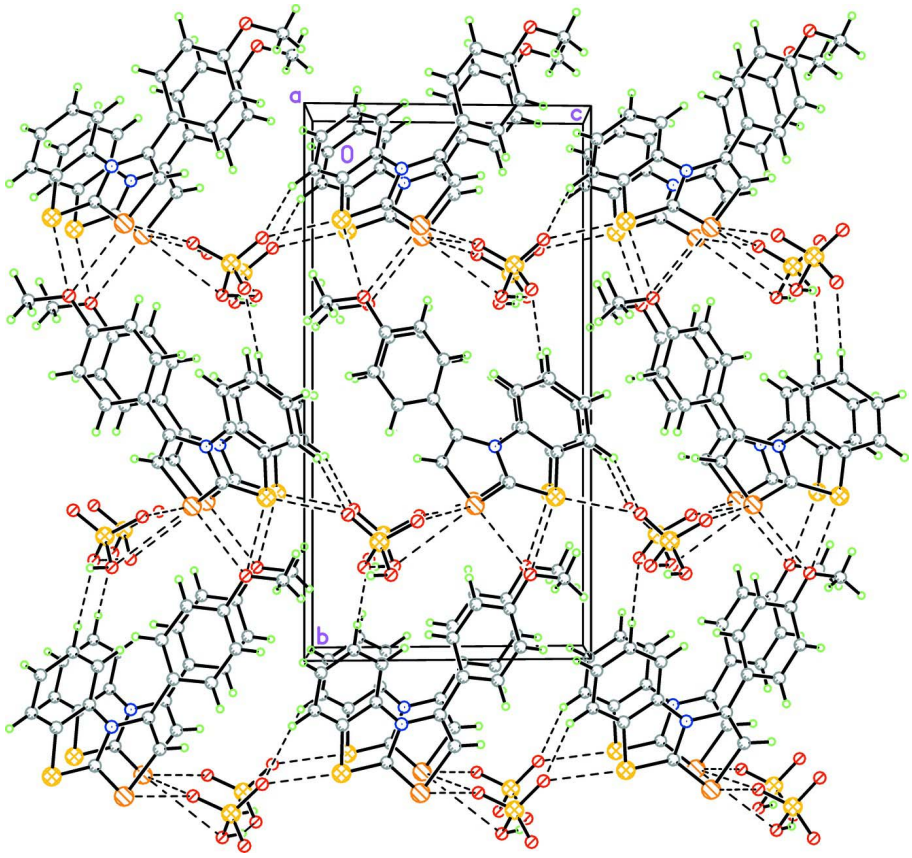

Figure 3

A portion of crystal packing of **I** viewed approximately down the *a* axis. Dashed lines indicate the intermolecular O—H···O and C—H···O hydrogen bonds as well as the non-valent Se···O and S···O attractive interactions.

3-(4-Methoxyphenyl)-1,3-selenazolo[2,3-*b*][1,3]benzothiazol-4-ium hydrogen sulfate

Crystal data

$C_{16}H_{12}NOSSe^{+}\cdot HO_4S^{-}$
$M_r = 442.35$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 4.6408\ (8)$ Å
$b = 18.263\ (3)$ Å
$c = 9.4482\ (16)$ Å
$\beta = 94.294\ (3)°$
$V = 798.6\ (2)$ Å^3
$Z = 2$
$F(000) = 444$
$D_x = 1.840$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2780 reflections
$\theta = 2.2–28.3°$
$\mu = 2.64$ mm^{-1}
$T = 100$ K
Plate, colourless
0.30 × 0.18 × 0.02 mm

Data collection

Bruker SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.505$, $T_{max} = 0.949$
8638 measured reflections
4145 independent reflections
3555 reflections with $I > 2\sigma(I)$

R_{int} = 0.052
θ_{max} = 29.0°, θ_{min} = 2.2°
h = −6→6
k = −24→24
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.085
S = 0.97
4145 reflections
227 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.001P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
Absolute structure: Flack (1983), 2075 Friedel pairs
Absolute structure parameter: 0.038 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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}
Se1	−0.35253 (8)	0.72534 (2)	0.59512 (4)	0.01626 (9)
C2	−0.3094 (9)	0.6448 (2)	0.4783 (4)	0.0173 (8)
H2	−0.4181	0.6389	0.3898	0.021*
C3	−0.1125 (9)	0.5955 (2)	0.5288 (4)	0.0165 (8)
N4	0.0200 (7)	0.61551 (17)	0.6630 (4)	0.0147 (7)
C4A	0.2352 (8)	0.5819 (2)	0.7546 (4)	0.0149 (8)
C5	0.3787 (8)	0.5164 (2)	0.7368 (4)	0.0168 (8)
H5	0.3330	0.4866	0.6559	0.020*
C6	0.5907 (9)	0.4956 (2)	0.8401 (4)	0.0186 (9)
H6	0.6911	0.4508	0.8296	0.022*
C7	0.6596 (9)	0.5392 (2)	0.9593 (4)	0.0182 (8)
H7	0.8068	0.5238	1.0282	0.022*
C8	0.5155 (9)	0.6048 (2)	0.9785 (5)	0.0180 (8)
H8	0.5608	0.6346	1.0596	0.022*
C8A	0.3030 (8)	0.6250 (2)	0.8747 (4)	0.0146 (8)
S9	0.0967 (2)	0.70586 (5)	0.87325 (11)	0.0174 (2)
C9A	−0.0728 (8)	0.6813 (2)	0.7133 (4)	0.0163 (8)
C10	−0.0297 (8)	0.5298 (2)	0.4485 (4)	0.0158 (8)
C11	0.1148 (8)	0.5411 (2)	0.3255 (4)	0.0172 (8)
H11	0.1567	0.5896	0.2972	0.021*

C12	0.1981 (9)	0.4824 (2)	0.2441 (4)	0.0182 (8)
H12	0.3004	0.4908	0.1622	0.022*
C13	0.1307 (8)	0.4114 (2)	0.2833 (4)	0.0156 (8)
C14	−0.0266 (9)	0.3998 (2)	0.4026 (5)	0.0205 (9)
H14	−0.0819	0.3516	0.4270	0.025*
C15	−0.1006 (8)	0.4583 (2)	0.4841 (4)	0.0192 (9)
H15	−0.2019	0.4498	0.5663	0.023*
O1	0.2001 (6)	0.35027 (15)	0.2094 (3)	0.0199 (6)
C16	0.3593 (9)	0.3608 (2)	0.0861 (4)	0.0198 (9)
H16A	0.3901	0.3134	0.0411	0.030*
H16B	0.5466	0.3833	0.1145	0.030*
H16C	0.2497	0.3930	0.0188	0.030*
S1	0.2806 (2)	0.78392 (5)	0.26484 (11)	0.0180 (2)
O2	0.3759 (7)	0.7346 (2)	0.1596 (3)	0.0333 (8)
O3	0.2090 (6)	0.74833 (15)	0.3937 (3)	0.0228 (6)
O4	0.0395 (6)	0.83188 (17)	0.2081 (3)	0.0256 (7)
O5	0.5298 (6)	0.83793 (17)	0.3069 (4)	0.0277 (7)
H5O	0.6634	0.8370	0.2413	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.01455 (16)	0.01458 (16)	0.02001 (18)	0.00098 (18)	0.00359 (13)	0.00010 (19)
C2	0.0167 (19)	0.018 (2)	0.018 (2)	−0.0019 (16)	0.0052 (16)	0.0018 (16)
C3	0.0159 (19)	0.0149 (18)	0.019 (2)	−0.0012 (15)	0.0058 (16)	0.0005 (16)
N4	0.0130 (15)	0.0124 (15)	0.0192 (17)	−0.0010 (13)	0.0049 (13)	−0.0009 (13)
C4A	0.0115 (18)	0.0145 (18)	0.019 (2)	−0.0025 (15)	0.0036 (15)	−0.0001 (15)
C5	0.017 (2)	0.0164 (19)	0.018 (2)	−0.0027 (16)	0.0047 (16)	−0.0004 (16)
C6	0.0153 (19)	0.0165 (19)	0.025 (2)	0.0015 (16)	0.0085 (17)	0.0024 (17)
C7	0.0135 (19)	0.022 (2)	0.019 (2)	0.0007 (16)	0.0020 (16)	0.0031 (17)
C8	0.016 (2)	0.0172 (19)	0.021 (2)	−0.0006 (16)	0.0050 (17)	0.0012 (17)
C8A	0.0156 (19)	0.0124 (18)	0.016 (2)	0.0009 (15)	0.0053 (15)	−0.0010 (15)
S9	0.0163 (4)	0.0168 (5)	0.0192 (5)	0.0003 (3)	0.0028 (4)	−0.0013 (4)
C9A	0.0155 (19)	0.0165 (18)	0.0175 (19)	−0.0055 (16)	0.0054 (15)	−0.0042 (16)
C10	0.0132 (18)	0.0137 (18)	0.021 (2)	−0.0009 (15)	0.0019 (16)	−0.0011 (16)
C11	0.0149 (19)	0.0165 (19)	0.020 (2)	−0.0005 (16)	0.0007 (16)	0.0008 (16)
C12	0.018 (2)	0.019 (2)	0.018 (2)	−0.0002 (16)	0.0034 (16)	0.0003 (16)
C13	0.0148 (19)	0.0155 (19)	0.016 (2)	0.0012 (15)	0.0000 (15)	−0.0035 (16)
C14	0.019 (2)	0.018 (2)	0.025 (2)	−0.0031 (17)	0.0067 (17)	0.0013 (17)
C15	0.0171 (19)	0.021 (2)	0.021 (2)	−0.0022 (16)	0.0055 (17)	−0.0016 (17)
O1	0.0223 (15)	0.0163 (14)	0.0223 (15)	−0.0003 (12)	0.0096 (13)	−0.0003 (12)
C16	0.021 (2)	0.021 (2)	0.018 (2)	−0.0003 (17)	0.0067 (17)	−0.0029 (17)
S1	0.0164 (5)	0.0182 (5)	0.0197 (5)	0.0014 (4)	0.0029 (4)	0.0002 (4)
O2	0.0372 (17)	0.036 (2)	0.0270 (14)	0.0050 (17)	0.0053 (13)	−0.0125 (16)
O3	0.0204 (15)	0.0232 (15)	0.0252 (15)	0.0021 (12)	0.0041 (12)	0.0073 (12)
O4	0.0152 (15)	0.0258 (16)	0.0353 (18)	0.0019 (12)	−0.0007 (13)	0.0102 (14)
O5	0.0167 (15)	0.0263 (17)	0.0406 (18)	−0.0014 (13)	0.0064 (14)	−0.0019 (15)

Geometric parameters (Å, º)

Se1—C9A	1.834 (4)	C10—C15	1.394 (5)
Se1—C2	1.859 (4)	C10—C11	1.399 (6)
C2—C3	1.345 (5)	C11—C12	1.391 (6)
C2—H2	0.9500	C11—H11	0.9500
C3—N4	1.415 (5)	C12—C13	1.390 (6)
C3—C10	1.485 (5)	C12—H12	0.9500
N4—C9A	1.373 (5)	C13—O1	1.367 (5)
N4—C4A	1.412 (5)	C13—C14	1.404 (6)
C4A—C5	1.385 (5)	C14—C15	1.376 (6)
C4A—C8A	1.397 (5)	C14—H14	0.9500
C5—C6	1.386 (6)	C15—H15	0.9500
C5—H5	0.9500	O1—C16	1.439 (5)
C6—C7	1.397 (6)	C16—H16A	0.9800
C6—H6	0.9500	C16—H16B	0.9800
C7—C8	1.391 (6)	C16—H16C	0.9800
C7—H7	0.9500	S1—O2	1.436 (3)
C8—C8A	1.388 (6)	S1—O3	1.441 (3)
C8—H8	0.9500	S1—O4	1.489 (3)
C8A—S9	1.759 (4)	S1—O5	1.549 (3)
S9—C9A	1.710 (4)	O5—H5O	0.9086
C9A—Se1—C2	84.92 (18)	C15—C10—C11	118.3 (4)
C3—C2—Se1	114.8 (3)	C15—C10—C3	123.9 (4)
C3—C2—H2	122.6	C11—C10—C3	117.7 (3)
Se1—C2—H2	122.6	C12—C11—C10	121.1 (4)
C2—C3—N4	112.5 (4)	C12—C11—H11	119.5
C2—C3—C10	123.7 (4)	C10—C11—H11	119.5
N4—C3—C10	123.7 (3)	C11—C12—C13	119.6 (4)
C9A—N4—C4A	113.2 (3)	C11—C12—H12	120.2
C9A—N4—C3	114.2 (3)	C13—C12—H12	120.2
C4A—N4—C3	132.6 (3)	O1—C13—C12	124.0 (4)
C5—C4A—C8A	120.3 (4)	O1—C13—C14	116.3 (4)
C5—C4A—N4	128.7 (4)	C12—C13—C14	119.7 (4)
C8A—C4A—N4	111.0 (3)	C15—C14—C13	119.9 (4)
C4A—C5—C6	118.3 (4)	C15—C14—H14	120.0
C4A—C5—H5	120.9	C13—C14—H14	120.0
C6—C5—H5	120.9	C14—C15—C10	121.3 (4)
C5—C6—C7	121.3 (4)	C14—C15—H15	119.4
C5—C6—H6	119.4	C10—C15—H15	119.4
C7—C6—H6	119.4	C13—O1—C16	117.3 (3)
C8—C7—C6	120.9 (4)	O1—C16—H16A	109.5
C8—C7—H7	119.6	O1—C16—H16B	109.5
C6—C7—H7	119.6	H16A—C16—H16B	109.5
C8A—C8—C7	117.4 (4)	O1—C16—H16C	109.5
C8A—C8—H8	121.3	H16A—C16—H16C	109.5
C7—C8—H8	121.3	H16B—C16—H16C	109.5

C8—C8A—C4A	121.9 (4)	O2—S1—O3	113.9 (2)
C8—C8A—S9	125.9 (3)	O2—S1—O4	112.44 (19)
C4A—C8A—S9	112.2 (3)	O3—S1—O4	110.80 (18)
C9A—S9—C8A	90.01 (19)	O2—S1—O5	108.31 (19)
N4—C9A—S9	113.6 (3)	O3—S1—O5	106.59 (18)
N4—C9A—Se1	113.5 (3)	O4—S1—O5	104.13 (18)
S9—C9A—Se1	132.9 (2)	S1—O5—H5O	110.3

C9A—Se1—C2—C3	0.2 (3)	C4A—N4—C9A—S9	0.3 (4)
Se1—C2—C3—N4	0.6 (4)	C3—N4—C9A—S9	−178.3 (3)
Se1—C2—C3—C10	−175.7 (3)	C4A—N4—C9A—Se1	−180.0 (3)
C2—C3—N4—C9A	−1.3 (5)	C3—N4—C9A—Se1	1.5 (4)
C10—C3—N4—C9A	174.9 (4)	C8A—S9—C9A—N4	0.1 (3)
C2—C3—N4—C4A	−179.5 (4)	C8A—S9—C9A—Se1	−179.6 (3)
C10—C3—N4—C4A	−3.3 (6)	C2—Se1—C9A—N4	−0.9 (3)
C9A—N4—C4A—C5	−179.1 (4)	C2—Se1—C9A—S9	178.8 (3)
C3—N4—C4A—C5	−0.9 (7)	C2—C3—C10—C15	−110.1 (5)
C9A—N4—C4A—C8A	−0.6 (4)	N4—C3—C10—C15	74.1 (5)
C3—N4—C4A—C8A	177.6 (4)	C2—C3—C10—C11	66.4 (5)
C8A—C4A—C5—C6	−0.5 (6)	N4—C3—C10—C11	−109.4 (4)
N4—C4A—C5—C6	177.9 (4)	C15—C10—C11—C12	−2.9 (6)
C4A—C5—C6—C7	−0.1 (6)	C3—C10—C11—C12	−179.6 (4)
C5—C6—C7—C8	0.4 (6)	C10—C11—C12—C13	1.6 (6)
C6—C7—C8—C8A	−0.2 (6)	C11—C12—C13—O1	179.2 (4)
C7—C8—C8A—C4A	−0.3 (6)	C11—C12—C13—C14	1.5 (6)
C7—C8—C8A—S9	−178.7 (3)	O1—C13—C14—C15	178.9 (4)
C5—C4A—C8A—C8	0.7 (6)	C12—C13—C14—C15	−3.3 (6)
N4—C4A—C8A—C8	−177.9 (4)	C13—C14—C15—C10	1.9 (6)
C5—C4A—C8A—S9	179.3 (3)	C11—C10—C15—C14	1.2 (6)
N4—C4A—C8A—S9	0.7 (4)	C3—C10—C15—C14	177.7 (4)
C8—C8A—S9—C9A	178.1 (4)	C12—C13—O1—C16	1.7 (5)
C4A—C8A—S9—C9A	−0.4 (3)	C14—C13—O1—C16	179.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*O*···O4^{i}	0.91	1.80	2.610 (4)	147
C6—H6···O4^{ii}	0.95	2.54	3.494 (5)	178
C8—H8···O2^{iii}	0.95	2.26	3.022 (5)	137

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