



# The synthesis and crystal structure of 2-(chloroselanyl)pyridine 1-oxide: the first monomeric organoselenenyl chloride stabilized by an intramolecular secondary Se···O interaction

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Received 27 November 2016

Accepted 27 November 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

**Keywords:** crystal structure; synchrotron radiation; organoselenenyl chloride; intramolecular stabilization; secondary interactions.

**CCDC reference:** 1519449

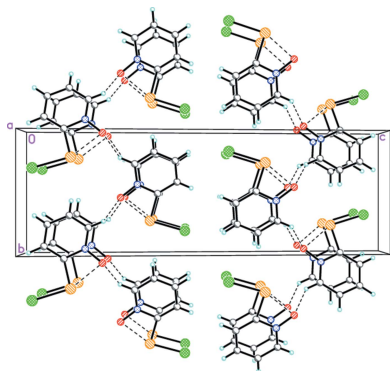
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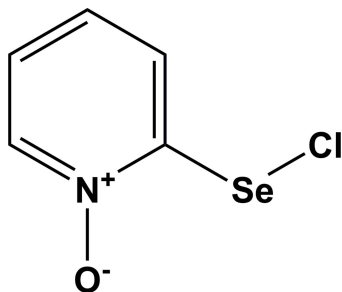
The title compound, C<sub>5</sub>H<sub>4</sub>ClNOSe, is the product of the reaction of sulfonyl chloride and 2-selanyl-1-pyridine 1-oxide in dichloromethane. The molecule has an almost planar geometry (r.m.s. deviation = 0.012 Å), and its molecular structure is stabilized by an intramolecular secondary Se···O interaction of 2.353 (3) Å, closing a four-membered N—C—Se···O ring. The title compound represents the first monomeric organoselenenyl chloride stabilized intramolecularly by an interaction of this type. The non-valent attractive Se···O interaction results in a substantial distortion of the geometry of the *ipso*-carbon atom. The *endo*-cyclic N—C—Se [102.1 (3)°] and *exo*-cyclic C—C—Se [136.9 (3)°] bond angles deviate significantly from the ideal value of 120° for an *sp*<sup>2</sup>-hybridized carbon atom, the former bond angle being much smaller than the latter. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming zigzag chains propagating along [010]. The chains, which stack along the *a*-axis direction, are linked by offset  $\pi$ - $\pi$  interactions [intercentroid distance = 3.960 (3) Å], forming corrugated sheets parallel to the *ab* plane.

## 1. Chemical context

Organoselenenyl halides *RSeX* (*X* = Cl, Br) play an important role in modern organic synthesis and are used as reagents for the functionalization of many classes of compounds, including organoselenium compounds with a broad spectrum of biological activities (Ranganathan *et al.*, 2004; Selvakumar *et al.*, 2010, 2011; Ninomiya *et al.*, 2011; Singh & Wirth, 2011; Zade & Singh, 2014; Elsherbini *et al.*, 2016). An essential aspect of the chemistry of selenenyl halides is the factors responsible for the stability of these reagents (Coles, 2006; Mukherjee *et al.*, 2010; Nakanishi *et al.*, 2013; Takaluoma *et al.*, 2015). Recently, we have developed a new effective method for the stabilization of heteroarenselenenyl and -tellurenyl chlorides by the transformation of them to T-shaped zwitterionic adducts with hydrochloric acid (Khrustalev *et al.*, 2012, 2014, 2016). Moreover, we have established another stabilization method of heteroarenselenenyl and -tellurenyl chlorides by intermolecular secondary Ch···N (Ch = Se, Te)



interactions with the formation of dimers (Borisov *et al.*, 2010*a,b,c*; Khrustalev *et al.*, 2016). Herein, we report on the synthesis and structural characterization of the first monomeric 2-(chloroselanyl)pyridine 1-oxide stabilized by an intramolecular secondary  $\text{Se}\cdots\text{O}$  interaction.



## 2. Structural commentary

The title compound, Fig. 1, is the product of the reaction of sulfuryl chloride and 2-selanyl-1-pyridine 1-oxide in dichloromethane. It has an almost planar geometry (r.m.s. deviation = 0.012 Å), and its molecular structure is stabilized by an intramolecular secondary  $\text{Se1}\cdots\text{O1}$  interaction of 2.353 (3) Å, closing the four-membered  $\text{N1}-\text{C2}-\text{Se1}\cdots\text{O1}$  ring (Fig. 1). The non-valent attractive  $\text{Se1}\cdots\text{O1}$  interaction results in the substantial distortion of the geometry of the *ipso*-C2 carbon atom. The *endo*-cyclic  $\text{N1}-\text{C2}-\text{Se1}$  [102.1 (3)°] and *exo*-cyclic  $\text{C3}-\text{C2}-\text{Se1}$  [136.9 (3)°] bond angles deviate significantly from the ideal value of 120° for an  $sp^2$ -hybridized carbon atom, the former angle being much smaller than the latter. The title compound represents the first monomeric organoselenenyl chloride stabilized intramolecularly by an interaction of this type. Previously, the analogous stabilization of monomeric organoselenenyl chlorides by intramolecular secondary  $\text{Se}\cdots\text{S}$  (Tiecco *et al.*, 2006)

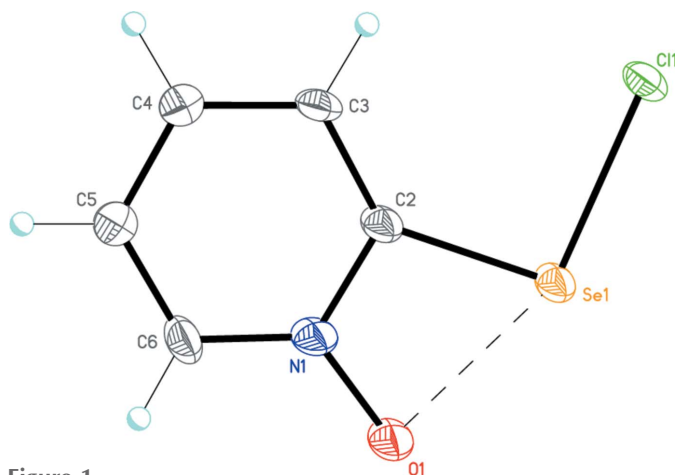


Figure 1

The molecular structure of the title compound, with atom labelling and displacement ellipsoids drawn at the 50% probability level. The dashed line indicates the intramolecular secondary attractive  $\text{Se1}\cdots\text{O1}$  interaction.

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O1}^i$	0.95	2.34	3.101 (6)	137

Symmetry code: (i)  $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$ .

and  $\text{Se}\cdots\text{N}$  (Panda *et al.*, 1999; Klapötke *et al.*, 2004; Kulcsar *et al.*, 2007; Pöllnitz *et al.*, 2011) interactions have been reported.

## 3. Supramolecular features

In the crystal, molecules are linked by  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1 and Fig. 2), forming zigzag chains propagating along the *b*-axis direction. The chains stack along the *a*-axis direction and are linked by offset  $\pi-\pi$  interactions, forming corrugated sheets parallel to the *ab* plane [ $Cg\cdots Cg^{iii}$  = 3.960 (3) Å,  $Cg$  is the centroid of the  $\text{N1}/\text{C2}-\text{C6}$  ring, interplanar distances = 3.590 (2) Å, slippages = 1.671 Å, symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x + 1, y, z$ ].

## 4. Synthesis and crystallization

The synthesis of the title compound is illustrated in Fig. 3. It was synthesized according to the procedure described previously by Borisov *et al.* (2010*a,b,c*). A solution of sulfuryl chloride (0.27 g, 2 mmol) in dichloromethane (15 ml) was added to a solution of 2-selanyl-1-pyridine 1-oxide (0.35 g, 2 mmol) in dichloromethane (20 ml) at 293 K. After one h it was filtered to give the title compound (yield 0.33 g, 80%). The

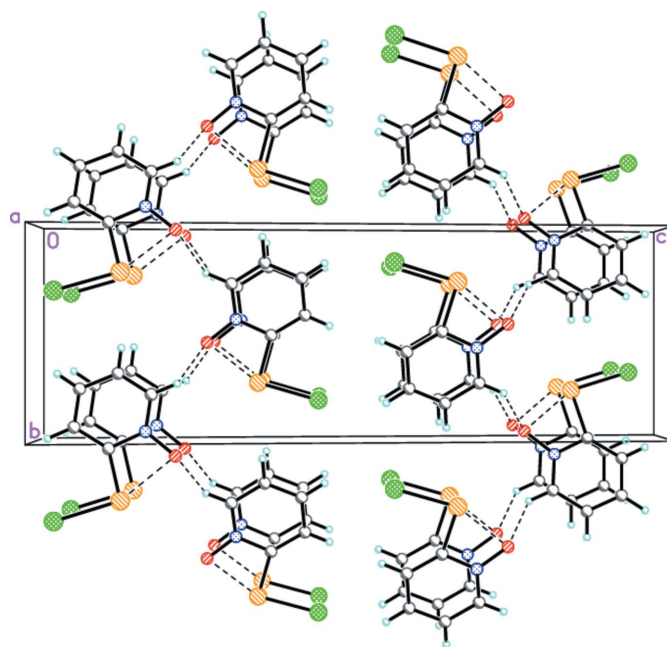
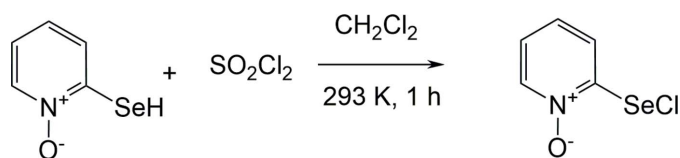


Figure 2

The crystal packing of the title compound viewed along the *a* axis. The intramolecular secondary  $\text{Se}\cdots\text{O}$  interactions and the intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds are shown as dashed lines (see Table 1).



**Figure 3**  
The synthesis of the title compound; the reaction of 2-selanyl-1-pyridine 1-oxide with sulfuryl chloride in dichloromethane.

filtrate was evaporated *in vacuo* and recrystallization of the residue from dichloromethane solution gave an additional 0.06 g (15%) of the title compound. Colourless prismatic crystals of the title compound were obtained after recrystallization of the crude product from dichloromethane (m.p. 433–435 K). IR (KBr,  $\text{cm}^{-1}$ ),  $\nu$  1617, 1462, 1423, 1254, 1151, 836, 748, 621.  $^1\text{H}$  NMR (DMSO- $d_6$ , 300 MHz, 300 K):  $\delta$  = 8.28 (d, 1H,  $^3J$  = 5.9, H6); 7.52 (d, 1H,  $^3J$  = 7.3, H3); 7.43 (dd, 1H,  $^3J$  = 7.8,  $^3J$  = 7.3, H4); 7.30 (dd, 1H,  $^3J$  = 7.8,  $^3J$  = 5.9, H5). Analysis calculated for  $\text{C}_5\text{H}_4\text{ClNOSe}$ : C 24.81; H 1.93; N 6.72. Found: 24.43; H 1.83; N 6.65.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were placed in calculated positions and refined as riding: C–H = 0.95 Å with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Acknowledgements

The work was supported by the Ministry of Education of the Russian Federation (Agreement number 02.a03.21.0008 of June 24, 2016) and the Russian Foundation for Basic Research (Grant No. 14–03–00914).

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**Table 2**  
Experimental details.

Crystal data	$\text{C}_5\text{H}_4\text{ClNOSe}$
Chemical formula	208.50
$M_r$	Monoclinic, $P2_1/c$
Crystal system, space group	100
Temperature (K)	3.9601 (8), 7.5102 (15), 22.350 (5)
$a, b, c$ (Å)	94.32 (3)
$\beta$ (°)	662.8 (2)
$V$ (Å <sup>3</sup> )	4
$Z$	Synchrotron, $\lambda = 0.96990$ Å
Radiation type	13.68
$\mu$ (mm <sup>-1</sup> )	0.05 × 0.03 × 0.03
Crystal size (mm)	
Data collection	
Diffractometer	Rayonix SX-165 CCD
Absorption correction	Multi-scan (SCALA; Evans, 2006)
$T_{\text{min}}, T_{\text{max}}$	0.550, 0.660
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	5526, 1310, 1121
$R_{\text{int}}$	0.083
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.636
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.074, 0.175, 1.01
No. of reflections	1310
No. of parameters	83
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.26, -1.58

Computer programs: *Automar* (MarXperts, 2015), *iMosflm* (Battye *et al.*, 2011), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2014/6* (Sheldrick, 2015).

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## supporting information

*Acta Cryst.* (2016). E72, 1864-1866 [https://doi.org/10.1107/S2056989016018946]

## The synthesis and crystal structure of 2-(chloroselanyl)pyridine 1-oxide: the first monomeric organoselenenyl chloride stabilized by an intramolecular secondary Se...O interaction

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### Computing details

Data collection: *Automar* (MarXperts, 2015); cell refinement: *iMosflm* (Battye *et al.*, 2011); data reduction: *iMosflm* (Battye *et al.*, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### 2-(Chloroselanyl)pyridine 1-oxide

#### Crystal data

C<sub>5</sub>H<sub>4</sub>ClN<sub>2</sub>OSe

$M_r = 208.50$

Monoclinic,  $P2_1/c$

$a = 3.9601$  (8) Å

$b = 7.5102$  (15) Å

$c = 22.350$  (5) Å

$\beta = 94.32$  (3)°

$V = 662.8$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 400$

$D_x = 2.089$  Mg m<sup>-3</sup>

Synchrotron radiation,  $\lambda = 0.96990$  Å

Cell parameters from 600 reflections

$\theta = 5.0\text{--}35.0^\circ$

$\mu = 13.68$  mm<sup>-1</sup>

$T = 100$  K

Prism, colourless

$0.05 \times 0.03 \times 0.03$  mm

#### Data collection

Rayonix SX-165 CCD  
diffractometer

$\omega$  scan

Absorption correction: multi-scan  
(*SCALA*; Evans, 2006)

$T_{\min} = 0.550$ ,  $T_{\max} = 0.660$

5526 measured reflections

1310 independent reflections

1121 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.083$

$\theta_{\max} = 38.1^\circ$ ,  $\theta_{\min} = 5.0^\circ$

$h = -4 \rightarrow 4$

$k = -9 \rightarrow 9$

$l = -28 \rightarrow 28$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.074$

$wR(F^2) = 0.175$

$S = 1.01$

1310 reflections

83 parameters

0 restraints

Primary atom site location: difference Fourier  
map

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 1.6P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.26 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.58 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL,

$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.054 (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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.51523 (13)	0.26936 (7)	0.34782 (2)	0.02716 (17)
Cl1	0.4514 (3)	0.18592 (14)	0.44303 (4)	0.0331 (3)
O1	0.6571 (9)	0.4577 (4)	0.26942 (12)	0.0347 (8)
N1	0.7603 (10)	0.5643 (5)	0.31523 (14)	0.0290 (8)
C2	0.7093 (11)	0.4927 (5)	0.36941 (16)	0.0266 (9)
C3	0.7969 (12)	0.5838 (6)	0.42160 (17)	0.0301 (10)
H3	0.7578	0.5342	0.4596	0.036*
C4	0.9449 (14)	0.7515 (6)	0.4172 (2)	0.0334 (13)
H4	1.0115	0.8173	0.4524	0.040*
C5	0.9941 (12)	0.8213 (7)	0.36099 (19)	0.0343 (12)
H5	1.0906	0.9365	0.3579	0.041*
C6	0.9047 (14)	0.7257 (5)	0.3095 (2)	0.0317 (12)
H6	0.9436	0.7720	0.2710	0.038*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Se1	0.0427 (4)	0.0202 (3)	0.0200 (3)	-0.00320 (19)	0.0117 (3)	-0.00209 (16)
Cl1	0.0522 (7)	0.0277 (5)	0.0208 (4)	-0.0077 (5)	0.0122 (4)	0.0037 (4)
O1	0.058 (2)	0.0284 (15)	0.0190 (12)	-0.0061 (14)	0.0139 (13)	-0.0045 (12)
N1	0.044 (2)	0.0265 (17)	0.0177 (14)	0.0022 (16)	0.0106 (13)	-0.0035 (13)
C2	0.041 (2)	0.0217 (19)	0.0183 (16)	0.0003 (18)	0.0111 (15)	-0.0008 (14)
C3	0.049 (3)	0.028 (2)	0.0144 (16)	-0.0006 (19)	0.0089 (16)	0.0008 (15)
C4	0.049 (3)	0.027 (2)	0.024 (2)	-0.0035 (19)	0.004 (2)	-0.0028 (15)
C5	0.051 (3)	0.026 (2)	0.0267 (19)	-0.002 (2)	0.0033 (19)	-0.0008 (19)
C6	0.048 (3)	0.0180 (18)	0.030 (2)	0.0009 (18)	0.009 (2)	0.0062 (15)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Se1—C2	1.892 (4)	C3—H3	0.9500
Se1—Cl1	2.2506 (11)	C4—C5	1.389 (7)
O1—N1	1.339 (4)	C4—H4	0.9500
N1—C6	1.350 (6)	C5—C6	1.381 (6)

N1—C2	1.354 (5)	C5—H5	0.9500
C2—C3	1.374 (6)	C6—H6	0.9500
C3—C4	1.395 (6)		
C2—Se1—C11	94.48 (11)	C5—C4—C3	119.6 (4)
O1—N1—C6	124.8 (3)	C5—C4—H4	120.2
O1—N1—C2	112.9 (3)	C3—C4—H4	120.2
C6—N1—C2	122.3 (4)	C6—C5—C4	120.9 (4)
N1—C2—C3	121.0 (4)	C6—C5—H5	119.6
N1—C2—Se1	102.1 (3)	C4—C5—H5	119.6
C3—C2—Se1	136.9 (3)	N1—C6—C5	118.1 (4)
C2—C3—C4	118.0 (4)	N1—C6—H6	120.9
C2—C3—H3	121.0	C5—C6—H6	120.9
C4—C3—H3	121.0		
O1—N1—C2—C3	-179.4 (4)	Se1—C2—C3—C4	178.9 (4)
C6—N1—C2—C3	1.4 (7)	C2—C3—C4—C5	0.9 (7)
O1—N1—C2—Se1	0.7 (4)	C3—C4—C5—C6	-1.3 (8)
C6—N1—C2—Se1	-178.5 (4)	O1—N1—C6—C5	179.2 (4)
C11—Se1—C2—N1	-179.0 (3)	C2—N1—C6—C5	-1.7 (7)
C11—Se1—C2—C3	1.0 (5)	C4—C5—C6—N1	1.6 (8)
N1—C2—C3—C4	-1.0 (7)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6...O1 <sup>i</sup>	0.95	2.34	3.101 (6)	137

Symmetry code: (i)  $-x+2, y+1/2, -z+1/2$ .