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An unusually stable pyridine-2-selenenyl chloride: structure and reactivity

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Abstract According to an X-ray diffraction study, pyridine-2-selenenyl chloride (1) characterized by unusually high stability both in solutions and in the solid state adopts a dimeric structure formed by two secondary intermolecular Se…N interactions. However, it slowly transforms into zwitterionic T-shaped pyridinium-2-selenenyl dichloride (2) in a dichloromethane solution. Conformational features, electronic structures, and reactivities of 1 and 2 are discussed on the basis of experimental and theoretical (quantum chemical calculations) data.

Keywords Pyridine-2-selenenyl chloride · T-shaped adduct · Conformational analysis · Molecular structure · DFT calculation · Crystal structure

This paper is dedicated to Prof. Vladimir Shevchenko (Institute of Silicate Chemistry of Russian Academy of Sciences, Saint-Petersburg, Russia) on the occasion of his 75th anniversary.

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Introduction

The stabilization of arenechalcogenyl halides is typically achieved via the intermolecular coordination of the chalcogen atom to electron-donor functional groups (often nitrogen- or oxygen-containing ones) in the ortho-position with respect to the chalcogenyl halide group [1-15]. Recently, we have synthesized the very first representative of hetarenetellurenyl halides bearing pyridine as a hetaryl fragment—2-pyridinetellurenyl chloride (1a), and the dimeric structure of this compound was established [16]. With this respect, it was important to further elucidate factors governing the prominent stability of its close analogue, 2-pyridineselenyl chloride (1b) actually synthesized more than 30 years ago [17]. As we have found recently, 1a slowly spontaneously converts into the T-shaped adduct 2a in a dichloromethane solution [18]. Furthermore, we have shown that complexes 1a and 2a can act as efficient reagents in the polar cycloaddition to multiple bonds [18-20].

In the present paper, we establish the molecular and crystal structures of 2-pyridineselenyl chloride and study reasons for its high stability in relation to capabilities of its further transformations and modifications.

Experimental

Synthesis of 1b and 2b

Starting reagents were purchased from Sigma-Aldrich and used without further purification. Melting points were measured on a "Boetius" bench. Elemental analysis was accomplished with an automated PerkinElmer 2400 CHN microanalyzer. **1b** Pyridine-2-selenenyl chloride was obtained by the method described previously [17], but using dichloromethane as a solvent instead of ethyl acetate. *M*p 136–138 °C ([17]: 118–119 °C). C_5H_4NCISe (192.51): calcd. C 31.20, H 2.09, N 7.28; found C 31.15, H 2.21, N 7.37.

2b Pyridine-2-selenenyl chloride (0.05 g, 0.26 mmol) was dissolved in dichloromethane (100 mL) at room temperature. After 168 h, the solvent was evaporated in *vacuo*. The precipitate contained 0.059 g (100 %) of a yellow powder T-shaped 1*H*-pyridine-2-selenenyl dichloride (**2b**). *M*p 145–146 °C. $C_5H_5NCl_2Se$ (228.97): calcd. C 26.23, H 2.20, N 6.12; found C 26.17, H 2.34, N 6.22. Single crystals of **2b** suitable for an X-ray diffraction analysis were prepared by a slow evaporation of a solution in dimethylformamide/diethyl ether (9:1) solvent mixture at room temperature.

X-ray crystallography

Data were collected using Bruker APEX CCD (for 1b) and APEX-II CCD (for **2b**) diffractometers $[\lambda(MoK_{\alpha})-radia$ tion, graphite monochromator, ω and φ scanning modes] and corrected for absorption using the SADABS program [21]. For details, see Table 1. The crystal structures were determined by the direct methods and refined by a fullmatrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. The crystal of **2b** contained a solvate dimethylformamide (DMFA) molecule. The pyridinium NH hydrogen atom in 2b was objectively localized in the difference-Fourier map and refined isotropically with fixed isotropic displacement parameters $[U_{iso}(H) = 1.2U_{eq}(N)]$. The other hydrogen atoms in both complexes were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters $[U_{iso}(H) = 1.5U_{eq}(C)$ for the CH₃ groups and $1.2U_{eq}(C)$ for other groups]. All calculations were carried out using the SHELXTL program [22]. Crystallographic data for 1b and 2b DMFA have been deposited with the Cambridge Crystallographic Data Center.

Computational details

All theoretical calculations of geometry and normal coordinate analysis (NCA) for **1b** and **2b** were performed using the Gaussian 03 [23] program at the DFT level of theory using the PBE0 [24] and M06-2X [25] functionals; 6-311++G(d,p) [26, 27] valence basis sets were utilized for all atoms. The R. Bader's QTAIM analysis of electron density was performed in the AIMAll program [28] at the M06-2X/6-311++G(d,p) level of theory.

Results and discussion

Molecular and crystal structures

Molecules of **1b** occur in the crystal structure as dimers formed by the Se \leftarrow N interactions (Fig. 1), exactly as in the case of tellurium analogue **1a**.

The molecule of **1b** adopts a *butterfly* conformation with the fold angle on the Se…Se line of $70.07(7)^{\circ}$. The Cl1– Se1 \leftarrow N2 and Cl2–Se2 \leftarrow N1 fragments are almost linear (177.93(7) and 175.30(7)°, respectively). The C2–Se1 and C7–Se2 distances of 1.926(3) and 1.918(3) Å are equal to each other and correspond well to single bonds. The Se1 \leftarrow N2 and Se2 \leftarrow N1 distances of 2.141(3) and 2.189(3) Å fall in the range of those within the related T-shaped selenium(II) complexes (1.931(4)–2.204(5) Å [29]).

It is interesting to point out that the Cl1 atom forms secondary interactions with the both selenium atoms [Se1…Cl1 (-x, 1 - y, 2 - z) 3.6603(9) and Se2…Cl1 (1 - x, -y, 2 - z) 3.7500(8) Å], whereas the Cl2 atom remains free of any non-valent contacts. Due to the intermolecular Se…Cl interactions, the selenium atoms have a distorted square-planar coordination (Fig. 2). Moreover, just these additional interactions result in the elongation of the Se1–Cl1 bond [2.4041(3) Å] as compared to the Se2–Cl2 one [2.3657(3) Å].

In the crystal, molecules of 1b form the ribbons parallel to (110) via the intermolecular secondary Se…Cl interactions described above (Fig. 2).

Earlier based on NMR data, we suggested that strong proton acceptors (DMSO, DMFA, etc.) can cleave the stabilizing intramolecular N–H···Cl H-bond in zwitterionic T-shaped hetarylselenenyl chlorides giving rise to a "propeller"-type molecular motion in such solvents (Scheme 1) [30]. Making such a suggestion, we kept in mind that an H-bond is *directional*, which makes it similar to a normal polar covalent bond, only a weak one [31]. Our arguments were well stipulated, but still the formation of a *bifurcate* H-bond with the proton bonding simultaneously intermolecularly to a solvent molecule and intramolecularly to a chlorine atom of the –SeCl₂ moiety cannot be totally ruled out.

Remarkably, upon recrystallization, we have isolated the H-bonded complex of **2b** with a molecule of DMFA in the solid state and studied its structure by single-crystal X-ray crystallography. It appeared that the DFMA molecule being a stronger proton acceptor actually cleaves the intramolecular N–H···Cl H-bond avoiding the formation of a *bifurcate*-type H-bond (Fig. 3). The parameters of the intermolecular N–H···O hydrogen bond are following: N–H 0.80(2) Å, H···O 1.90(2) Å, N···O 2.6563(19) Å, \angle N–H···O 159(2)°. Furthermore, the 2-pyridineselenyl chloride

 Table 1
 Crystal data and experimental parameters for 1b and 2b

Compounds	1b	2b·DMFA
Molecular formula	$C_{10}H_8Cl_2N_2Se_2$	C ₈ H ₁₂ Cl ₂ N ₂ OSe
Formula weight	385.00	302.06
Crystal system	Triclinic	Monoclinic
Space group	$P\overline{1}$	$P2_{1}/c$
a (Å)	7.4651 (4)	12.0570 (4)
<i>b</i> (Å)	8.6227 (4)	11.5026 (4)
<i>c</i> (Å)	10.2077 (5)	8.5326 (3)
α (°)	77.229 (1)	90
β (°)	83.049 (1)	94.585 (1)
γ (°)	72.354 (1)	90
V (Å ³)	609.62 (5)	1179.57 (7)
Ζ	2	4
$d (\text{g cm}^{-3})$	2.097	1.701
Absorption coefficient (mm ⁻¹)	6.475	3.607
F(000)	368	600
Crystal size (mm)	$0.20\times0.15\times0.10$	$0.15 \times 0.15 \times 0.10$
θ range for data collection (°)	2.53-26.99	2.45-30.99
Reflections collected	4067	16,421
Independent reflections	2622	3764
Reflections with $I > 2\sigma(I)$	2390	3224
Number of parameters	145	132
Goodness-of-fit on F^2	1.050	1.015
$R_1 \left[I > 2\sigma(I) \right]$	0.0333	0.0259
$wR_2 \ [I > 2\sigma(I)]$	0.0866	0.0668
T_{\min}, T_{\max}	0.336, 0.565	0.606, 0.707
Largest diff. peak and hole ($e \text{ Å}^{-3}$)	0.852 and -0.333	0.749 and -0.264
CCDC no. ^a	922,925	1,055,674

^a Copies of the data can be obtained free of charge on application to The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (http://www.ccdc.cam.ac.uk)



Fig. 1 Molecular structure of 1b

molecule adopts the *twist* conformation with a twisting angle between the pyridyl and $-\text{SeCl}_2$ planes of $48.49(5)^{\circ}$ rather than the *planar* conformation typical of other analogous zwitterionic T-shaped selenium complexes stabilized by a strong intramolecular N–H···Cl H-bond (Fig. 4) [30]. This solidly and directly supports the mechanism actuating the molecular dynamics of T-shaped hetarylselenyl chlorides in proton-acceptor solvents, and thus zwitterionic structure of T-shaped chalcogenide complexes with a common formula [H(hetAr)]ChHal₂, where hetAr is a hetaryl substituent [32].

The C–Se distance of 1.9195(15) Å in **2b** is representative of single bonds {the lengths of C=Se bonds in 1-methylbenzoimidazoleselone, benzothiazoleselone, and *N*-methylbenzothiazole-2-selone are 1.838(2) Å [33], 1.8236(11) Å [34], and 1.817(7) Å [35], respectively}.

The Cl2 atom in **2b** is involved in the intermolecular secondary Se…Cl interaction [Se1…Cl2 $(x, \frac{1}{2} - y, \frac{1}{2} - y)$]



Fig. 2 Crystal packing of 1b demonstrating the ribbons parallel to (110). The *dashed lines* are indicative of the intermolecular secondary Se…Cl interactions



Scheme 1 Dynamic *propeller*-like process in solution of zwitterionic T-shaped hetarylselenenyl chlorides

 $-\frac{1}{2} + z$) 3.3786(4) Å]. Thus, the selenium atom in **2b** adopts a distorted square-planar coordination (Fig. 5). Due to the intermolecular Se…Cl interaction, molecules of **2b** form the *zigzag*-like chains along the crystallographic *c* axis (Fig. 5). As a result of the intermolecular interaction, the SeCl₂ moiety in **2b** has asymmetric geometry with the Se–Cl2 bond [2.4566(4) Å] being longer than the Se–Cl1 bond [2.3929(4) Å]. The mean value of the two Se–Cl bond lengths in **2b** [2.4248(4) Å] is significantly larger than those in the two-coordinate selenenyl(II) chlorides {[2.177(1) and 2.184(1) Å [2], 2.164(2) Å [6], 2.188(3) Å] [36]}.

Calculation results

In order to gain a deeper insight into the stabilization mechanism of 2-pyridineselenyl chloride, we performed quantum chemical calculations for its real dimeric (1d) and



Fig. 3 Molecular structure of 2b-DMFA. The intermolecular N-H \cdots O hydrogen bond is drawn by *dashed line*

hypothetical monomeric (1m) forms. The results obtained using two different functionals PBE0 and M06-2X are virtually identical and self-consistently indicate that the dimer formation is energetically favorable both in the solid



Fig. 4 Planar conformation of benzothiazolium-2-selenenyl dichloride stabilized by the intramolecular N-H…Cl hydrogen bond. The intramolecular N-H…Cl hydrogen bond is drawn by *dashed line*



Fig. 5 Crystal structure of 2b demonstrating the *zigzag*-like chains along the *c* axis. The *dashed lines* are indicative of the intermolecular N–H···O hydrogen bonds and secondary Se···Cl interactions

1	Functional	$\Delta E_{\rm tot}$, a.u.	$\Delta H^{\rm o}$, a.u.	ΔG^{o} , a.u.
Monomer (1m)	PBE0	-3108.662365	-3108.653912	-3108.697340
	M06-2X	-3109.307793	-3109.299351	-3109.343286
Dimer (1d)	PBE0	-6217.353919	-6217.336839	-6217.400251
	M06-2X	-6218.645118	-6218.628021	-6218.691764
ΔE , kcal/mol ^a	PBE0	-18.32	-18.21	-3.50
	M06-2X	-18.53	-18.40	-3.26

^a ZPVE correction is applied

state and in solutions (Tables 2, 3). It is also of note that the hypothetical planar dimer is not realized as a local minimum of the potential energy surface: It undergoes a nearly barrierless transformation into the butterfly conformation with a folding angle of $\sim 100^{\circ}$.

Table 2 Results of calculationfor the 2-pyridylselenenylchloride dimerization

The barrier to rotation of the $-\text{SeCl}_2$ linear fragment around the C–Se bond in **2b** is 9.0 kcal/mol (Fig. 6), which

is slightly lower than for similar benzimidazole and benzothiazole derivatives (11–13 kcal/mol [30]).

We applied QTAIM analysis in order to identify dimerforming attractive interactions. The respective results are summarized in Fig. 7 and Table 4. As it can be clearly seen in molecular graph **1d** (see Fig. 7), the dimer is formed by two strong Se \leftarrow N bonds with energy of 10.8 kcal/mol each

Table 3 Geometrical (X-rayand calculated) parameters for1m, 1d, and 2b

Molecule	Method	Se–C, Å	Se–Cl, Å	Se←N, Å	C=N, Å	N–C–Se, deg.	C-Se-Cl, deg.
1m	PBE0	1.926	2.163	_	1.315	119.7	100.1
	M06-2X	1.930	2.165	-	1.315	119.5	99.4
1d	X-ray	1.926(3)	2.4041(8)	2.141(3)	1.341(4)	116.8(2)	91.69(9)
	PBE0	1.923	2.286	2.371	1.331	116.7	99.1
	M06-2X	1.932	2.261	2.458	1.329	116.3	94.2
2b	X-ray	1.9195(15)	2.3929(4)	-	1.344(2)	118.91(12)	89.21(5)
			2.4566(4)				89.35(5)
	M06-2X	1.919	2.326	-	1.346	117.6	93.2
			2.566				88.8



Fig. 6 Potential energy surface (PES) scanning for [PyH]SeCl₂ (2b) along the rotational angle coordinate calculated at the M06-2x/6-311++G(d,p) level

as estimated according to the Espinosa-Lecompte correlation [37].

Furthermore, both bonding paths and critical points are present between the $Cl\cdots H(C)$ and $N\cdots N$ atomic pairs. The

short N…N contact of ~2.8 Å can be regarded as a topological artifact due to nearly convergence of two ring critical points (3; +1) with the bonding critical point (3; -1), which is especially distinct in the molecular graph calculated using the PBE0 functional. All expected bonding critical points and paths are actually observed in the monomer molecular graph **1m** without extra intramolecular Se \leftarrow N interactions. Therefore, we may conclude that the planar monomeric structure in **1m** is exclusively due to a partial double character of the Se–C bond therein. This statement is evident from MO plots of HOMO[-5] and HOMO[-6] (Fig. 8).

QTAIM analysis results for the adduct **2b** including both molecular graph and topological parameters are essentially equivalent to those reported for a benzimidazole analogue [30] except for a somewhat higher energy of the N–H…Cl intramolecular bond (14.0 vs. \sim 8 kcal/mol).

The Se–Cl bond energies in 1m, 1d, and 2b were also estimated using the Espinosa-Lecompte correlation (see Table 4), which enabled us to trace how this energy changes upon the formation of extra contacts. In particular, the dimerization of 1m into 1d results in a weakening of the Se–Cl bond by ~8 kcal/mol, whereas the hydrochloration affording the adduct 2b results in even more prominent weakening by ~12 kcal/mol. The observed energy changes correlate well with respective bond length changes.



Fig. 7 Molecular graphs for 1m, 1d, and 2b calculated at the M06-2X/6-311+G(d,p) level. The critical points: red—bond (3; -1); yellow—ring (3; +1)

Table 4 QTAIM parameterscalculated at the M06-2X/6-311+G(d,p) level

Bond critical points $(3; -1)$	$\rho(r)$, a.u.	$\Delta \rho(r)$, a.u.	<i>v</i> (<i>r</i>), a.u.	$E_{\rm cont}$, kcal(kJ)/mol
Monomer 1m				
Se-Cl	+0.114997	+0.021017	-0.111411	34.96 (146.27)
Dimer 1d				
Se-Cl	+0.096368	+0.041305	-0.087215	27.36 (114.47)
Se←N	+0.044810	+0.098518	-0.034429	10.8 (45.19)
H…Cl	+0.011589	+0.044549	-0.007026	2.20 (9.20)
$N \cdots N$	+0.014642	+0.058762	-0.010739	3.37 (14.10)
[PyH]SeCl ₂ 2b				
$H \cdots Cl(C)$	+0.018241	+0.066719	-0.011636	3.65 (15.27)
Se-Cl	+0.085811	+0.053845	-0.072690	22.80 (95.40)
Cl···H(N)	+0.050497	+0.083931	-0.044617	14.00 (58.58)
Se-Cl _{bonded}	+0.054058	+0.071169	-0.039157	12.29 (51.42)



Fig. 8 MO plots for 2b indicating a partial double-bond character of Se–C bond





Scheme 2 Selenocyclization of olefins and acetylenes



Reactivity studies

Selen-containing electrophilic reagents, in particular organylselenenyls, are widely used in contemporary organic synthesis for the functionalization of different types of substances, such as unsaturated compounds [12–14]. For instance, the selenocyclization of olefins and acetylenes with the ring closure by nucleophilic fragments of the unsaturated substrate has proven to be a powerful and useful approach to the synthesis of heterocyclic compounds. Nitrogen, oxygen, and other atoms can act as internal nucleophiles in such cyclization processes (Scheme 2).

Recently, we have proposed a novel approach to the synthesis of chalcogen- and nitrogen-containing heterocycles based on tandem addition-cyclization reactions of chalcogen-centered electrophiles at multiple bonds with the ring closure by the nitrogen atom from the reactant's organyl moiety, which is currently under further development [18–20, 30, 38–42]. In particular, we have demonstrated for the first time that the introduction of a moiety bearing a nitrogenous base, i.e. pyridine, into the selenenyl chloride structure enables a novel avenue in the olefin selenation affording cyclization products with the pyridine nitrogen atom responsible for the ring closure [39–42].

As we have shown earlier [39-42], the reaction of selenenyl chloride **1b** with different alkenes, including styrene, 1-ethynyl-4-methoxybenzene, cyclopentene, and 3,4-dihydro-2*H*-pyran, in methylene chloride affords the respective heterocyclization products via the ring closure by the nucleophilic nitrogen atom of the reactant's hetaryl moiety (Scheme 3). This implies that the dimeric reactant **1b** dissociates under reaction conditions into transient monomeric species similar to pyridine-2-selenenyl

chloride, which are actually responsible for the formation of target heterocyclization product. Taking into account data on self-transformation of **1b** reported in this paper, we performed additional studies on reactions of T-shaped selenenyl dichloride **2b** with alkenes in methylene chloride. These reactions yield condensed heterocyclic compounds fully identical to aforementioned ones. Thus, it becomes clear that in this case also the reaction is actuated by the dissociation of **2b** to generate highly reactive monomeric pyridine-2-selenenyl chloride.

Conclusions

In conclusion, we have prepared and structurally characterized two new selenenyl chloride compounds, viz., dimeric pyridine-2-selenium chloride (1b) and H-bonded complex of pyridinium-2-selenium dichloride with DMFA (2b·DMFA). The experimental and theoretical data obtained (1) clearly explain the relatively high stability of 1b, (2) directly confirm the presence of the propeller-like free rotation of the SeCl₂ moiety around the essentially ordinary C-Se bond in solutions of T-shaped hetarylselenenyl dichlorides, (3) prove that the transformation of hetarylselenenyl chlorides into T-shaped hetarylselenenyl dichlorides in solution is energetically favorable, and thus (4) contribute to understanding of mechanism of the novel heterocyclization reaction. Furthermore, our results revealed that the investigated selenenyl chlorides 1b and 2b can serve as a source of difficult-to-obtain, unstable organoselenenyl chlorides, which should open new opportunities for the study of low-valent chalcogens.

Supplementary materials

Full crystal data as CIFs and optimized geometry of the most stable conformers of **1b** and **2b**·**DMFA** are included as electronic supplement.

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