Synthesis and Structure of Organoantimony(III) Compounds Containing Antimony−Selenium and −Tellurium Terminal Bonds[†]

Libor Dostál,*[,‡] Roman Jambor,[‡] Aleš Růžička,[‡] Antonín Lyčka,[§] Jiří Brus,[||] and
Frank de Proft[⊥]

Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, nám. Čs. legií 565, CZ 532 10, Pardubice, Czech Republic, Research Institute for Organic Syntheses (VUOS), Rybitví 296, CZ 533 54, Pardubice 20, Czech Republic, Institute of Macromolecular Chemistry of the Academy of Science of the Czech Republic, Heyrovsky sq. 2, CZ 162 06, Prague 6, Czech Republic, and Eenheid Algemene Chemie (ALGC), Vrije Universiteit Brussel (VUB), Faculteit Wetenschappen, Pleinlaan 2, B-1050 Brussels, Belgium

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Summary: The reactions of the organoantimony(I) compound Sb_4Ar_4 (where Ar is the N,C,N chelating ligand C_6H_3-2,6-$(CH_2NMe_2)_2$) with elemental Se and Te give the unprecedented monomeric compounds ArSbE (E = Se, Te) with the terminal Sb−E bond being retained both in solution and in the solid state.

The syntheses of stable organometallic compounds containing double bonds between heavier main-group elements have recently attracted considerable attention.[1] The majority of these compounds were stabilized using effective steric hindrance by several types of bulky substituents. Double-bonded systems between heavier group 15 elements were prepared in a similar way. Power and Tokitoh have reported the syntheses of kinetically stabilized *trans*-distibenes and -dibismuthenes (*trans*-RM═MR, M = Sb, Bi and R = bulky ligand; Chart 1).[2] Reactions of double-bonded BbtM═MBbt and TbtM═MTbt compounds (Bbt = 2,6-bis[bis(trimethylsilyl)methyl]-4-[tris(trimethylsilyl)methyl]phenyl; Tbt = 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl) with elemental chalcogens give the dimeric centrosymmetric oxides $(BbtMO)_2$ and $(TbtMO)_2$ with central four-membered rings in the case of oxygen and mixtures of cyclic sulfides and polysulfides in the reaction with sulfur.[3] On the other hand, reactions with selenium and Bu_3PTe yielded selena- and telluradistibarane and selena- and telluradibismirane as examples of the heaviest three-membered heteroatom ring systems reported to date.[3,4] Trimeric $(TbtMSe)_3$ (M = Sb, Bi) and $(BbtSbSe)_3$ compounds with a six-membered core have recently been obtained as stable compounds.[2a,b,3] Nevertheless, any evidence for organoantimony compounds bearing an unsupported terminal Sb−Se or Sb−Te double bond is still missing. The presence of a terminal antimony−selenium double bond was suggested by Breunig in the case of a tungsten complex, $(CO)_5W(CH(SiMe_3)_2)Sb{=}Se$, in benzene solution. However, the possibility of the dimeric nature of this complex in solution was in fact not excluded and, furthermore, this compound was shown to be dimeric with the central Sb_2Se_2 core in the solid state by X-ray studies.[5]

Recently, we have demonstrated that the so-called N,C,N pincer-type ligand C_6H_3-2,6-$(CH_2NMe_2)_2$ (denoted as Ar hereafter) can be used for stabilization of low-valent metal centers in the case of both heavier group 14 and 15 elements.[6] This ligand can be used as an alternative to sterically demanding ligands, because it also offers, in addition to its slight steric protection, significant thermodynamic stabilization of reactive metal centers by the coordination of its two pendant CH_2NMe_2 functionalities. In this study, we employed this ligand for stabilization of terminal Sb−Se and Sb−Te bonds in the monomeric compounds ArSbSe (**2**) and ArSbTe (**3**).

The reaction of the cyclic organoantimony(I) compound Ar_4Sb_4 (**1**)[6b] with an excess (~20%) of elemental selenium and tellurium in THF (Scheme 1) gave the corresponding selenide **2** and telluride **3** in moderate yields as yellow and orange highly air-sensitive crystalline solids, respectively.[7] Compound **2** melts

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* To whom correspondence should be addressed. E-mail: libor.dostal@upce.cz.

[†] Dedicated to Prof. Marcel Gielen on the occasion of his 70th birthday and his outstanding contribution to main-group chemistry.

[‡] University of Pardubice.

[§] Research Institute for Organic Syntheses (VUOS).

[||] Institute of Macromolecular Chemistry of the Academy of Science of the Czech Republic.

[⊥] Vrije Universiteit Brussel (VUB).

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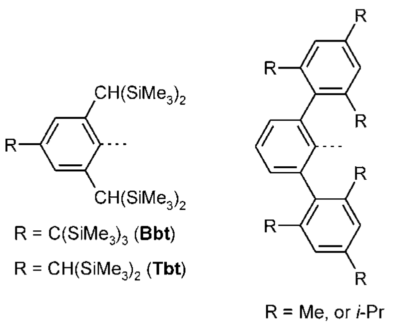
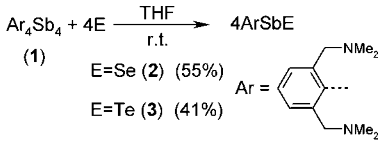
(7) Data for **2** are as follows. Yield: 236 mg (55%). Mp: 174−176 °C. Anal. Calcd for $C_{12}H_{19}N_2SbSe$ (mol wt 392.01): C, 36.8; H, 4.9. Found: C, 37.0; H, 4.7. ^1H NMR ($CDCl_3$): δ 2.57 (6H, s, $(CH_3)_2N$), 2.65 (6H, s, $(CH_3)_2N$), 3.59 and 4.06 (4H, AX pattern, NCH_2), 7.08 (2H, d, Ar-H3,5), 7.23 (1H, t, Ar-H4). ^{13}C NMR ($CDCl_3$): δ 46.06 (s, $(CH_3)_2N$), 46.53 (s, $(CH_3)_2N$), 64.26 (s, NCH_2), 125.29 (s, Ar-C3,5), 129.2 (s, Ar-C4), 143.15 (s, Ar-C2,6), 151.76 (s, Ar-C1). ^{77}Se NMR ($CDCl_3$): δ −197. ^{77}Se CP/MAS NMR: δ −153. Data for **3** are as follows. Yield: 115 mg (41%). Mp: 165 °C dec. Anal. Calcd for $C_{12}H_{19}N_2SbTe$ (mol wt 440.65): C, 32.7; H, 4.4. Found: C, 38.0; H, 4.7. ^1H NMR (THF): δ 2.55 (6H, s, $(CH_3)_2N$), 2.60 (6H, s, $(CH_3)_2N$), 3.52 and 3.96 (4H, AX pattern, NCH_2), 7.07 (2H, d, Ar-H3,5), 7.17 (1H, t, Ar-H4). ^{13}C NMR (THF): δ 45.46 (s, $(CH_3)_2N$), 47.79 (s, $(CH_3)_2N$), 64.70 (s, NCH_2), 125.74 (s, Ar-C3,5), 129.22 (s, Ar-C4), 144.28 (s, Ar-C2,6), 151.88 (s, Ar-C1). ^{125}Te NMR (THF): δ −655.

10.1021/om800945g CCC: $40.75

Chart 1



Scheme 1. Synthesis of Compounds ArSbSe (2) and ArSbTe (3)



without decomposition, but telluride **3** decomposes at elevated temperatures. Compounds **2** and **3** were both characterized by a combination of ^{1}H, ^{13}C, ^{77}Se, and ^{125}Te NMR spectroscopy, elemental analysis, and X-ray crystallography (Figure 1).

The molecular structures of **2** and **3** were unambiguously determined by X-ray diffraction techniques[8] (Figure 1) in the solid state. Both compounds are monomeric. There are no close intermolecular contacts between chalcogen atoms (Se(1) in **2** and Te(1) in **3**) and other atoms in the unit cell, indicating well-isolated and -preserved Sb−Se (**2**) and Sb−Te (**3**) terminal bonds. The Sb(1)−Se(1) bond length of 2.4396(7) Å in **2** is approximately 9% shorter than the normal single covalent bond Sb−Se ($\sum_{\text{cov}}$(Sb−Se) = 2.68 Å), and a similar situation was observed also in the tellurium analogue **3** with the Sb(1)−Te(1) bond distance 2.6620(1) Å ($\sum_{\text{cov}}$(Sb−Te) = 2.93 Å). Such a shortening of bond lengths may be indicative of the multiple character of chemical bonds, as was previously shown for example in organotin selenides and also other double-bonded main-group-element systems[9] (see below for further discussion). Both Sb−Se (in **2**) and Sb−Te (in **3**) bond distances are slightly shorter than those found in three-membered Sb$_2$E rings (E = Se, Te) and, to the best of our knowledge, represent one of the shortest bonds between these elements detected by X-ray diffraction to date. Some examples of analogously short bonds were found only in the case of several Zintl phases, such as [Sb$_4$Se$_9$]$^{4-}$, [Sb$_2$Se$_5$]$^{4-}$, [SbTe$_4$]$^{3-}$, etc.[10] The N,C,N ligand is coordinated to the central antimony atom Sb(1) in a tridentate fashion in **2** and **3**. As a consequence of the presence of strong intramolecular Sb−N interactions (Sb−N distances 2.461(3) and 2.518(3) Å in **2** and 2.448(5) and 2.526(5) Å in **3**; $\sum_{\text{vdW}}$(Sb−N) = 3.74 Å), the coordination polyhedron around the antimony atoms can be described as a distorted Ψ-trigonal bipyramid. Both nitrogen donor atoms occupy the axial positions (N(1)−Sb(1)−N(2) angles are 145.14(12)° for **2** and 145.70(18)° for **3**; the deviation from the ideal value of 180° is caused by significant ligand rigidity). The ipso carbon atom C(1) and chalcogen atoms (Se(1) or Te(1)) are located in the equatorial plane (Figure 1). The angles C(1)−Sb(1)−Se(1) = 102.90(11)° in **2** and C(1)−Sb(1)−Te(1) = 102.69(16)° in **3** are slightly smaller than 120°, reflecting the presence of a lone pair of electrons on the central atom.

Compounds **2** and **3** both preserve their monomeric structure in solution. ^{1}H and ^{13}C NMR spectra revealed only one set of signals, consistent with the structure found for both compounds in the solid state. In the ^{1}H NMR spectra, an AX pattern was obtained for the NCH$_2$ moieties and two signals in a 1:1 intensity ratio were detected for the NMe$_2$ groups. Similarly, two signals for NMe$_2$ groups were present in the ^{13}C NMR spectra.[11] Only one signal was observed in the ^{77}Se spectrum of **2** (−197 ppm) and in the ^{125}Te NMR spectrum of **3** (−655 ppm). Both values closely resemble those found by Tokitoh in ^{77}Se and ^{125}Te NMR spectra of Sb$_2$E ring compounds.[4] Unambiguous evidence that the monomeric structure of **2** was retained on going from the solid state to solution was provided by the ^{77}Se CP/MAS NMR spectra of **2** and the value δ_{iso} −153 ppm, which resembles that found in solution (−197 ppm). This small discrepancy in ^{77}Se chemical shifts between solution and the solid state might also be caused by different strengths of the Sb−Se bond in both phases. These findings point to an essentially identical chemical environment around the selenium atom both in solution and in the solid state. Analogous behavior can most probably be expected also for compound **3**, according to ^{1}H and ^{13}C NMR data and theoretical calculations (vide infra).[12]

We have also carried out a theoretical analysis of compounds **2** and **3** by performing a geometry optimization of these compounds, starting from their gas-phase structures. These geometry optimizations were performed at the B3LYP[13] level of theory using the cc-pVTZ basis set[14] for C, N, H, and Se and the SDB-cc-pVTZ basis set[15] for Sb and Te using Gaussian 03.[16] Both optimized geometries were confirmed to be minima on the potential energy surface by frequency analysis and correspond well to the experimental geometries. The computed bond length of Sb(1)−Se(1) in **2** is 2.430 Å, whereas the Sb(1)−Te(1) bond length in **3** was computed to be 2.639 Å, in very good agreement with the experimental findings (Sb(1)−Se(1) = 2.4396(7) Å, Sb(1)−Te(1) = 2.6620(1) Å).

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(8) Data for **2**: C$_{12}$H$_{19}$N$_2$SbSe, M_r = 392.0, orthorhombic, *Pbca*, a = 9.8540(8) Å, b = 15.4940(8) Å, c = 18.5060(19) Å, V = 2825.5(4) Å^3, Z = 8, T = 150(1) K, 25 990 total reflections, 3245 independent (R_{int} = 0.126, R1 (obsd data) = 0.040, wR2 (all data) = 0.061), CCDC 688753. Data for **3**: C$_{12}$H$_{19}$N$_2$SbTe, M_r = 440.64, orthorhombic, *Pbca*, a = 9.8740(9) Å. b = 15.6460(15) Å, c = 18.913(2) Å, V = 2921.8(5) Å^3, Z = 8, T = 150(1) K, 10 638 total reflections, 3249 independent (R_{int} = 0.082, R1 (obsd data) = 0.046, wR2 (all data) = 0.097), CCDC 688752.

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(11) If compounds **2** and **3** were dimers in solution, two sets of signal should be detected in the ^{1}H and ^{13}C NMR spectra due to the possible formation of cis and trans isomers with regard to the mutual position of both ligands on the hypothetical central Sb$_2$E$_2$ core, similarly to Sb$_2$S$_2$ and Sn$_2$S$_2$ analogues. See: (a) Dostál, L. et al. To be submitted for publication. (b) Dostál, L.; Jambor, R.; Růžička, A.; Jirásko, R.; Taraba, J.; Holeèek, J. *J. Organomet. Chem.* **2007**, *692*, 3750.

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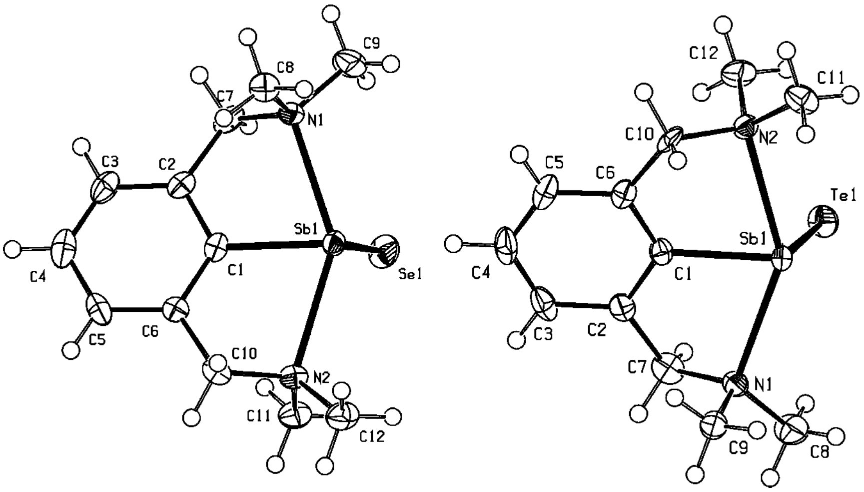
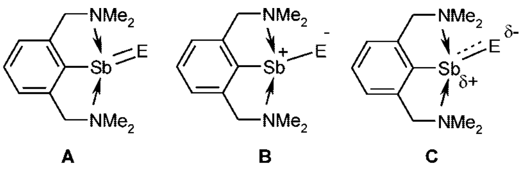


Figure 1. ORTEP plot of molecules of **2** (left) and **3** (right) showing 50% probability displacement ellipsoids. Selected bond lengths (Å) and angles (deg): for **2**, Sb(1)−Se(1) = 2.4396(7), Sb(1)−N(1) = 2.461(3), Sb(1)−N(2) = 2.518(3), Sb(1)−C(1) = 2.135(4), N(1)−Sb(1)−N(2) = 145.14(12), C(1)−Sb(1)−Se(1) = 102.90(11); for **3**, Sb(1)−Te(1) = 2.6620(1), Sb(1)−N(1) = 2.448(5), Sb(1)−N(2) = 2.526(5), Sb(1)−C(1) = 2.133(6), N(1)−Sb(1)−N(2) = 145.70(18), C(1)−Sb(1)−Te(1) = 102.69(16).

Chart 2



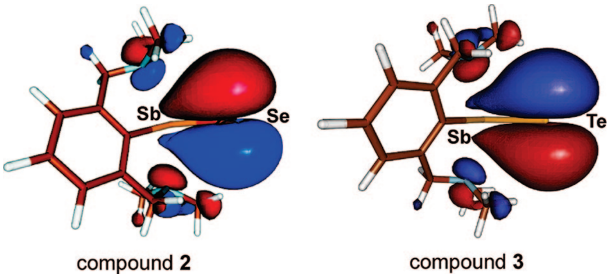


Figure 2. Plot of the molecular orbital corresponding to the terminal bond between Sb and Se (left) and Sb and Te (right) in compounds **2** and **3**, respectively (in both compounds, this is the orbital below the HOMO). The value of the isosurface plotted is 0.02 au in both cases.

Regarding the nature of the terminal Sb−E (E = Se, Te) bonds in **2** and **3**, there are two different descriptions (Chart 2A,B).[17]

First, both bonds can be viewed as “regular Sb═E double bonds” (Chart 1A). The molecular orbitals describing the situation in the Sb−Se (**2**) and Sb−Te (**3**) terminal bonds are depicted in Figure 2. In both cases, this molecular orbital is the orbital directly below the highest occupied molecular orbital, and the electron density distribution seems to have π symmetry in these bonds (in accord with the double-bond formulation). Also, the significant shortening of the bond length (as determined in the solid state by X-ray studies) in comparison to the single covalent bond length points to a double-bond character in **2** and **3**.[9]

On the other hand, there is an alternative possibility (Chart 1B) to describe these bonds as “polarized single bonds $Sb^+−E^-$”.[17] As is apparent from Figure 2, the electron density is quite strongly polarized to chalcogen atoms Se (**2**) and Te (**3**). The positive charge on the central antimony atom is then of course reflected in the presence of strong intramolecular Sb−N interactions present both in **2** and **3**.[18] However, as shown by the bond lengths Sb−N, these dative bonds are still weaker than those observed in the true cationic species $[2,6\text{-}(CH_2NMe_2)_2C_6H_3SbCl]^+[CB_{11}H_{12}]^-$ (the values of Sb−N bond lengths 2.369(8) and 2.437(7) Å) and $[2\text{-}(CH_2NMe_2)\text{-}C_6H_4]_2Sb^+[PF_6]^-$ (2.412(3) and 2.416(4) Å),[18c,19] where the anion is well-separated from the cationic antimony center (with formal charge 1+ at the Sb atom). This finding, in fact, rules out the possibility of a fully polarized single bond as depicted in Chart 1B. In order to gain further insight into the precise nature of the Sb−Se and Sb−Te bonding in **2** and **3**, we have performed an NBO analysis[20] at the same level of theory used for the geometry optimizations.

In compounds **2** and **3**, the charges on the central Sb atom are +0.999 and +0.854, respectively, the charges on Se and Te amounting to −0.788 and −0.658. The NBO analysis reveals

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(17) We are deeply indebted to one of the referees of this manuscript for helpful suggestions especially proposal of the second alternative description of the nature of the Sb-Se and Sb-Te terminal bonds as strongly polarized single bonds was really stimulating for us.

(18) The coordination of organoantimony or organobismuth cations by C,Y chelating ligands has been already well established. See: (a) Dostál, L.; Novák, P.; Jambor, R.; Rùžička, A.; Císařová, I.; Jirásko, R.; Holeček, J. *Organometallics* **2007**, *26*, 2911. (b) Dostál, L.; Jambor, R.; Císařová, I.; Beneš, L.; Rùžička, A.; Jirásko, R.; Holeček, J. *J. Organomet. Chem.* **2007**, *692*, 2350. (c) Carmalt, C. J.; Walsh, D.; Cowley, A. H.; Norman, N. C. *Organometallics* **1997**, *16*, 3597.

(19) Dostál, L. Unpublished material.

that next to the single bond between Sb and the chalcogen (Se or Te), there is a large back-donation of the lone-pair orbital of the chalcogen into the empty orbital on Sb. The lone-pair orbitals on Se and Te contain 1.738 and 1.727 electrons, respectively (for a perfect lone pair this value should be 2); the empty lone p orbital on Sb contains 0.513 and 0.531 electron for compounds **2** and **3**.

We have also computed the Wiberg bond order[21] for the Sb−Se and Sb−Te bonds. For compound **2**, the Wiberg bond order for the Sb−Se bond order is 1.409, whereas in the case of the Sb−Te bond it is 1.426. For a perfect ionic bond, the Wiberg bond order should be equal to 0; for perfectly covalent single and double bonds, the values should be 1 and 2, respectively. This result thus implies that the bonds between Sb and Se or Te thus lie between a single and a double bond. From this analysis, it can thus be concluded that the bonding between Sb and the chalcogen atoms can be described as intermediate between a polarized single bond and a double bond. Similar bonding situations for lighter elements (Si) have been described elsewhere.[22]

To summarize, taking all aforementioned experimental and theoretical data into account, the terminal Sb−Se (**2**) and Sb−Te (**3**) bonds are probably best described as having appreciable double-bond character, although the electron density is strongly polarized in the chalcogen atom direction (Chart 1C).

In conclusion, compounds **2** and **3** containing unique Sb−Se and Sb−Te terminal bonds, which are retained both in solution and in the solid state, were prepared and characterized. Effective support of the N,C,N pincer type ligand seems to be crucial for stabilization of these monomeric compounds, because using bulky ligands gave the trimeric selenides only. Studies concerning the reactivity of **2** and **3** and further utilization of the N,C,N ligand in similar multiple or terminal bond stabilization are currently underway in our group.

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Supporting Information Available: Text, figures, tables, and CIF files giving all experimental details, including syntheses, experimental measurements, copies of all NMR spectra, all crystal data and structure refinement details, atomic coordinates, anisotropic displacement parameters, and geometric data for compounds and details of theoretical calculations. This material is available free of charge via the Internet at http://pubs.acs.org.

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