Supplementary materials for:

Monomeric Organoantimony(III) Sulphide and Selenide with Terminal Sb-S(Se) Bond. Syntheses, Structures and Theoretical Consideration.

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Details of DFT calculations

All molecular structures were computed using the Gaussian 09 program[S1] at the B3LYP level of theory[S2] using the cc-pVTZ basis set[S3] on all atoms, except for Sb and Te for which the SDB-cc-pVTZ basis set [S4] was used.
On the optimized structures, given below, an NBO analysis[S5] was performed in order to probe the bonding features of the Sb-E bond; in addition, the Wiberg bond order[S6] for these bonds were computed.
Molecular structures of compounds 3 and 4 were optimized previously, see ref. S7.

[1] Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[2] (a) Becke, A.D. *J. Chem. Phys*. **1993**, *98*, 5648.
(b) Lee, C.; Yang, W.; Parr, R.G. *Phys. Rev. B* **1988**, *37*, 785.
(c) Stephens, P.J.; Devlin, F.J.; Chabalowski, C.F.; Frisch, M.J. *J. Phys. Chem.* **1994**, *98*, 11623.

[3] Hydrogen and 1st-row: Kendall, R.A.; Dunning, T.H.; Harrison, R.J. *J. Chem. Phys*. **1992**, *96*, 6796. 2nd row: Woon, D.E.; Dunning T.H. *J. Chem. Phys*. **1993**, *98*, 1358. 3rd row: Wilson, A.K.; Woon, D.E.; Peterson, K.A.; Dunning Jr., T.H. *J. Chem. Phys.* **1999**, *110*, 7667.

[4] Martin, J. M. L.; Sunderman, A. *J. Chem. Phys*. **2001**, *114*, 3408.

[5] (a) Foster, J. P.; Weinhold, F. *J. Am. Chem. Soc.* **1980**, *102*, 7211.
(b) Reed, A. E.; Weinhold, F. *J. Chem. Phys.* **1983**, *78*, 4066.
(c) Reed, A. E.; Curtiss, L. A. Weinhold, F. *Chem. Rev.* **1988**, *88*, 899.
(d) Weinhold, F. In *Encyclopedia of Computational Chemistry*, Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R. Eds., John Wiley & Sons, Chichester, UK, 1998, *Vol. 3*, p. 1792.
(e) Weinhold, F.; Landis, C. *Valency and Bonding, A Natural Bond Orbital Donor-Acceptor Perspective*; Cambridge University Press: Cambridge, 2005.

[6] Wiberg, K. B. *Tetrahedron* **1968**, *24*, 1083.

[7] L. Dostál, R. Jambor, A. Růžička, A. Lyčka, J. Brus, F. de Proft, *Organometallics* **2008**, *27*, 6059.

1. Cartesian coordinates (Å) for compound 1

Sb	−0.000197	−0.537399	0.085187
S	−0.000251	−1.086668	−2.140218
N	−2.381337	0.283141	0.144051
C	0.000032	1.633074	0.093787
C	4.141611	−0.924802	−1.052120
C	3.500352	−0.599324	0.153906
N	2.381466	0.283084	0.143810
C	0.000078	4.426378	0.118880
H	0.000108	5.507581	0.119062
C	4.928717	−2.103023	1.364056
H	5.231664	−2.560371	2.297289
C	2.475166	1.561552	0.137521
C	−1.209897	2.334133	0.115699
C	3.722850	−0.303970	−2.357644
H	4.005742	0.751194	−2.410820
H	4.205910	−0.811881	−3.190817
H	2.642209	−0.365805	−2.494382
C	3.879641	−1.186703	1.371155
C	−3.500221	−0.599304	0.154057
C	1.209997	2.334073	0.115593
C	−2.475057	1.561625	0.137765
C	−4.141663	−0.924410	−1.051978
C	3.784813	2.300784	0.165353
H	4.624270	1.614298	0.210641
H	3.887481	2.922155	−0.725705
H	3.826237	2.966044	1.029087
C	−3.784697	2.300838	0.165817
H	−4.624160	1.614354	0.211032
H	−3.826009	2.965918	1.029687
H	−3.887458	2.922401	−0.725106
C	3.184054	−0.831645	2.658867
H	3.306748	0.224592	2.910056
H	2.110696	−1.019435	2.599414
H	3.584875	−1.417545	3.484364
C	5.578244	−2.436919	0.184964
H	6.385504	−3.156948	0.194807
C	5.183296	−1.850067	−1.007844
H	5.682717	−2.115209	−1.930788
C	−1.202219	3.733582	0.122400
H	−2.128420	4.290640	0.129557
C	−3.879298	−1.187076	1.371172
C	1.202348	3.733521	0.122323
H	2.128565	4.290550	0.129490
C	−4.928320	−2.103462	1.363948
H	−5.231078	−2.561132	2.297082
C	−5.183299	−1.849732	−1.007828

H	−5.682890	−2.114568	−1.930764
C	−3.183575	−0.832343	2.658905
H	−3.306076	0.223880	2.910242
H	−3.584460	−1.418293	3.484333
H	−2.110252	−1.020316	2.599384
C	−3.723085	−0.303212	−2.357386
H	−2.642518	−0.365536	−2.494510
H	−4.206703	−0.810529	−3.190593
H	−4.005431	0.752121	−2.410023
C	−5.578014	−2.437006	0.184856
H	−6.385227	−3.157091	0.194581

E (B3LYP) = –1520.63398 a.u.

2. Cartesian coordinates (Å) for compound 2

Sb	0.000000	−0.428696	0.273225
Se	−0.000120	−1.277674	−2.011622
N	2.378702	0.384081	0.249400
C	0.000017	1.722800	0.053045
N	−2.378678	0.384122	0.249432
C	−4.176350	−0.911159	−0.794524
C	3.497552	−0.491870	0.361100
C	2.474045	1.656332	0.117184
C	−3.497514	−0.491846	0.361145
C	4.176349	−0.911213	−0.794595
C	−1.210699	2.422216	0.007580
C	4.891226	−1.888417	1.730805
H	5.167372	−2.266693	2.706731
C	3.842823	−0.976746	1.632953
C	−3.842736	−0.976756	1.633009
C	−4.891112	−1.888449	1.730874
H	−5.167233	−2.266744	2.706802
C	1.210738	2.422194	0.007551
C	−1.202367	3.815065	−0.127457
H	−2.128649	4.369881	−0.175026
C	−2.474015	1.656369	0.117215
C	3.805267	−0.396449	−2.159422
H	4.114604	0.643709	−2.296540
H	4.297370	−0.984745	−2.932197
H	2.728095	−0.449038	−2.321905
C	3.784410	2.394145	0.089531
H	4.620860	1.715723	0.224386
H	3.905527	2.916170	−0.861052
H	3.811480	3.147907	0.877722
C	0.000035	4.503714	−0.202548
H	0.000041	5.579343	−0.312009
C	5.574171	−2.316846	0.602307
H	6.379918	−3.032797	0.693974
C	5.215322	−1.828591	−0.644693
H	5.741917	−2.166214	−1.528003
C	1.202426	3.815048	−0.127485
H	2.128716	4.369847	−0.175089
C	−3.784382	2.394175	0.089490
H	−4.620809	1.715790	0.224674
H	−3.811376	3.148216	0.877418
H	−3.905610	2.915860	−0.861265
C	3.118110	−0.514829	2.869906
H	3.508036	−1.020131	3.751950
H	3.227406	0.560834	3.026938
H	2.047682	−0.717621	2.809273
C	−5.574084	−2.316876	0.602384

H	−6.379809	−3.032848	0.694069
C	−3.805366	−0.396332	−2.159354
H	−4.297561	−0.984559	−2.932121
H	−4.114666	0.643845	−2.296378
H	−2.728206	−0.448958	−2.321928
C	−3.117997	−0.514856	2.869951
H	−3.507942	−1.020130	3.752003
H	−2.047578	−0.717703	2.809316
H	−3.227235	0.560813	3.026970
C	−5.215295	−1.828579	−0.644609
H	−5.741901	−2.166194	−1.527915

E (B3LYP) = –3524.05086 4a.u.

3. Cartesian coordinates (Å) for the hypothetical compound PhSbS

Sb	−0.571154	−0.440044	−0.511533
S	1.484436	−1.206256	−0.991746
C	−0.254006	1.668134	−0.187388
C	0.041033	4.407922	0.253967
H	0.158014	5.469992	0.424566
C	−1.362021	2.458364	0.139196
C	1.003999	2.26744	−0.290072
C	−1.215869	3.823294	0.359217
H	−2.077173	4.427719	0.611423
C	1.150286	3.629658	−0.070704
H	2.126964	4.088627	−0.151803
H	1.862601	1.65714	−0.542557
H	−2.346884	2.01206	0.223588

E (B3LYP) = –635.40566 a.u.

4. Cartesian coordinates (Å) for the hypothetical compound PhSbSe

Sb	−0.719617	−0.936814	−0.000041
Se	−2.127645	0.979287	0.000042
C	1.276269	−0.119143	0.000065
C	1.554214	1.250307	−0.000027
C	2.339676	−1.029568	0.000103
C	2.867431	1.698258	−0.000081
H	3.075661	2.760243	−0.000204
C	3.918638	0.783668	−0.000027
H	4.941509	1.136465	−0.000036
C	3.655475	−0.581176	0.000066
H	4.470838	−1.292494	0.0002
H	2.146277	−2.096509	0.000167
H	0.735892	1.959996	−0.000044

E (B3LYP) = –2638.82405 4a.u.

5. Cartesian coordinates (Å) for the hypothetical compound PhSbTe

Sb	−0.680205	−0.411392	−0.484781
Te	1.590682	−1.425701	−1.157866
C	−0.276371	1.6854	−0.176163
C	0.057133	4.424164	0.267444
H	0.189481	5.48433	0.438384
C	−1.362191	2.483868	0.203869
C	0.978644	2.279135	−0.330568
C	−1.197051	3.84651	0.424805
H	−2.043079	4.45392	0.718222
C	1.144215	3.638917	−0.110374
H	2.120289	4.09012	−0.232528
H	1.824393	1.669664	−0.624258
H	−2.345714	2.045116	0.329966

E (B3LYP) = –245.27752 a.u.