Electronic Supplementary Material (ESI) for Chemical Communications.

Bismuthanylstibanes

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Electronic Supporting Information

General

Synthetic procedures

All manipulations were performed using standard Schlenk and glovebox techniques under an atmosphere of dry nitrogen. Solvents were dried over Na/benzophenone (pentanes, hexanes, tetrahydrofuran, benzene-d_6) or over calcium hydride (dichloromethane, chloroform-d) and distilled prior to use. Reaction glassware was baked in a 160 ^{o}C oven for at least 1 h prior to use and assembled under nitrogen while hot.

Solution NMR spectroscopy

Nuclear magnetic resonance spectra are referenced to tetramethylsilane (^{1}H, ^{13}C) on a Bruker AV-300 spectrometer or a Bruker AV-500 spectrometer with residual solvent used for chemical shift calibration. Samples for NMR spectroscopy were prepared and sealed inside the glovebox with Parafilm before removal into ambient atmosphere.

Vibrational spectroscopy

Infrared spectra were obtained on an Agilent Technologies Cary 630 FTIR instrument equipped with a ZnSe ATR module. Infrared spectra were obtained on a Thermo Scientific Nicolet NXR 9650 FT-Infrared Spectrometer instrument equipped with a 1064 nm Nd:YVO_4 laser and InGaAs detector.

Melting points

Melting points were obtained for samples sealed in glass capillaries and are uncorrected.

Crystallography

Single crystals diffraction experiments were performed on a Bruker D8-Quest Photon II diffractometer. Reflections were integrated using the APEX III software and solved and refined using Olex2 software. Details for individual compounds are given with their characterization data. Crystallographic data has been deposited with the Cambridge Structural Database under numbers: 1975977-1975980

Mass Spectrometry

Atmospheric Pressure Chemical Ionization (APCI) spectra were obtained on a Bruker micrOTOF.

Commercial reagents: Naphthalenediamine was obtained from Oakwood Chemicals. Chlorosilanes were obtained from Alfa. nButylltihium (1.6 M in hexanes) was obtained from Acros. $SbCl_3$ and $BiCl_3$ was obtained from Alfa and sublimed prior to use. $LiHBEt_3$ (1.0 M in THF) and $LiNMe_2$ were obtained from Alfa.

Starting materials

^{R}SbH and ***^{R}SbCl*** were synthesized according to the procedure of Chitnis *et. al.*[1]
^{R}BiNMe$_2$ and ***^{R}BiCl*** were synthesized according to the procedure of Roesky *et. al.* [2]

Representative synthetic procedure for $^{R}BiSb^{R'}$:

^{Et}SbH (1.4460 g, 2.85 mmol) was dissolved in hexane (ca. 50 mL) and cooled to –30 °C. To this, $^{Me}BiNMe_2$ (1.5792 g, 2.85 mmol) in a solution of hexane (ca. 50 mL) was slowly added, resulting in the formation of a dark red solution. The solution was warmed to room temperature and stirred for 5 hours. The reaction mixture was concentrated and placed in the freezer for recrystallization at –25 °C which gave the respective diaminostibanes as a red powder.

$^{Me}BiSb^{Et}$:
Yield: 2.2047 g, 76%

Melting Point: 151.3-155.1 °C, decomp.

^{1}H NMR (300 MHz, benzene-d_6): δ 7.30-7.08 (m, 12H, Ar-H), 0.89-0.86 (m, 18H, 2 x Et_3Si), 0.70-0.69 (m, 12H, 2 x Et_3Si), 0.15 (s, 18H, 2 x Me_3Si).

^{13}C{^{1}H} NMR (75 MHz, benzene-d_6): δ 154.3 (CAr), 151.4 (CAr), 138.2 (CAr), 137.7 (CAr), 136.9 (CAr), 126.2 (CAr), 124.7 (CAr), 124.4 (CAr), 122.1 (CAr), 120.4 (CAr), 116.8 (CAr), 116.01 (CAr), 7.4 (2 x Et_3Si), 6.7 (2 x Et_3Si), 3.13 (2 x Me_3Si).

FTIR (cm^{-1} (relative int.)): 3051(7), 2950(25), 2906(2), 2872(5), 1959(13), 1555(55), 1511(1), 1460(1), 1453(6), 1429(2), 1422(19), 1384(4), 1371(34), 1324(33), 1312(3), 1271(100), 1249(33), 1174(7), 1155(1), 1126(3), 1103(1), 1057(81), 1039(14), 1018(4), 1002(29), 958(<1), 887(12), 872(15), 856(72), 838(21), 809(26), 781(22), 763(30), 751(81), 736(1), 720(1), 693(2), 682(<1), 675(9), 658(3), 624(<1), 618(4), 599(2), 589(7), 572(1), 530(14), 521(6), 481(11).

HRMS (APCI, $[M]^+$): calculated = 1014.2732 m/z, observed = 1014.2734 m/z, error = 0.24 ppm

Elemental analysis: Calcd. C: 44.92, H: 5.95, N: 5.51; Expt. C: 43.05, H: 6.44, N: 5.47

X-ray**:** Crystals were grown from a hexane solution. $C_{38}H_{60}BiN_4SbSi_4$ (M =1029.93 g/mol): monoclinic, space group C2/c (no. 15), a = 20.7764(8) Å, b = 9.9748(4) Å, c = 42.2992(15) Å, β = 100.049(2)°, V = 8631.6(6) Å^3, Z = 8, T = 120.0 K, μ(CuKα) = 14.180 mm^{-1}, $Dcalc$ = 1.585 g/cm^3, 60586 reflections measured (4.242° ≤ 2Θ ≤ 144.412°), 8363 unique (R_{int} = 0.0536, R_{sigma} = 0.0306) which were used in all calculations. The final R_1 was 0.0334 (I > 2σ(I)) and wR_2 was 0.0809 (all data).

$^{Me}BiSb^{iPr}$:
Yield: 0.3975 mg, 69%

Melting Point: 135.0-140.2 °C, decomp.

^{1}H NMR (300 MHz, benzene-d_6): δ 7.30-7.09 (m, 12H, Ar-H), 1.39-1.33 (m, 6H, 2 x iPr_3Si), 1.15-1.13 (d, 18H, 2 x iPr_3Si), 0.99-0.97 (d, 18H, 2 x iPr_3Si), 0.17 (s, 18H, 2 x Me_3Si).

^{13}C{^{1}H} NMR (75 MHz, benzene-d_6): δ 153.7 (CAr), 151.8 (CAr), 138.2 (CAr), 137.7 (CAr), 136.9 (CAr), 124.8 (CAr), 124.0 (CAr), 122.4 (CAr), 120.5 (CAr), 117.6 (CAr), 116.5 (CAr), 19.2 (2 x iPr_3Si), 19.1 (2 x iPr_3Si), 14.9 (2 x iPr_3Si), 3.27 (2 x Me_3Si).

FTIR (cm^{-1} (relative int.)): 3053(13), 2945(60), 2927(1), 2924(1), 2889(4), 2865(25), 1959(24), 1598(3), 1578(2), 1556(63), 1465(19), 1425(22), 1384(12), 1370(33), 1325(24), 1313(6), 1270(100), 1248(22), 1173(5), 1165(2), 1124(5), 1098(1), 1059(68), 1049(8), 1039(8), 1016(7), 988(3), 884(15), 868(36), 842(100), 794(33), 780(16), 758(47), 748(6), 734(23), 674(4), 654(19), 557(7), 524(20), 515(3).

HRMS (APCI, $[M]^+$): calculated = 1098.3671 m/z, observed = 1098.3634 m/z, error = 3.32 ppm

Elemental analysis: Calcd. C: 48.04, H: 6.60, N: 5.09; Expt. C: 43.67, H: 6.39, N: 5.32

X-ray**:** Crystals were grown from benzene solutions. $C_{47}H_{75}BiN_4SbSi_4$ (*M* =1139.20 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 11.7148(10) Å, *b* = 24.8374(17) Å, *c* = 17.6977(10) Å, *β* = 98.486(2)°, *V* = 5093.0(6) Å^3, *Z* = 4, *T* = 120.0 K, μ(CuKα) = 12.067 mm^{-1}, *Dcalc* = 1.486 g/cm^3, 82000 reflections measured (6.178° ≤ 2Θ ≤ 127.002°), 8287 unique (R_{int} = 0.0579, R_{sigma} = 0.0298) which were used in all calculations. The final R_1 was 0.0592 (I > 2σ(I)) and wR_2 was 0.1426 (all data).

***^{Et}BiSb^{Et}*:**
Yield: 0.2609 g, 58%

Melting Point: 193.8-197.1 °C, decomp.

^{1}H NMR (300 MHz, benzene-d_6): δ 7.31-7.08 (m, 12H, Ar-H), 0.91-0.80 (m, 36H, 4 x Et_3Si), 0.77-0.70 (m, 24H, 4 x Et_3Si).

^{13}C{^{1}H} NMR (75 MHz, benzene-d_6): δ 154.9 (CAr), 151.5 (CAr), 138.0 (CAr), 137.7 (CAr), 136.5 (CAr), 126.5 (CAr), 124.5 (CAr), 124.3 (CAr), 122.2 (CAr), 120.3 (CAr), 117.4 (CAr), 115.5 (CAr), 7.5 (1 x Et_3Si), 7.1 (1 x Et_3Si), 6.9 (2 x Et_3Si).

FTIR (cm^{-1} (relative int.)): 2950(20), 2932(2), 2920(3), 2906(1), 2870(8), 2851(1), 1959(23), 1556(17), 1463(2), 1454(7), 1434(2), 1413(8), 1384(17), 1370(6), 1322(1), 1311(11), 1271(4), 1235(100), 1205(2), 1182(3), 1153(8), 1127(17), 1062(16), 1039(13), 1019(4), 999(29), 984(8), 879(23), 860(13), 845(27), 804(47), 788(17), 779(8), 763(8), 747(36), 719(11), 691(14), 652(2), 588(5), 530(4), 521(8).

HRMS (APCI, [M]$^+$): calculated = 1098.3671 m/z, observed = 1098.3680 m/z, error = 0.89 ppm

Elemental analysis: Calcd. C: 48.04, H: 6.60, N: 5.09; Expt. C: 45.30, H: 6.24, N: 4.53

X-ray**:** Crystals were grown from hexane solutions. $C_{44}H_{72}BiN_4SbSi_4$ (*M* =1100.14 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 10.5482(4) Å, *b* = 12.2644(5) Å, *c* = 19.2011(8) Å, *β* = 101.6560(10)°, *V* = 2432.77(17) Å^3, *Z* = 2, *T* = 115.0 K, μ(CuKα) = 12.609 mm^{-1}, *Dcalc* = 1.502 g/cm^3, 130846 reflections measured (8.608° ≤ 2Θ ≤ 144.474°), 4778 unique (R_{int} = 0.1761, R_{sigma} = 0.0378) which were used in all calculations. The final R_1 was 0.0350 (I > 2σ(I)) and wR_2 was 0.0959 (all data).

^{Me}BiSSb^{Et}*: *^{Et}SbBi^{Me} (0.2561 g, 0.252 mmol) was dissolved in toluene (ca. 5 mL) and added to a pressure vessel containing S_8 (0.0081 g, 0.031 mmol). The solution was heated to 100 °C and stirred for 1 hour. The solvent was removed and the residual solid was dissolved in pentane and placed in the freezer for recrystallization at –25 °C which gave the respective thiobismuthanylstibane as a brown solid.

Yield: 46%

Melting Point: 72.6-74.5 °C, melt.

^{1}H NMR (300 MHz, benzene-d_6): δ 7.43-7.09 (m, 12H, Ar-H), 0.87-0.80 (m, 18H, 2 x Et_3Si), 0.79-0.71 (m, 12H, 2 x Et_3Si), 0.21 (s, 18H, 2 x Me_3Si).

^{13}C{^{1}H} NMR (75 MHz, benzene-d_6): δ 148.1 (CAr), 145.6 (CAr), 137.9 (CAr), 137.7 (CAr), 132.1 (CAr), 127.1 (CAr), 126.4 (CAr), 123.6 (CAr), 121.8 (CAr), 119.7 (CAr), 118.0 (CAr), 116.2 (CAr), 7.2 (2 x Et_3Si), 6.0 (2 x Et_3Si), 2.6 (2 x Me_3Si).

FTIR (cm^{-1} (relative int.)): 3223(10), 3054(17), 3027(6), 2955(108), 2933(3), 2874(21), 2029(11), 1959(43), 1598(5), 1579(10), 1562(78), 1512(14), 1494(21), 1460(33), 1453(5), 1420(51), 1416(2), 1384(14), 1375(40), 1332(11), 1313(17), 1293(6), 1274(100), 1263(5), 1251(37), 1175(6), 1162(2), 1154(6), 1092(2), 1080(6), 1059(111), 1043(17), 1031(8), 1017(6), 1002(27), 870(32), 859(2), 842(92), 815(40), 783(13), 767(30), 755(127), 730(16), 698(60), 659(3), 648(2), 627(2), 621(10), 605(32), 588(8), 532(13).

HRMS (APCI): decomposed in spectrometer.

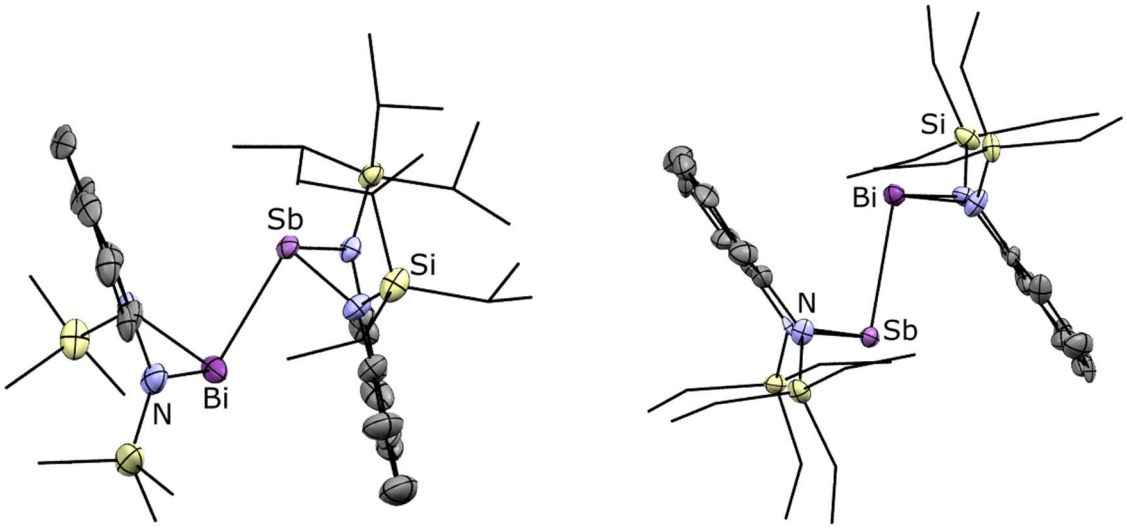
Elemental analysis: Calcd. C: 43.55, H: 5.77, N: 5.35; Expt. C: 39.55, H: 5.56, N: 4.73

X-ray**:** Crystals were grown from a saturated hexane solution. $C_{38}H_{60}BiN_4SSbSi_4$ (*M* =917.87 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 16.5940(6) Å, *b* = 12.7708(4) Å, *c* = 21.9816(8) Å, *β* = 108.2140(10)°, *V* = 4424.9(3) $Å^3$, *Z* = 4, *T* = 116 K, μ(CuKα) = 14.183 mm^{-1}, *Dcalc* = 1.378 g/cm^3, 106069 reflections measured (5.606° ≤ 2Θ ≤ 144.504°), 8717 unique (R_{int} = 0.0309, R_{sigma} = 0.0126) which were used in all calculations. The final R_1 was 0.0178 (I > 2σ(I)) and wR_2 was 0.0440 (all data).

***(^{Et}Sb)$_4$Sb$_8$*:**
Spectroscopic data could not be obtained for this product due to poor solubility and a mixture of solids precipitating out of solution. Note that this compound was formed as a byproduct and is not of immediate interest to the findings of this study.

Xray: Crystals were grown from a solution of ether. $C_{30}H_{40}N_2Sb_3Si_2$ (*M* =850.07 g/mol): monoclinic, space group $P2_1$ (no. 4), *a* = 18.3686(6) Å, *b* = 11.8349(4) Å, *c* = 25.5125(8) Å, *β* = 92.574(2)°, *V* = 5540.6(3) $Å^3$, *Z* = 8, *T* = 125.0 K, μ(MoKα) = 3.016 mm^{-1}, *Dcalc* = 2.038 g/cm^3, 147121 reflections measured (3.972° ≤ 2Θ ≤ 53.406°), 22856 unique (R_{int} = 0.0470, R_{sigma} = 0.0261) which were used in all calculations. The final R_1 was 0.0200 (I > 2σ(I)) and wR_2 was 0.0411 (all data).

Figure S1. X-ray crystal structure of bismuthanylstibanes $^{Me}BiSb^{iPr}$ and $^{Et}BiSb^{Et}$. The latter is for connectivity only.



NMR Spectra

Figure S2. ***Crude ^{1}H NMR spectrum*** of $^{Et}SbNMe_2$ obtained from the combination of **$LiNMe_2$** and $^{Et}SbCl$.

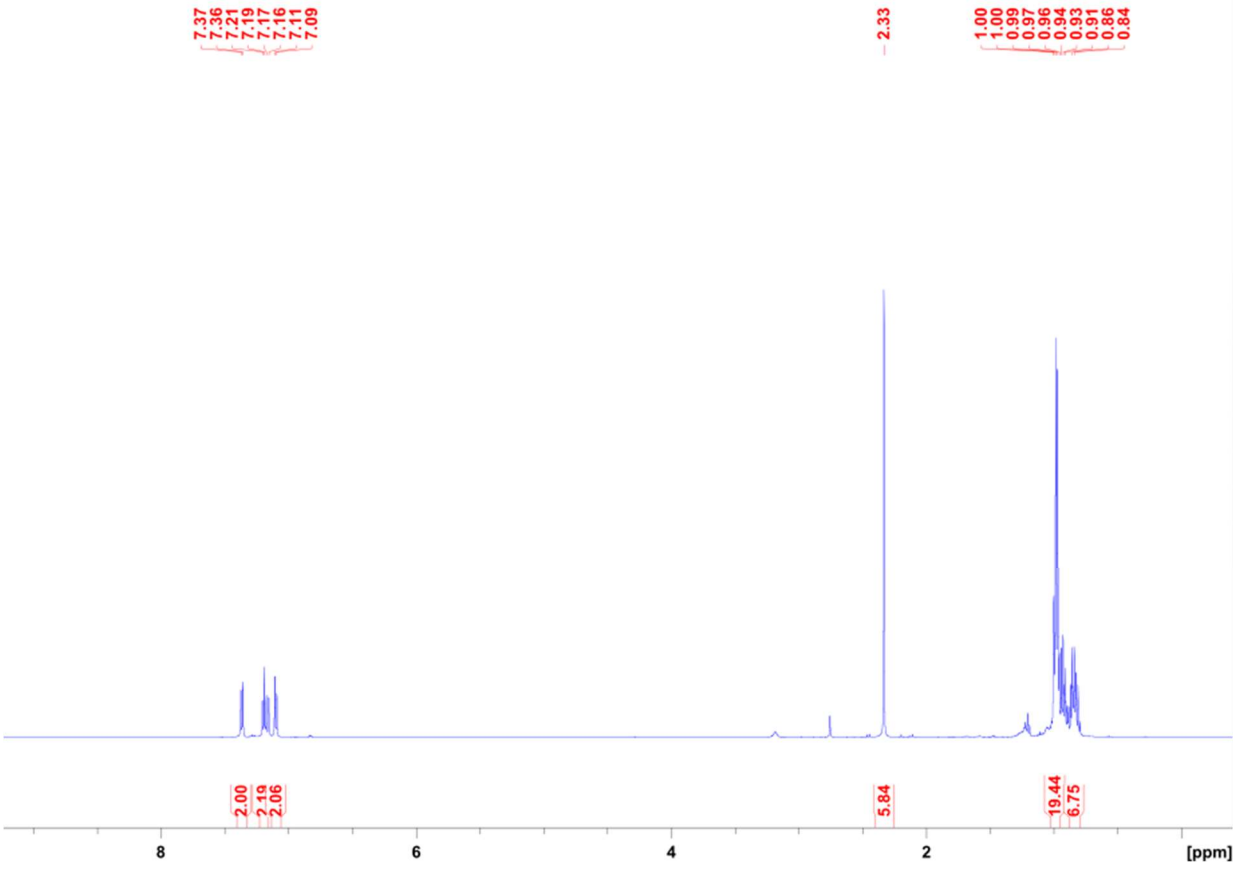


Figure S3. ^{1}H NMR spectrum of ***^{Me}BiSb^{Et}***.

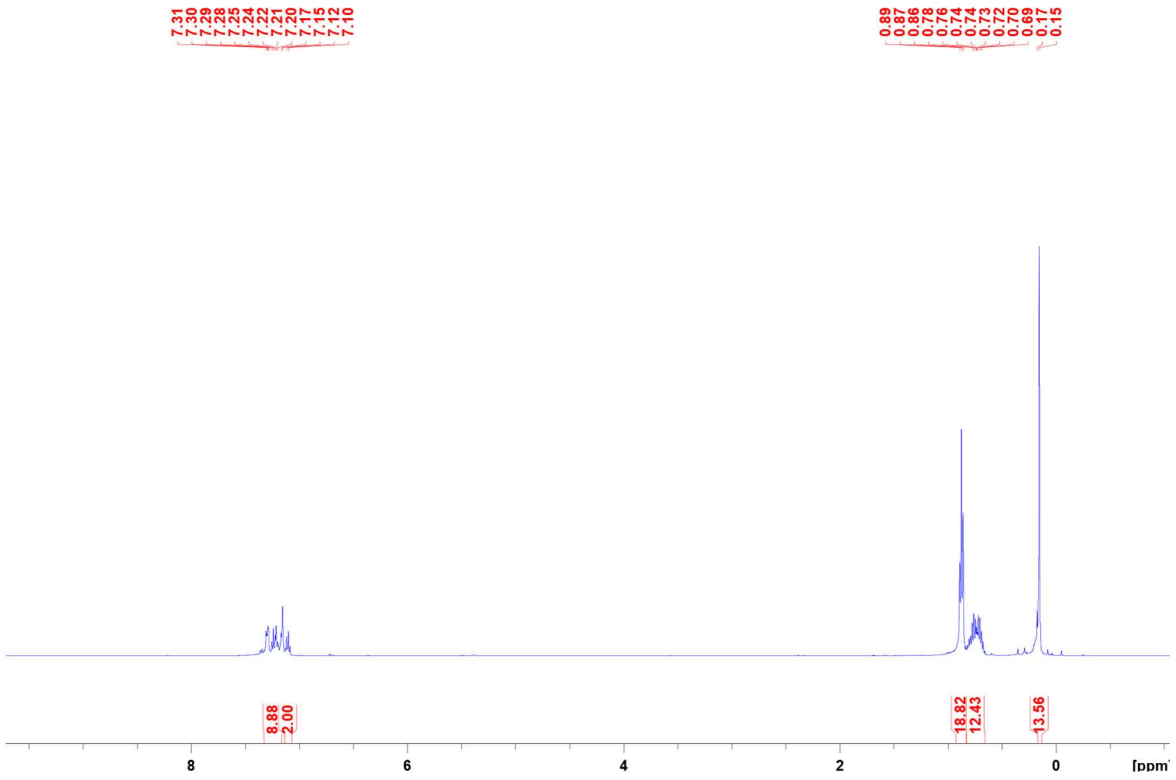


Figure S4. ^{13}C NMR spectrum of ***^{Me}BiSb^{Et}***.

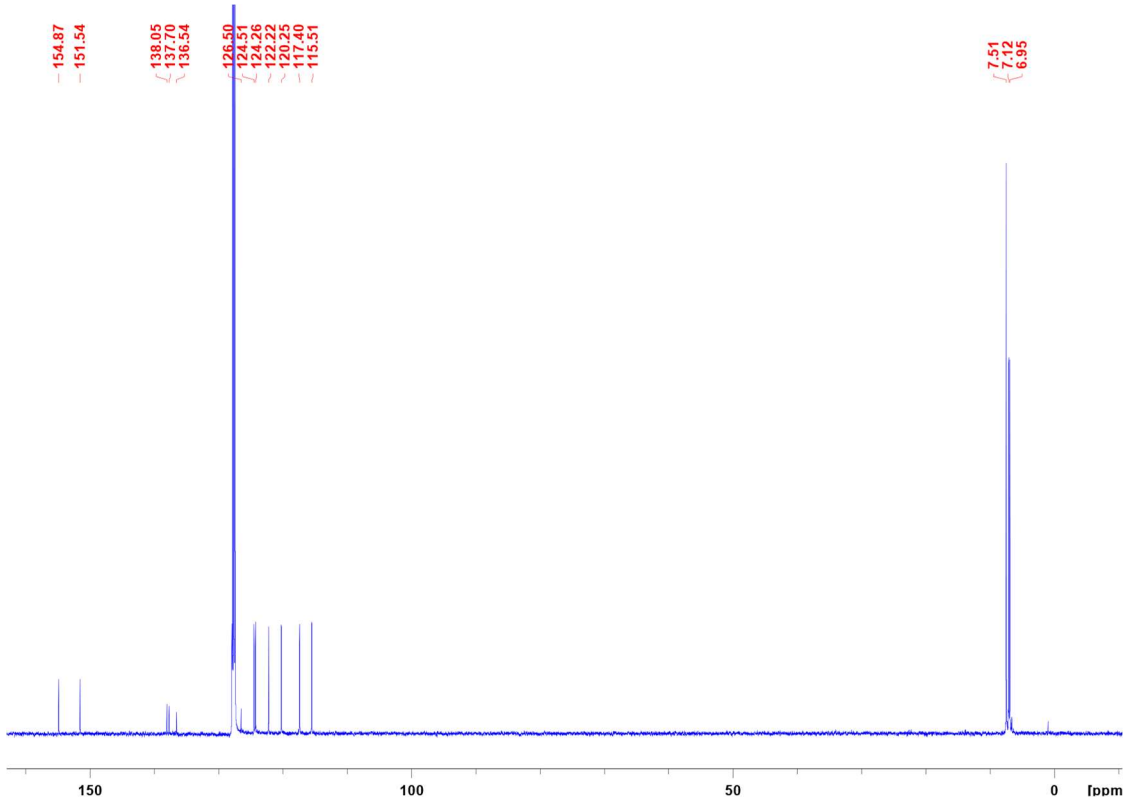


Figure S5. ^{1}H NMR spectrum of ***^{Et}BiSb^{Et}***.

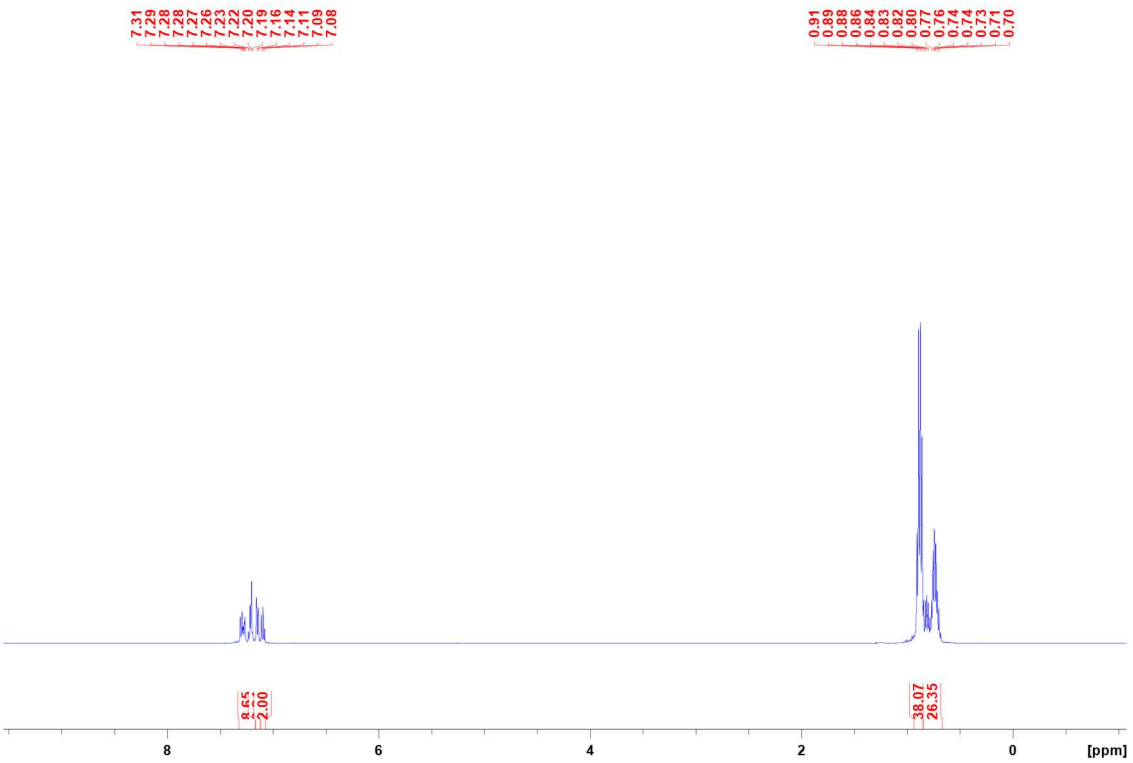


Figure S6. ^{13}C NMR spectrum of ***^{Et}BiSb^{Et}***.

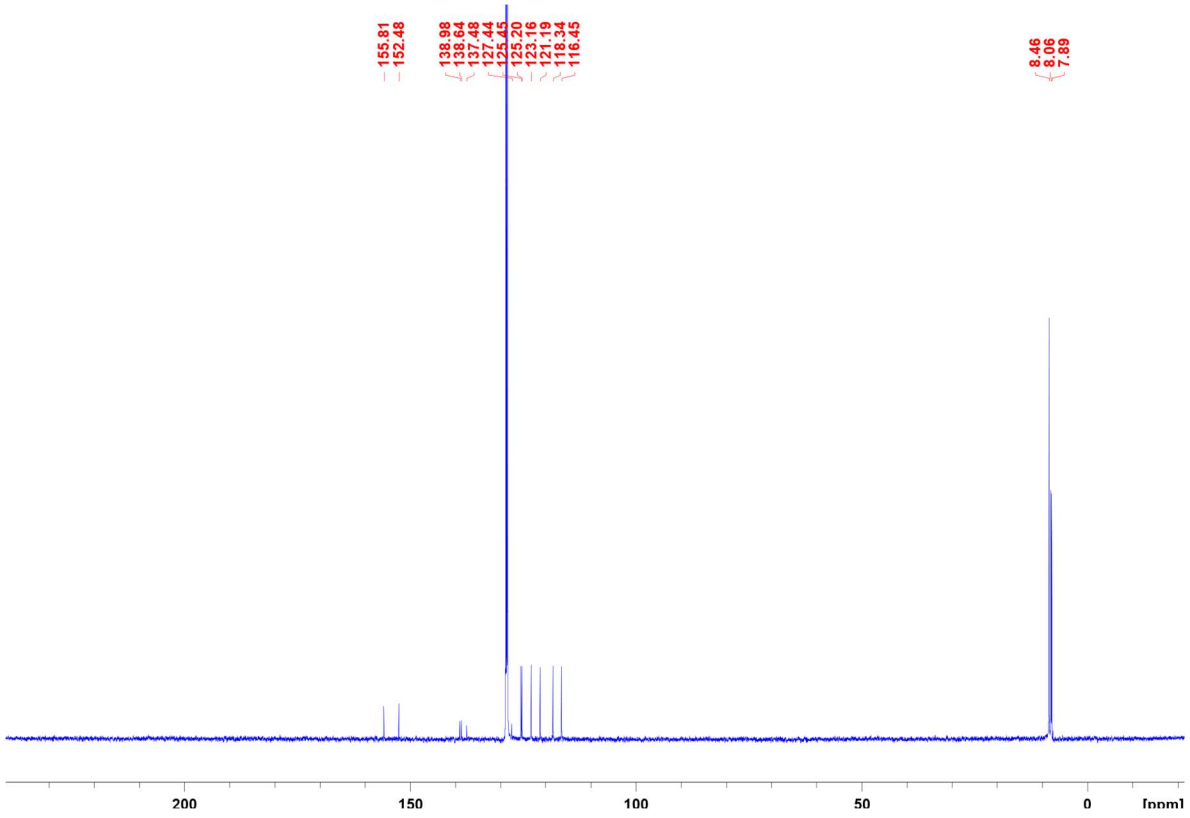


Figure S7. ^{1}H NMR spectrum of ***^{Me}BiSb^{iPr}***.

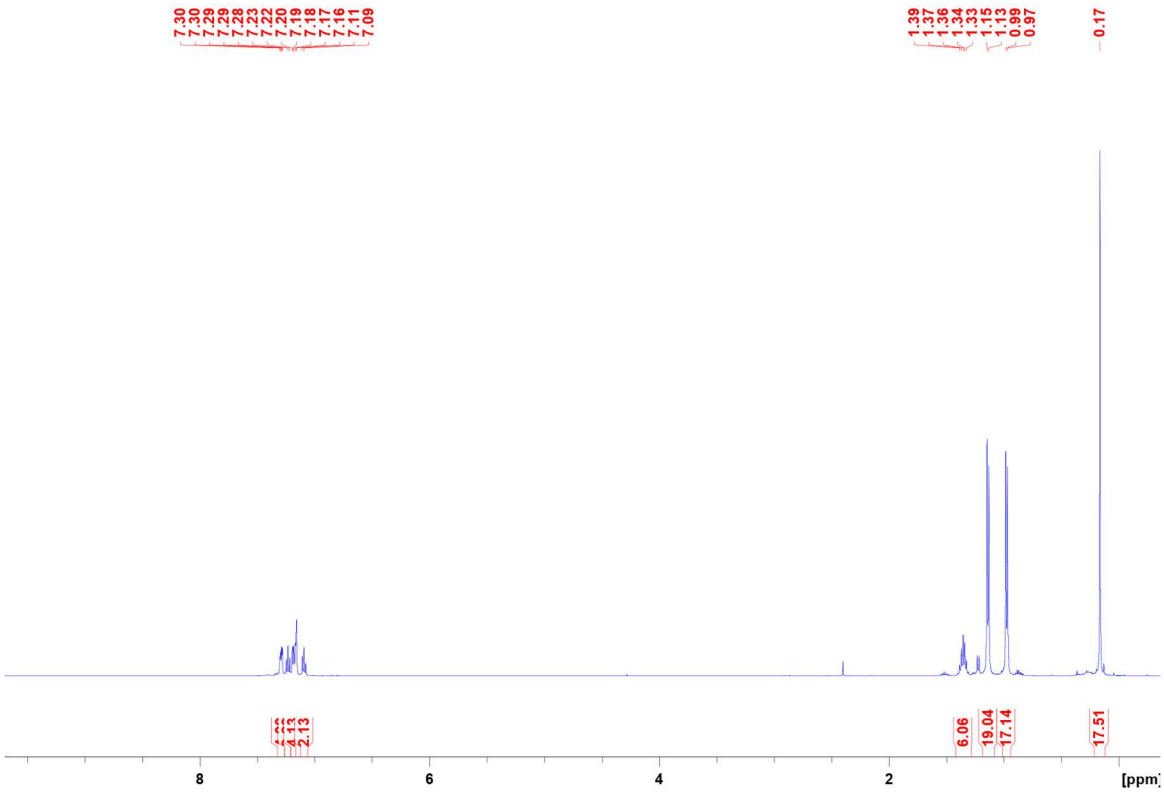


Figure S8. ^{13}C NMR spectrum of ***^{Me}BiSb^{iPr}***.

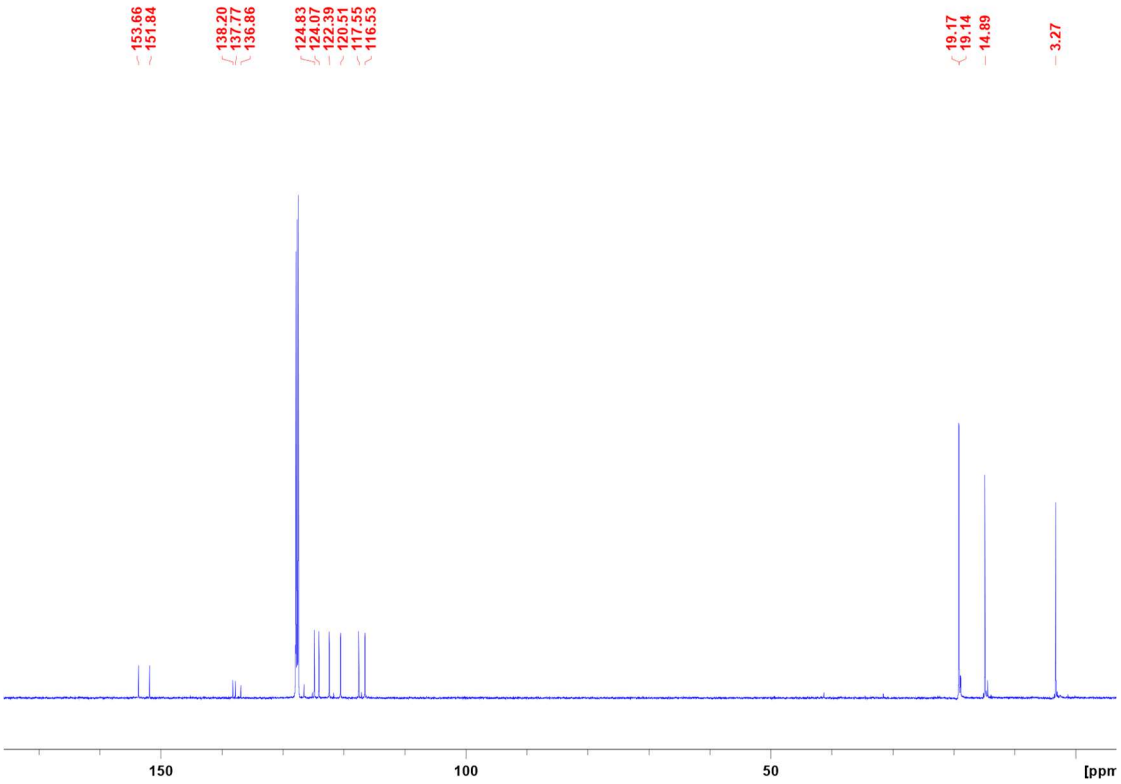


Figure S9. ^{1}H NMR spectrum of ***^{Me}BiSSb^{Et}***.

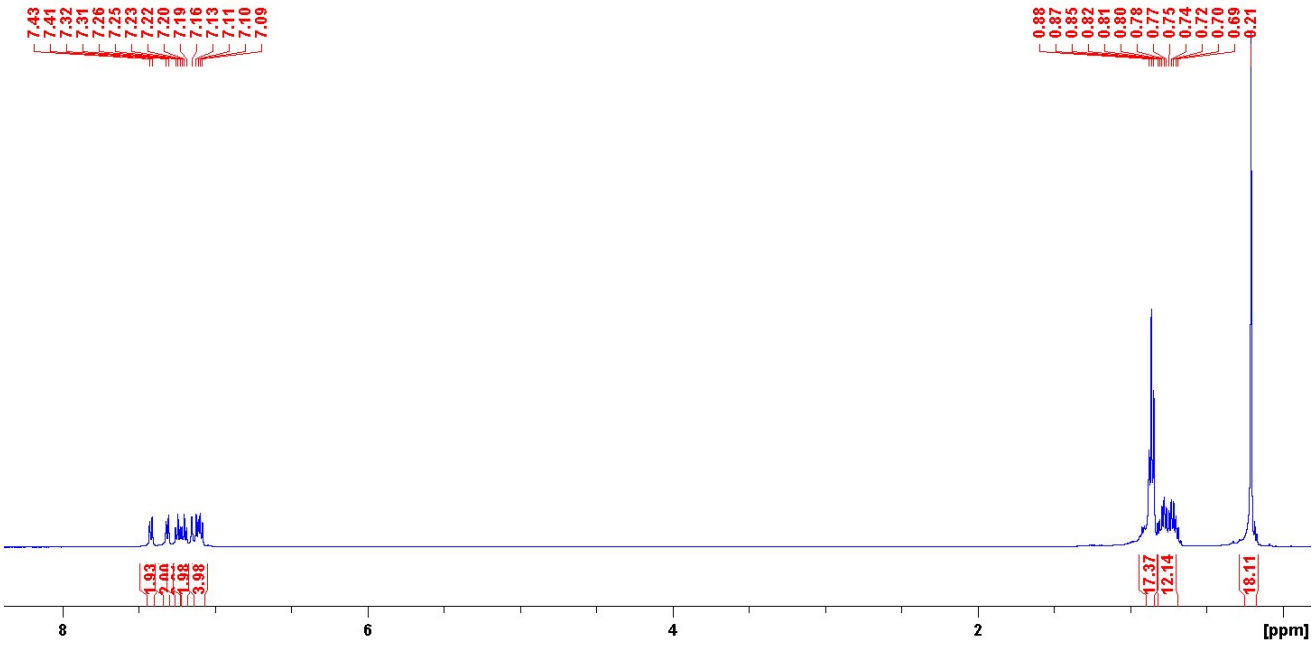
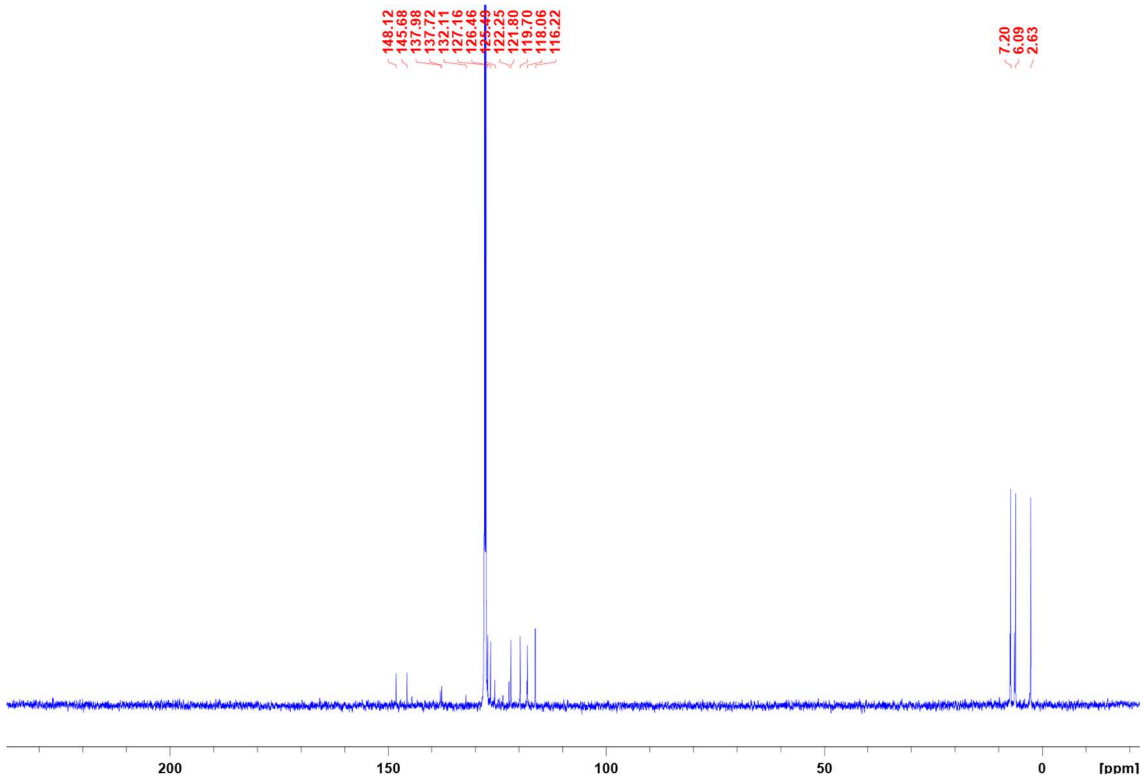
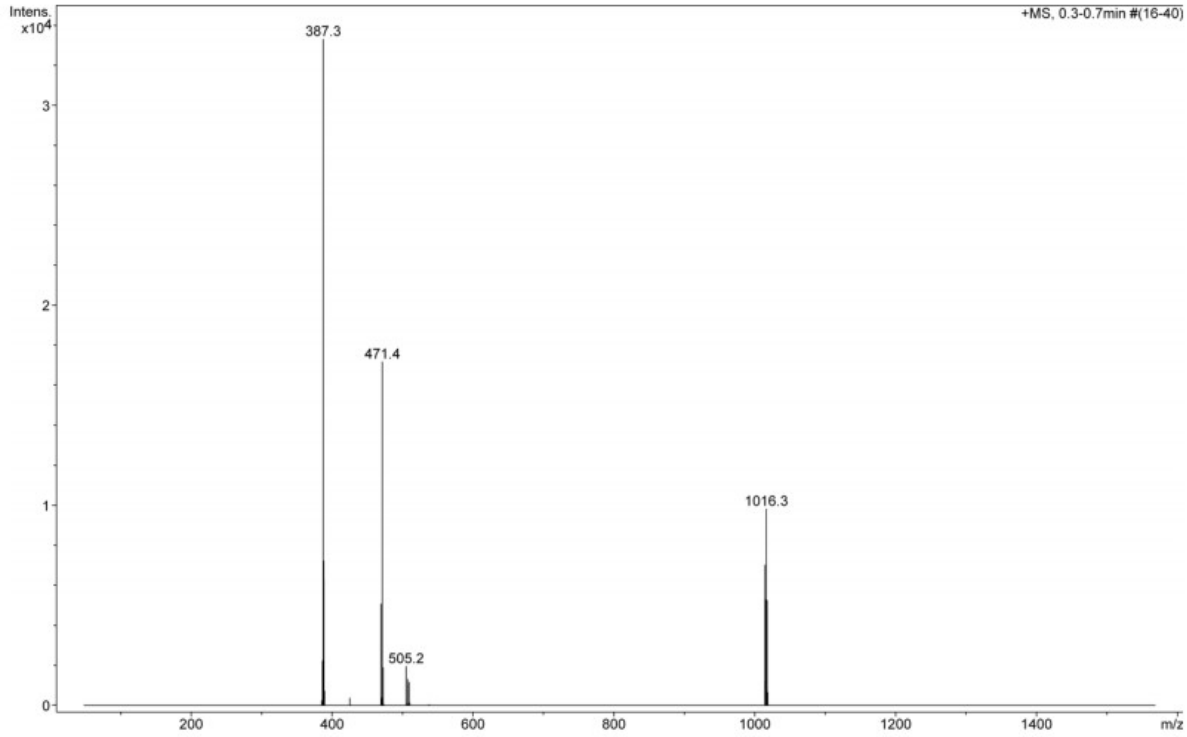


Figure S10. ^{13}C NMR spectrum of ***^{Me}BiSSb^{Et}***.



HRMS

Figure S11. HRMS spectrum of ***^{Me}BiSb^{Et}***:



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 38 H 60 Bi 1 N 4 Sb 1 Si 4	0.09	1014.2732	-0.24	-1.38	18.00	-	odd

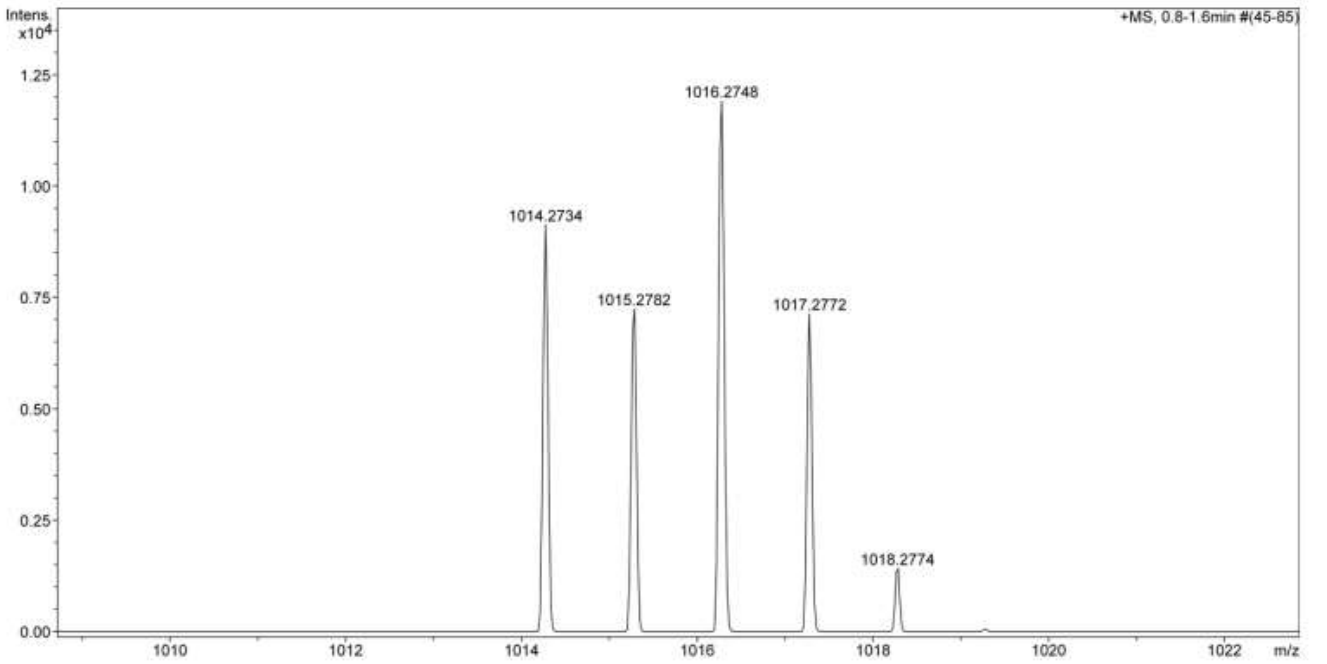
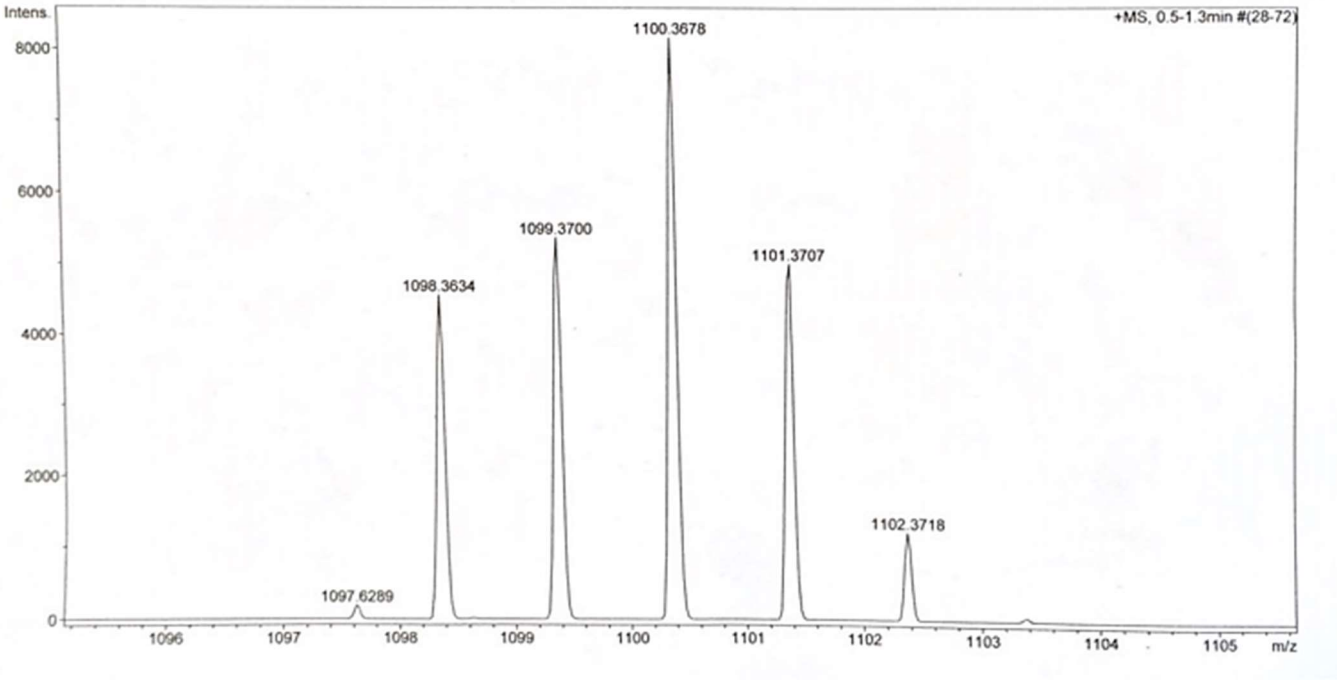


Figure S12. HRMS spectrum of ***Me*BiSb*iPr***:

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 44 H 72 Bi 1 N 4 Sb 1 Si 4	0.14	1098.3671	3.32	0.12	18.00	-	odd



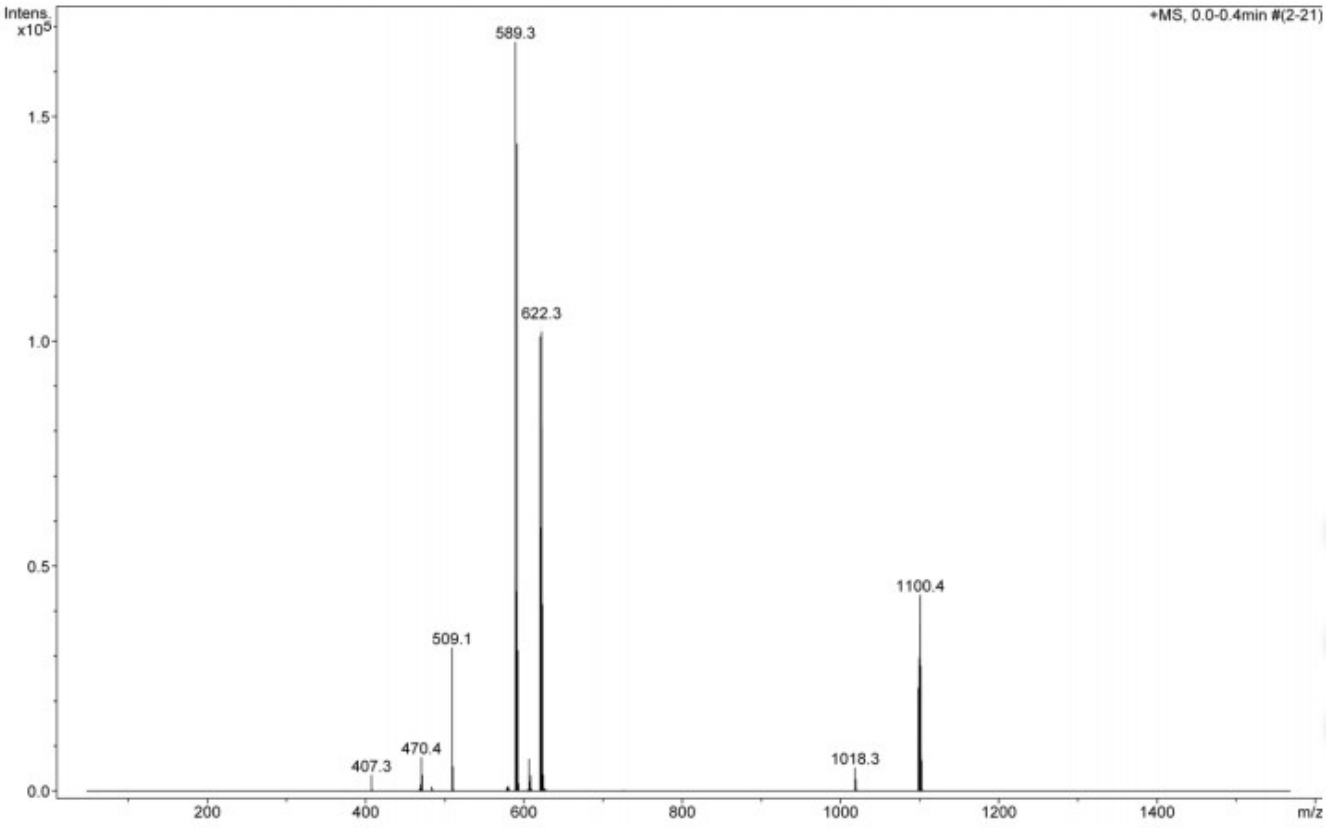


Figure S13. HRMS spectrum of ***^{Et}BiSb^{Et}***:

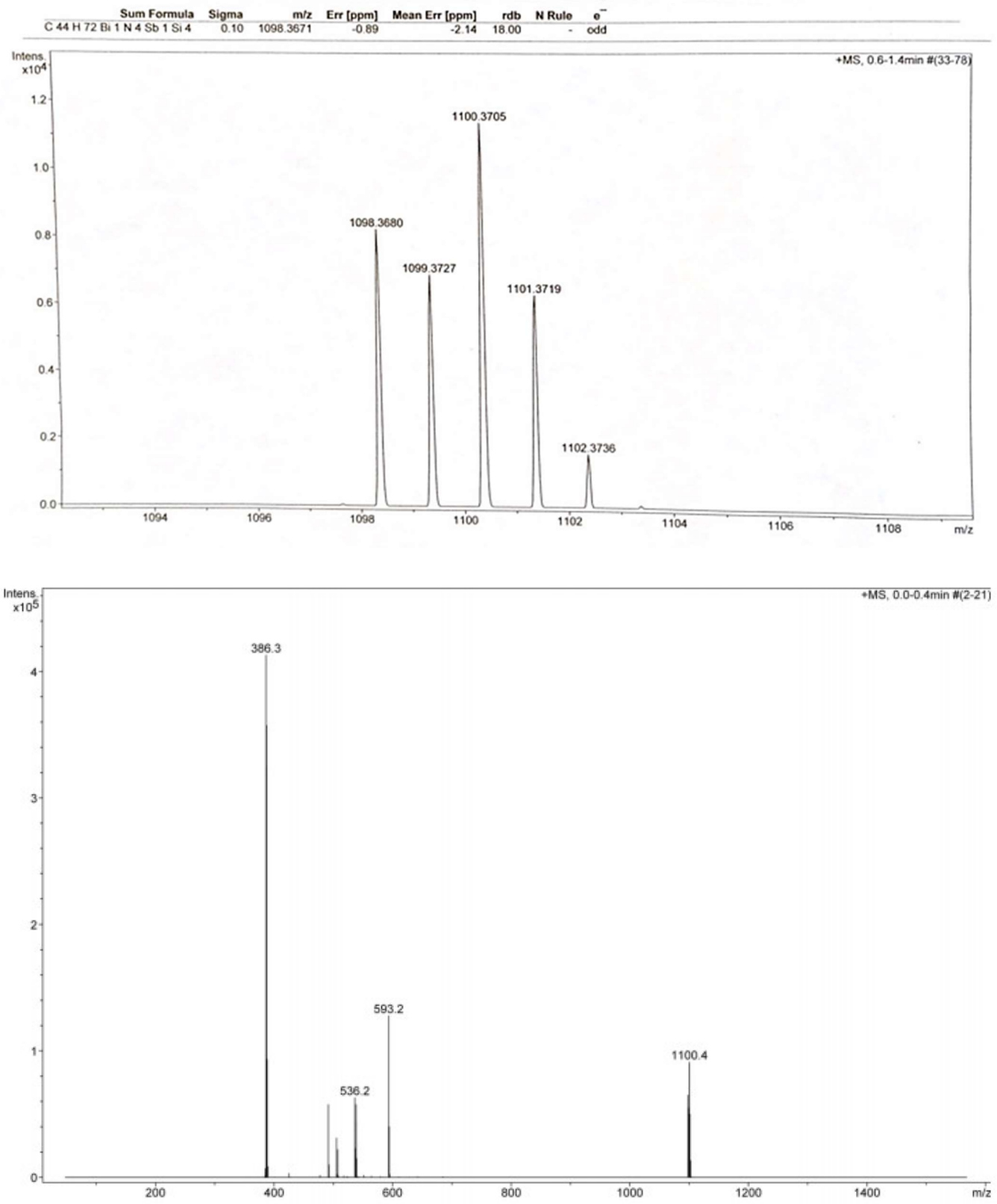
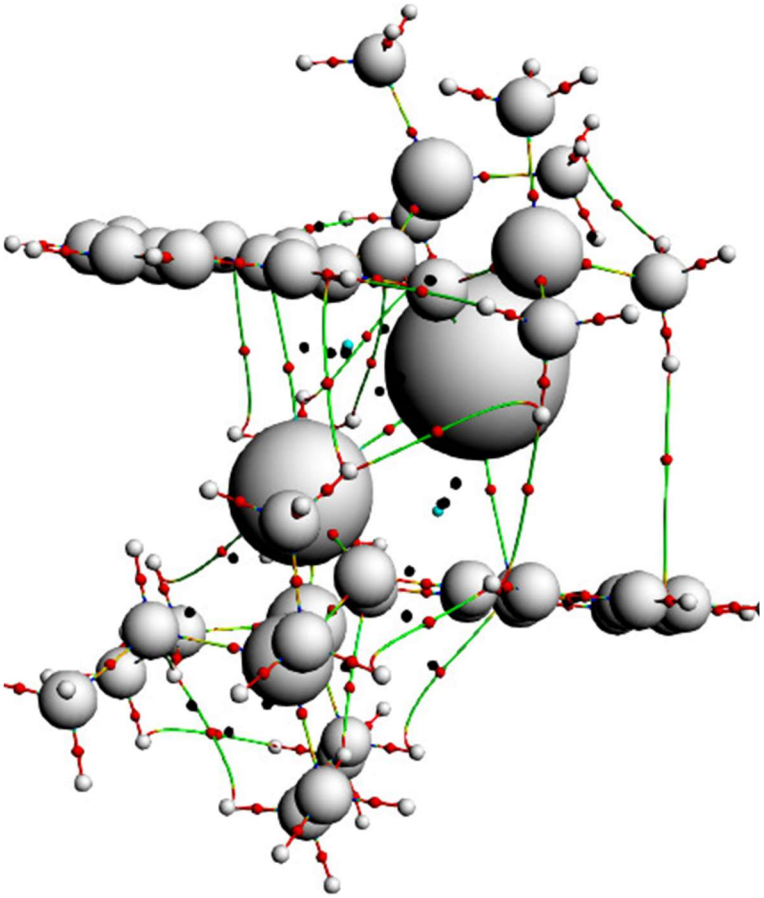


Figure S14. QTAIM molecular graph for $^{Me}BiSb^{Et}$:



Computational details

All calculations were performed using the 2017 Amsterdam Density Functional (ADF) suite.

EDA calculations: The BP86 functional was used with Grimme's D3 correction and Becke-Johnson dampening. The TZ2P basis set was employed with a small frozen core approximation and scalar relativistic correction. Homolytic dissociation of the Sb-Bi bond into two doublet fragments was assumed due to their similar electronegativities. All optimized species were confirmed as minima by frequency analysis.

NBO calculations: The BP86 functional was used with Grimme's D3 correction and Becke-Johnson dampening. The TZ2P basis set was employed without any frozen core approximation. Scalar relativistic correction was employed. NBO analysis Homolytic dissociation of the Sb-Bi bond into two doublet fragments was assumed due to their similar electronegativities.

Reference for ADF: G.te Velde, F.M. Bickelhaupt, E.J. Baerends, C. Fonseca Guerra, S.J.A. van Gisbergen, J.G. Snijders and T. Ziegler, *Chemistry with ADF*, Journal of Computational Chemistry 22, 931 (2001)

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Optimized geometry for ^{Et}Sb

1 C	15.231937	4.350333	22.383142
2 Sb	11.428188	5.789843	24.510863
3 Si	14.466444	4.643137	24.092901
4 Si	9.138195	5.029135	22.200799
5 H	14.528910	3.744687	21.793015
6 H	15.272397	5.326726	21.874694
7 N	9.871560	4.689285	23.766668
8 N	12.736221	4.231558	24.067151
9 H	11.891391	3.914317	21.556512

10	H	11.497154	4.926658	20.159845
11	C	9.801267	3.362641	24.271229
12	C	12.301308	2.903922	23.988073
13	C	15.324200	3.702697	25.489669
14	H	15.590704	2.683204	25.181435
15	H	16.279026	4.212530	25.694127
16	C	11.292719	3.958517	20.637591
17	C	10.937465	2.484908	24.251029
18	C	14.600463	6.487233	24.499566
19	H	13.981122	7.072407	23.801640
20	H	14.203429	6.685710	25.507843
21	H	11.662755	3.173572	19.964383
22	C	14.460604	3.656291	26.759800
23	C	13.244631	1.905397	23.712808
24	H	14.253962	2.192550	23.429996
25	C	11.717564	0.127719	24.266260
26	H	11.496914	-0.926755	24.428630
27	C	9.796965	3.789380	20.943781
28	H	9.606586	2.782097	21.347118
29	H	9.200604	3.860839	20.020165
30	H	14.170019	4.663874	27.089712
31	C	10.687502	1.079526	24.466486
32	H	14.991747	3.177820	27.593515
33	C	9.625774	6.790797	21.727149
34	H	9.342287	7.476490	22.541429
35	H	10.722703	6.856439	21.649877
36	H	13.535484	3.093321	26.582024
37	C	8.980558	7.244878	20.407591
38	H	9.257323	6.580510	19.577335
39	H	9.292094	8.261665	20.132267
40	H	7.884258	7.243898	20.474672
41	C	16.057513	6.978539	24.414787
42	C	16.623127	3.699476	22.384279
43	H	17.016318	3.582984	21.365329
44	H	16.599365	2.700950	22.842065
45	H	17.349851	4.294990	22.953124
46	C	7.257686	4.918282	22.287510
47	H	6.864906	5.104487	21.274709
48	H	6.976021	3.882048	22.526009
49	C	9.392032	0.638519	24.842398
50	H	9.239770	-0.427389	25.011921
51	H	16.477132	6.818055	23.412619
52	C	12.960207	0.539708	23.843977
53	H	13.746432	-0.187342	23.641953
54	C	8.354065	1.529848	24.978876
55	H	7.365298	1.187842	25.284243
56	H	16.703244	6.452742	25.130805
57	H	16.132363	8.051787	24.633786
58	C	6.629159	5.895618	23.290875
59	H	5.539962	5.771100	23.362842
60	H	6.821895	6.939151	23.005898
61	H	7.049088	5.757414	24.297148
62	C	8.560414	2.887505	24.681651

63 H	7.735547	3.594522	24.732609

Optimized geometry for ^{Me}Bi

1 Bi	9.999079	3.348686	27.271983
2 C	6.946403	2.523504	28.645217
3 H	7.123240	1.937358	27.732598
4 H	5.959406	2.225243	29.029237
5 Si	6.929379	4.384004	28.343846
6 Si	11.978795	3.303674	30.066549
7 H	7.695954	2.227052	29.390631
8 C	6.468711	5.259946	29.938891
9 N	8.560122	4.856130	27.887259
10 N	11.268625	4.258897	28.776655
11 C	11.445155	5.648597	28.649657
12 H	7.171994	4.985145	30.736273
13 H	5.456559	4.976381	30.259706
14 H	6.499101	6.350287	29.826568
15 C	5.627970	4.686697	27.010964
16 C	9.024120	6.183103	27.920635
17 C	11.999459	8.427127	28.596673
18 H	12.189412	9.500012	28.582731
19 C	10.915795	1.761857	30.273981
20 H	9.869355	2.020249	30.483201
21 C	8.432246	8.551983	27.634889
22 H	7.671227	9.291379	27.385628
23 H	11.293605	1.178059	31.126183
24 H	10.933934	1.099729	29.397505
25 H	5.356828	5.743858	26.898225
26 H	4.708280	4.134840	27.253828
27 H	5.985661	4.327430	26.035755
28 C	12.991451	7.535876	28.927005
29 H	13.995676	7.883214	29.169644
30 C	10.700281	7.970257	28.259505
31 C	11.933001	4.293978	31.661209
32 C	10.383261	6.557164	28.265285
33 H	12.566423	5.187317	31.611339
34 H	12.277289	3.676437	32.502583
35 H	10.906982	4.622710	31.873310
36 C	9.712136	8.938292	27.950448
37 H	9.994785	9.990518	27.967726
38 C	8.109234	7.189158	27.602252
39 H	7.111162	6.891346	27.288671
40 C	12.711344	6.162868	28.933209
41 H	13.509341	5.456705	29.153967
42 C	13.732458	2.714939	29.699330
43 H	13.767269	2.179824	28.739825
44 H	14.076238	2.022197	30.481152
45 H	14.455236	3.539081	29.646155

Optimized geometry for $^{Me}BiSb^{Et}$

1	Bi	10.423608	3.297479	27.343490
2	Sb	11.277435	5.362379	25.343804
3	Si	14.142333	4.301718	24.050673
4	Si	9.297447	5.782624	22.695612
5	Si	7.136319	3.706239	28.055698
6	Si	11.918503	3.793689	30.397936
7	N	9.783997	4.749203	24.038124
8	N	12.471647	3.897579	24.422468
9	N	8.662455	4.524362	27.778120
10	N	11.329131	4.511589	28.919306
11	C	9.500178	3.372123	24.057837
12	C	11.935682	2.608561	24.438895
13	C	15.250054	4.018008	25.560558
14	H	15.463838	2.946433	25.690584
15	H	16.226316	4.492141	25.372095
16	C	8.858712	5.909283	27.781962
17	C	10.510748	2.353608	24.280508
18	C	14.159809	6.149922	23.657218
19	H	13.381502	6.334287	22.899967
20	H	13.861742	6.734091	24.541066
21	C	7.881524	8.114526	27.293569
22	H	7.008371	8.687079	26.980909
23	C	12.790115	1.521986	24.651096
24	H	13.847450	1.722920	24.813019
25	C	10.993214	-0.073965	24.558578
26	H	10.619058	-1.096273	24.602268
27	C	9.856752	4.942340	21.104963
28	H	9.342727	3.969498	21.050842
29	H	9.496806	5.521351	20.239953
30	C	10.206168	7.990680	27.957724
31	C	10.065865	0.976521	24.344190
32	C	10.120385	6.554472	28.129285
33	C	10.178257	7.435620	22.941175
34	H	9.906810	7.850986	23.924855
35	H	11.265346	7.267172	22.983950
36	C	9.082524	8.740255	27.531427
37	H	9.189036	9.818746	27.418073
38	C	7.784471	6.723216	27.407769
39	H	6.848310	6.241407	27.140275
40	C	12.440312	6.633193	28.941660
41	H	13.317454	6.095926	29.297379
42	C	16.202952	2.955588	22.520900
43	H	16.478950	2.423420	21.600263
44	H	16.458446	2.302657	23.366403
45	H	16.847674	3.841950	22.593293
46	C	7.439804	6.115571	22.638463
47	H	7.263786	6.870385	21.854732
48	H	6.910011	5.214511	22.294915
49	C	8.696056	0.653001	24.170499
50	H	8.400215	-0.394149	24.227418
51	C	11.292019	5.887264	28.669779
52	C	12.333831	0.197747	24.701196

53 H	13.047150	-0.608105	24.873282
54 C	7.769018	1.639043	23.927337
55 H	6.715794	1.390884	23.797454
56 C	11.407392	8.686065	28.252286
57 H	11.430355	9.764117	28.094929
58 C	11.034622	2.140490	30.589688
59 H	9.944323	2.274419	30.598509
60 H	11.322325	1.673600	31.542468
61 H	11.285328	1.426466	29.792778
62 C	8.172675	2.980601	23.881700
63 H	7.430389	3.762263	23.745996
64 C	14.713176	3.329606	22.532347
65 H	14.096881	2.423372	22.446785
66 H	14.466028	3.938649	21.648550
67 C	11.480724	4.915242	31.837565
68 H	11.963249	5.896178	31.745455
69 H	11.795282	4.468216	32.790674
70 H	10.395578	5.079472	31.874839
71 C	14.623993	4.586982	26.841431
72 H	14.399953	5.658727	26.746717
73 H	15.282039	4.470187	27.712659
74 H	13.676886	4.083833	27.086310
75 C	9.856982	8.452293	21.833811
76 H	10.129716	8.065657	20.841962
77 H	10.402253	9.394272	21.981185
78 H	8.786269	8.694428	21.807265
79 C	15.519840	6.648258	23.143308
80 H	15.820111	6.124132	22.225851
81 H	16.313828	6.491185	23.886266
82 H	15.495804	7.722135	22.914629
83 C	6.884555	6.598980	23.983743
84 H	5.798490	6.761764	23.952546
85 H	7.353568	7.541958	24.294584
86 H	7.095644	5.873837	24.780065
87 C	12.506077	8.018533	28.738680
88 H	13.429332	8.553894	28.960591
89 C	13.770675	3.444282	30.383093
90 H	14.043021	2.836673	29.509214
91 H	14.069914	2.890733	31.284830
92 H	14.365998	4.366066	30.346258
93 C	11.376931	4.738773	21.035810
94 H	11.677660	4.173427	20.143389
95 H	11.739475	4.194296	21.917734
96 H	11.907274	5.701354	21.007998
97 C	6.446335	4.294020	29.700389
98 H	7.139833	4.045571	30.514853
99 H	5.475060	3.829650	29.919375
100 H	6.309712	5.383371	29.700266
101 C	5.841001	3.901668	26.698419
102 H	5.355162	4.884695	26.677582
103 H	5.052494	3.148454	26.842158
104 H	6.296779	3.722899	25.716662
105 C	7.509386	1.861024	28.118139

106 H	7.846161	1.471986	27.145963
107 H	6.577681	1.331782	28.367043
108 H	8.253081	1.588359	28.878509

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