Electronic Supplementary Material (ESI) for ChemComm.

- Supporting Information –

Bisstibane–Distibane conversion via consecutive single-electron oxidation and reduction reaction

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I. Experimental Details

General Considerations. All manipulations were performed in an atmosphere of purified argon using standard Schlenk and glovebox techniques. Toluene, *n*-hexane and Et_2O were dried using an mBraun Solvent Purification System (SPS). CH_2Cl_2 and fluorobenzene were dried over CaH_2, while THF was carefully dried over NaK. Dried solvents were degassed and stored over appropriate molecular sieves. thf-d_8, C_6D_6 and CD_2Cl_2 were dried over activated molecular sieves (4 Å, 3 Å CD_2Cl_2) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. Water was degassed through reflux in an argon atmosphere, followed by distillation. 1,8-Li_2Naph,[1] $Trip_2SbCl$,[2] $Trip_2BiCl$,[2] $FcBAr^F$,[3] KC_8[4] were prepared according to literature procedures. 1,8-Br_2Naph, TripBr, Mg, $NOSbF_6$ and ^{n}BuLi (2.5 M in hexane) were commercially available and used as received, whereas $SbCl_3$ and $BiCl_3$ were purified by sublimation prior to use. Microanalyses were performed at the Elemental Analysis Laboratory of the University of Duisburg-Essen. Melting points were measured using a Thermo Scientific 9300 apparatus. NMR spectra were recorded using a Bruker Avance Neo 400 (^{1}H: 400.1 MHz; ^{11}B = 128.4 MHz; ^{13}C{^{1}H}: 150.9 MHz;^{19}F: 376.5 MHz) or Bruker DMX300 (^{1}H: 300.1 MHz; ^{13}C{^{1}H}: 150.9 MHz) spectrometer, and the spectra were referenced to internal $CDHCl_2$ (^{1}H: δ = 5.32 ppm), C_6D_5H (^{1}H: δ = 7.16 ppm), C_7D_7H (^{1}H: δ = 2.08 ppm, ^{13}C: δ = 20.43 ppm) or C_4D_7HO (^{1}H: δ = 1.72 ppm; ^{13}C: δ = 25.31 ppm). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module in a glovebox to guarantee measurements under inert gas conditions. CV studies were performed in a glovebox using a Metrohm Autolab PGSTAT 204 potentiostat with a three-electrode setup consisting of a Pt-disk (*d* = 1 mm) working electrode, a Pt-wire counter electrode, and an Ag-wire pseudoreference electrode; and ferrocene was used as an internal standard. For **5**, the ferrocene redox couple was obscured; hence, decamethylferrocene was used as the internal reference (440 mV vs Fc in THF/0.1 M NBu_4PF_6).[5].

Synthesis of $(Trip_2Sb)_2$Naph (1). Li_2Naph (2 mmol, 369.8 mg) and $Trip_2SbCl$ (4 mmol, 2.29 g) were each dissolved in 20 mL of thf. The solutions were cooled to –78 °C, combined and stirred for 12 h. All volatiles were removed *in vacuo* and 20 mL of degassed water was added. The resulting mixture was stirred for 30 minutes, filtered and the residue dried *in vacuo*. Washing with ethanol (2 x 15 mL) and drying *in vacuo* gave **1** as a yellow powder.

Yield: 1.565 g (65 %); **m.p.:** 265.8 °C; **elemental analysis [wt-%]:** calcd. for $C_{70}H_{98}Sb_2$: C 71.1, H 8.35. found: C 70.7, H 8.43; **^{1}H NMR (400.1 MHz, 297 K, CD_2Cl_2): δ [ppm]** 8.16 (dd, $^3J_{HH}$ = 6.95 Hz, $^4J_{HH}$ = 1.07 Hz, 2 H, Naph-2,7-*H*), 7.86 (dd, $^3J_{HH}$ = 8.15 Hz, $^4J_{HH}$ = 1.26 Hz, 2 H, Naph-4,5-*H*), 7.31 (dd, $^3J_{HH}$ = 7.96 Hz, $^3J_{HH}$ = 7.04 Hz, 2 H, Naph-3,6-*H*), 6.91 (s (br), 8 H, Ph-*m*-*H*), 3.70 (s (br), 2 H, *o*-C*H*$(CH_3)_2$), 3.41 (s (br), 2 H, *o*-C*H*$(CH_3)_2$), 2.80 (s (br), 6 H, *o/p*-C*H*$(CH_3)_2$), 2.53 (s (br), 2 H, *o*-C*H*$(CH_3)_2$), 1.19 (d, $^3J_{HH}$ = 6.61 Hz, 36 H, *o/p*-CH(C*H*$_3)_2$), 0.96 (s (br), 12 H, *o*-CH(C*H*$_3)_2$), 0.45 (s (br), 12 H, *o*-CH(C*H*$_3)_2$), 0.19 (s (br), 12 H, *o*-

CH(CH_3)$_2$); **^{13}C{^{1}H} NMR (100.6 MHz, 297 K, CD_2Cl_2): δ [ppm]** 156.27 (br), 154.96 (br), 150.41 (br), 148.85 (br), 143.53, 143.30, 139.59 (Naph-2,7-*C*H), 137.26 (br), 136.94, 130.81 (Naph-4,5-*C*H), 125.12 (Naph-3,6-*C*H), 123.21 (br, Ph-*m*-*C*H), 122.22 (br, Ph-*m*-*C*H), 37.97 (br), 36.59 (br, *o*-*C*H(CH$_3$)$_2$), 34.93 (br, *o*-*C*H(CH$_3$)$_2$), 34.55 (*o/p*-*C*H(CH$_3$)$_2$), 26.05 (br, *o*-CH(*C*H$_3$)$_2$), 25.00 (br), 24.66 (br, *o*-CH(*C*H$_3$)$_2$), 24.22 (*o/p*-CH(*C*H$_3$)$_2$), 24.16 (*o*-CH(*C*H$_3$)$_2$), 23.21 (br, *o*-CH(*C*H$_3$)$_2$); **^{1}H NMR (300.1 MHz, 232 K, CD_2Cl_2): δ [ppm]** 8.08 (d, $^3J_{HH}$ = 6.78 Hz, 2 H, Naph-2,7-*H*), 7.84 (d, $^3J_{HH}$ = 7.63 Hz, 2 H, Naph-4,5-*H*), 7.29 (t, $^3J_{HH}$ = 7.38 Hz, 2 H, Naph-3,6-*H*), 6.98 (s, 2 H, Ph^1-*m*-*H*), 6.93 (s, 2 H, Ph^1-*m*-*H*), 6.79 (s, 2 H, Ph^2-*m*-*H*), 6.76 (s, 2 H, Ph^2-*m*-*H*), 3.63 (sept, $^3J_{HH}$ = 6.55 Hz, 2 H, Ph^1-*o*-C*H*(CH$_3$)$_2$), 3.31 (sept, $^3J_{HH}$ = 6.24 Hz, 2 H, Ph^2-*o*-C*H*(CH$_3$)$_2$), 2.85-2.65 (m, 6 H, Ph-*o/p*-C*H*(CH$_3$)$_2$), 2.48 (sept, $^3J_{HH}$ = 6.55 Hz, 2 H, Ph^2-*o*-C*H*(CH$_3$)$_2$), 1.16-1.10 (m, 36 H, Ph-*o/p*-CH(C*H*$_3$)$_2$), 0.92-0.89 (m, 12 H, Ph^1-*o*-CH(C*H*$_3$)$_2$), 0.38 (d, $^3J_{HH}$ = 6.69 Hz, 6 H, Ph^2-*o*-CH(C*H*$_3$)$_2$), 0.31 (d, $^3J_{HH}$ = 6.23 Hz, 6 H, Ph^2-*o*-CH(C*H*$_3$)$_2$), 0.20 (d, $^3J_{HH}$ = 6.46 Hz, 6 H, Ph^2-*o*-CH(C*H*$_3$)$_2$), 0.02 (d, $^3J_{HH}$ = 6.23 Hz, 6 H, Ph^1-*o*-CH(C*H*$_3$)$_2$); **^{13}C{^{1}H} NMR (75.5 MHz, 232 K, CD_2Cl_2): δ [ppm]** 155.55 (Ph^1-*o*-*C*), 155.11 (Ph^2-*o*-*C*), 154.13 (Ph^1-*o*-*C*), 153.31 (Ph^2-*o*-*C*), 149.83 (Ph-*p*-*C)*, 148.03 (Ph-*p*-*C)*, 142.66 (Naph-1,8-*C*), 142.27 (Naph-9-*C*), 142.23 (Ph^1-*ipso*-*C*), 138.80 (Naph-2,7-*C*H), 136.40 (Ph^2-*ipso*-*C*), 136.07 (Naph-10-*C*), 130.27 (Naph-4,5-*C*H), 124.55 (Naph-3,6-*C*H), 122.98 (Ph^1-*m*-*C*H), 122.34 (Ph^1-*m*-*C*H), 121.82 (Ph^2-*m*-*C*H), 121.17 (Ph^2-*m*-*C*H), 37.62 (Ph^1-*o*-*C*H(CH$_3$)$_2$), 36.29 (Ph^2-*o*-*C*H(CH$_3$)$_2$), 36.01 (Ph^2-*o*-*C*H(CH$_3$)$_2$), 34.34 (Ph^2-*o*-*C*H(CH$_3$)$_2$), 34.09 (Ph^1-*p*-*C*H(CH$_3$)$_2$), 33.95 (Ph^2-*p*-*C*H(CH$_3$)$_2$), 25.67 (Ph^2-*o*-CH(*C*H$_3$)$_2$), 25.40 (Ph^1-*o*-CH(*C*H$_3$)$_2$), 24.50 (Ph^1-*o*-CH(*C*H$_3$)$_2$), 24.00 (Ph^1-*o*-CH(*C*H$_3$)$_2$), 23.96 (Ph-*p*-CH(*C*H$_3$)$_2$), 23.81 (Ph-*p*-CH(*C*H$_3$)$_2$), 23.75 (Ph^2-*o*-CH(*C*H$_3$)$_2$), 22.72 (Ph^2-*o*-CH(*C*H$_3$)$_2$), 22.31 (Ph^1-*o*-CH(*C*H$_3$)$_2$), 22.26 (Ph^2-*o*-CH(*C*H$_3$)$_2$); **IR ν [cm^{-1}]**: 3033 (w), 2954 (s), 2923 (m), 2864 (m), 1594 (w), 1553 (w), 1535 (w), 1459 (m), 1415 (m), 1380 (m), 1360 (m), 1306 (w), 1258 (m), 1231 (w), 1191 (w), 1155 (w), 1129 (w), 1099 (m), 1066 (m), 1051 (m), 1007 (w), 935 (w), 876 (s), 816 (m), 773 (m), 744 (m), 668 (w), 643 (w), 629 (w), 613 (w), 563 (w), 511 (m), 470 (w), 450 (w), 433 (w), 395 (m).

Synthesis of (Trip$_2$Bi)$_2$Naph (2). Li_2Naph (1.99 mmol, 362 mg) and Trip$_2$BiCl (2.00 mmol, 1.3 g) were each dissolved in 20 mL of thf and the resulting solutions cooled to –30 °C. The yellow solution of Trip$_2$BiCl was added to Li_2Naph and stirred overnight. The reaction mixture was dried *in vacuo* and 25 mL of water were added, stirred for 30 minutes, filtered and the residue dried *in vacuo*. The solid was extracted with toluene and the resulting solution concentrated to 2 mL. Ethanol (10 mL) was added, yielding a precipitate that was dissolved in upon heating. Storage of the solution at +4 °C gave yellow crystals of **2**.

Yield: 754.8 mg (56 %); **m.p.:** 249.6 °C '(dec.); **elemental analysis [wt-%]:** calcd. for $C_{70}H_{98}Bi_2$: C 61.93, H 7.28. found: C 62.0, H 7.22; **^{1}H NMR (400.1 MHz, 297 K, CD_2Cl_2): δ [ppm]** 8.87 (dd, $^3J_{HH}$ = 6.88 Hz, $^4J_{HH}$ = 0.96 Hz, 2 H, Naph-2,7-C*H*), 7.88 (dd, $^3J_{HH}$ = 7.96 Hz, $^4J_{HH}$ = 0.93 Hz, 2 H, Naph-4,5-C*H*), 7.27 (t, $^3J_{HH}$ = 7.41 Hz, 2 H, Naph-3,6-C*H*), 7.07 (s, 8 H, Ph-*m*-*H*), 2.93 (sept, $^3J_{HH}$ = 6.45 Hz, 8 H, *o*-C*H*(CH$_3$)$_2$), 2.80 (sept, $^3J_{HH}$ = 6.94 Hz, 4 H, *p*-C*H*(CH$_3$)$_2$), 1.20 (d, $^3J_{HH}$ = 7.01 Hz, 24 H, *p*-CH(C*H*$_3$)$_2$), 0.81 (d, $^3J_{HH}$ = 6.42 Hz, 24 H,

o-CH(C*H*$_3$)$_2$), 0.70 (d, $^3J_{HH}$ = 4.67 Hz, 24 H, *o*-CH(C*H*$_3$)$_2$); **^{13}C{^{1}H} NMR (100.6 MHz, 297 K, CD_2Cl_2): δ [ppm]** 160.75 (Naph-*ipso*-*C*), 156.17 (Trip-*ipso*/*o*-*C*), 149.12 (Trip-*p*-*C*), 145.71 (Naph-10-*C*), 143.89 (Naph-2,7-*C*H), 139.26 (Naph-9-*C*), 129.98 (Naph-4,5-*C*H), 127.71 (Naph-3,6-*C*H), 123.67 (Ph-*m*-*C*H), 39.30 (*o*-*C*H(CH$_3$)$_2$), 34.60 (*p*-*C*H(CH$_3$)$_2$), 25.12 (*o*-CH(*C*H$_3$)$_2$), 24.42 (*o*-CH(*C*H$_3$)$_2$), 24.21 (*p*-CH(*C*H$_3$)$_2$), 24.14 (*p*-CH(*C*H$_3$)$_2$); **IR ν [cm^{-1}]**: 3015 (w), 2947 (s), 2914 (m), 2890 (m), 2855 (m), 1582 (w), 1549 (w), 1523 (w), 1453 (m), 1408 (m), 1375 (m), 1355 (m), 1302 (w), 1254 (w), 1226 (w), 1187 (w), 1152 (w), 1126 (w), 1093 (m), 1048 (m), 990 (m), 935 (w), 872 (m), 833 (w), 806 (m), 764 (m), 734 (m), 640 (w), 550 (w), 550 (w), 507 (w), 471 (w), 448 (w).

Synthesis of [(Trip$_2$Sb)(TripSb)Naph][BAr^F] (3). **1** (0.8 mmol, 1 g) and [Fc$^+$][BAr^F] (0.8 mmol, 723 mg) were each dissolved in 30 mL of thf. The solutions were cooled to –78 °C and the solution of [Fc$^+$][BAr^F] was added to **1**, yielding a deep purple reaction mixture, which was stirred for 12 h. Removal of all volatiles *in vacuo* gave an oily residue, that was washed with *n*-hexane until the hexane solution stayed colorless. Additional 50 mL of *n*-hexane were added, the resulting mixture stirred at 60 °C for 12 h and then filtered. Drying the solid residue *in vacuo* gave **3** as a green powder. Crystals suitable for single crystal X-ray diffraction were obtained by dissolving 100 mg of **3** in 2 mL of DCM, which was layered with 30 mL of *n*-hexane. Storage for a week at +4 °C resulted in the formation of green blocks of **3**.
Yield: 1.325 g (84 %); **m.p.:** 106.0 °C; **elemental analysis [wt-%]:** calcd. for $C_{79}H_{75}BF_{20}Sb_2$: C 57.21, H 4.56. found: C 56.5, H 4.22; **^{1}H NMR (400.1 MHz, 297 K, CD_2Cl_2): δ [ppm]** 8.21 (d, $^3J_{HH}$ = 8.43 Hz, 1 H, Naph-*H*), 8.11-8.06 (m, 3 H, Naph-*H*), 7.77 (dd, $^3J_{HH}$ = 8.05 Hz, $^3J_{HH}$ = 7.21 Hz, 1 H, Naph-*m*-*H*), 7.70 (dd, $^3J_{HH}$ = 8.26 Hz, $^3J_{HH}$ = 6.95 Hz, 1 H, Naph-*m*-C*H*), 7.17 (s, 2 H, Ph-*m*-*H*), 7.09 (s (br), 2 H, Ph-*m*-*H*), 7.06 (s, 2 H, Ph-*m*-*H*), 3.82 (s (br), 1 H, *o*-C*H*(CH$_3$)$_2$), 2.90 (sept, $^3J_{HH}$ = 6.85 Hz, 1 H, *p*-C*H*(CH$_3$)$_2$), 2.84 (sept, $^3J_{HH}$ = 6.91 Hz, 2 H, *p*-C*H*(CH$_3$)$_2$), 2.68 (sept, $^3J_{HH}$ = 6.58 Hz, 2 H, *o*-C*H*(CH$_3$)$_2$), 2.58 (sept, $^3J_{HH}$ = 6.58 Hz, 2 H, *o*-C*H*(CH$_3$)$_2$), 2.00 (s (br), 1 H, *o*-CH(C*H*$_3$)$_2$), 1.47 (s (br), 6 H, *o*-CH(C*H*$_3$)$_2$) 1.21-1.16 (m, 18 H, *p*-CH(C*H*$_3$)$_2$), 0.97 (d, $^3J_{HH}$ = 6.75 Hz, 6 H, *o*-CH(C*H*$_3$)$_2$), 0.91 (d, $^3J_{HH}$ = 6.51 Hz, 6 H, *o*-CH(C*H*$_3$)$_2$), 0.68 (d, $^3J_{HH}$ = 6.51 Hz, 6 H, *o*-CH(C*H*$_3$)$_2$), 0.64 (d, $^3J_{HH}$ = 6.75 Hz, 6 H, *o*-CH(C*H*$_3$)$_2$), 0.25 (s (br), 6 H, *o*-CH(C*H*$_3$)$_2$); **^{11}B NMR (128.4 MHz, 297 K, CD_2Cl_2): δ [ppm]** –16.75 (s); **^{13}C{^{1}H} NMR (100.6 MHz, 297 K, CD_2Cl_2): δ [ppm]** 157.63 (br), 155.81 (Trip-*C*), 154.89 (Trip-*C*), 154.35 (Trip-*C*), 153.87 (Trip-*C*), 153.63 (Trip-*C*), 149.79 (br, Trip-*C*), 147.35 (br, Trip-*C*), 142.35 (Naph-*ipso*-*C*), 141.11 (Naph-*C*), 140.12 (Naph-*ipso*-*C*), 139.86 (br, Trip-*C*), 138.43 (Naph-*CH*), 137.87 (br, Trip-*C*), 137.37 (Naph-10-*C*), 136.03 (Naph-*C*H), 135.47 (br, Trip-*C*), 134.54 (Naph-*C*H), 134.32, 132.36 (Naph-*C*H), 128.45 (Trip-*C*), 128.0 (Trip-*C*), 127.93 (Naph-3/5-*C*H), 127.85 (Naph-3/5-*C*H), 125.91 (Trip-*m*-*C*), 125.31 (Trip-*m*-*C*H), 124.07 (Trip-*m*-*C*H), 40.39 (*o*-C*H*(CH$_3$)$_2$), 38.73 (*o*-C*H*(CH$_3$)$_2$), 37.26 (*o*-C*H*(CH$_3$)$_2$), 34.78 (*p*-C*H*(CH$_3$)$_2$), 34.69 (*p*-C*H*(CH$_3$)$_2$), 34.54 (*p*-C*H*(CH$_3$)$_2$), 25.05 (*o*-CH(C*H*$_3$)$_2$), 24.46 (*o*-CH(C*H*$_3$)$_2$), 23.96 (*o*-CH(C*H*$_3$)$_2$), 23.83 (*p*-CH(C*H*$_3$)$_2$), 23.72 (*p*-CH(C*H*$_3$)$_2$), 23.68 (*p*-CH(C*H*$_3$)$_2$), 23.07 (br, *o*-CH(C*H*$_3$)$_2$), 14.28 (br, *o*-CH(C*H*$_3$)$_2$); **^{19}F NMR (376.5 MHz, 297 K, CD_2Cl_2): δ [ppm]** –133.26 (br-s, 2 F, BAr^F-*o*/*m*-C*F*), –163.84 (t, $^3J_{FF}$ = 20.55 Hz, 1 F, BAr^F-*p*-C*F*), –167.72 (br-t, $^3J_{FF}$

= 18.19 Hz, 2 F, BAr^F-*o/m*-C*F*); **^{1}H NMR (300.1 MHz, 242 K, CD_2Cl_2): δ [ppm]** 8.18 (d, $^3J_{HH}$ = 7.98 Hz, 1 H, Naph-*H*), 8.09-8.04 (m, 3 H, Naph-*H*), 7.76 (dd, $^3J_{HH}$ = 7.91 Hz, $^3J_{HH}$ = 7.38 Hz, 1 H, Naph-*m*-*H*), 7.68 (dd, $^3J_{HH}$ = 8.17 Hz, $^3J_{HH}$ = 6.81 Hz, 1 H, Naph-*m*-*H*), 7.16 (d, $^4J_{HH}$ = 1.61 Hz, 1 H, Sb^+-Ph-*m*-*H*), 7.12 (s, 2 H, Ph-*m*-*H*), 7.00 (s, 2 H, Ph-*m*-*H*), 7.00 (s, 2 H, Ph-*m*-*H*), 6.89 (d, $^4J_{HH}$ = 1.37 Hz, 1 H, Ph-*m*-*H*), 3.72 (sept, $^3J_{HH}$ = 6.57 Hz, 1 H, *o*-C*H*$(CH_3)_2$), 2.85 (sept, $^3J_{HH}$ = 6.72 Hz, 1 H, *p*-CH$(CH_3)_2$), 2.79 (sept, $^3J_{HH}$ = 6.47 Hz, 2 H, *p*-C*H*$(CH_3)_2$), 2.62 (sept, $^3J_{HH}$ = 6.22 Hz, 2 H, *o*-C*H*$(CH_3)_2$), 2.50 (sept, $^3J_{HH}$ = 6.22 Hz, 2 H, *o*-C*H*$(CH_3)_2$), 1.91 (sept, $^3J_{HH}$ = 6.72 Hz, 1 H, *o*-C*H*$(CH_3)_2$), 1.45 (d, $^3J_{HH}$ = 6.29 Hz, 3 H, CH(C*H*$_3)_2$), 1.26 (d, $^3J_{HH}$ = 6.29 Hz, 3 H, *o*-CH(C*H*$_3)_2$) 1.15-1.09 (m, 18 H, *p*-CH(C*H*$_3)_2$), 0.91 (d, $^3J_{HH}$ = 6.71 Hz, 6 H, *o*-CH(C*H*$_3)_2$), 0.82 (d, $^3J_{HH}$ = 6.29 Hz, 6 H, *o*-CH(C*H*$_3)_2$), 0.63 (d, $^3J_{HH}$ = 6.29 Hz, 6 H, *o*-CH(C*H*$_3)_2$), 0.56 (d, $^3J_{HH}$ = 6.71 Hz, 6 H, *o*-CH(C*H*$_3)_2$), 0.17 (d, $^3J_{HH}$ = 6.71 Hz, 3 H, *o*-CH(C*H*$_3)_2$), 0.12 (d, $^3J_{HH}$ = 6.71 Hz, 3 H, *o*-CH(C*H*$_3)_2$); **IR *ν* [cm^{-1}]**: 2955 (w), 2922 (w), 2859 (w), 1637 (w), 1587 (w), 1556 (w), 1506 (m), 1458 (s), 1412 (w), 1381 (w), 1359 (w), 1304 (w), 1255 (m), 1079 (m), 976 (s) 876 (w), 812 (m), 766 (m), 753 (m), 680 (m), 658 (m), 604 (w), 568 (w), 510 (w).

Synthesis of $(TripSb)_2Naph$ (4). 3 (0.06 mmol, 100 mg) and KC_8 (0.06 mmol, 8 mg) were dissolved in 10 mL of thf. The suspension was stirred for 12 h and then filtered, giving a pale-yellow solution. The solvent was removed *in vacuo*, and the remaining residue was extracted with *n*-hexane (3 x 5 mL) and concentrated until the formation of precipitate. The solid was redissolved in the heat and the solution was stored at +4 °C to give a yellow crystalline solid.

Yield: 17 mg (37 %); **m.p.:** 245.8 °C; **elemental analysis [wt-%]:** calcd. for $C_{40}H_{52}Sb_2$: C 61.88, H 6.75. found: C 61.8, H 6.56; **^{1}H NMR (400.1 MHz, 297 K, CD_2Cl_2): δ [ppm]** 7.86 (dd, $^3J_{HH}$ = 6.79 Hz, $^4J_{HH}$ = 1.21 Hz, 2 H, Naph-2/7-C*H*), 7.71 (dd, $^3J_{HH}$ = 8.21 Hz, $^4J_{HH}$ = 1.11 Hz, 2 H, Naph-4/5-C*H*), 7.38 (dd, $^3J_{HH}$ = 8.11 Hz, $^3J_{HH}$ = 6.85 Hz, 2 H, Naph-3/6-*H*), 6.94 (s, 4 H, Ph-*m*-*H*), 3.25 (sept, $^3J_{HH}$ = 6.78 Hz, 4 H, *o*-C*H*$(CH_3)_2$), 2.82 (sept, $^3J_{HH}$ = 6.97 Hz, 2 H, *p*-C*H*$(CH_3)_2$), 1.21 (dd, $^3J_{HH}$ = 6.88 Hz, $^4J_{HH}$ = 2.06 Hz, 12 H, *p*-CH(C*H*$_3)_2$), 1.14 (d, $^3J_{HH}$ = 6.84 Hz, 12 H, *o*-CH(C*H*$_3)_2$), 0.64 (d, $^3J_{HH}$ = 6.65 Hz, 12 H, *o*-CH(C*H*$_3)_2$); **^{13}C{^{1}H} NMR (100.6 MHz, 297 K, CD_2Cl_2): δ [ppm]** 156.69 (Ph-*o*-*C*), 150.20 (Ph-*p*-*C*), 147.95 (Naph-9-*C*), 145.02 (Naph-10-*C*), 138.75 (Naph-2/7-*C*H), 138.47 (Naph-1,8-*C*), 134.67 (Ph-*ipso*-*C*), 128.92 (Naph-4,5-*C*H), 125.91 (Naph-3,6-*C*H), 122.34 (Ph-*m*-*C*H), 38.20 (*o*-*C*H$(CH_3)_2$), 34.48 (*p*-*C*H$(CH_3)_2$), 25.27 (*o*-CH(*C*H$_3)_2$), 24.39 (*o*-CH(*C*H$_3)_2$), 24.06 (*p*-CH(*C*H$_3)_2$); **IR *ν* [cm^{-1}]**: 3030 (w), 2943 (s), 2914 (m), 2891 (m), 2854 (m), 1585 (w), 1546 (w), 1533 (w), 1451 (m), 1408 (m), 1375 (m), 1355 (m), 1339 (w), 1296 (w), 1255 (m), 1228 (w), 1191 (w), 1163 (w), 1092 (m), 1059 (m), 1048 (m), 1018 (m), 972 (w), 931 (w), 872 (m), 806 (s), 769 (s), 740 (m), 704 (w), 670 (w), 643 (w), 620 (w), 557 (w), 509 (w), 463 (w), 444 (w), 428 (w).

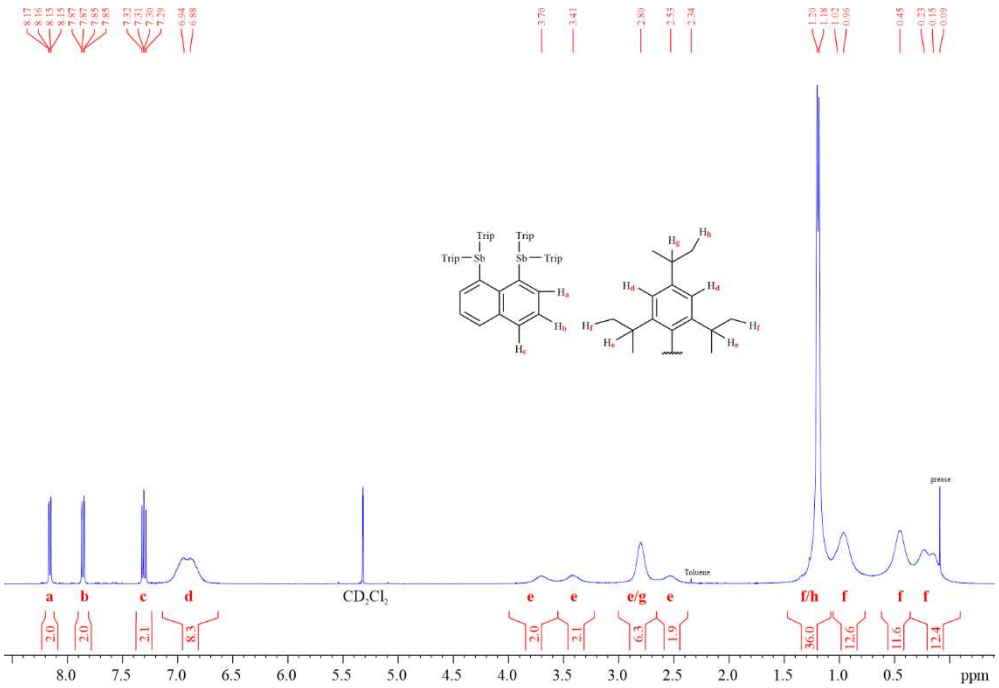


Figure S1. ^{1}H NMR spectrum of $(Trip_2Sb)_2Naph$ (**1**) in CD_2Cl_2.

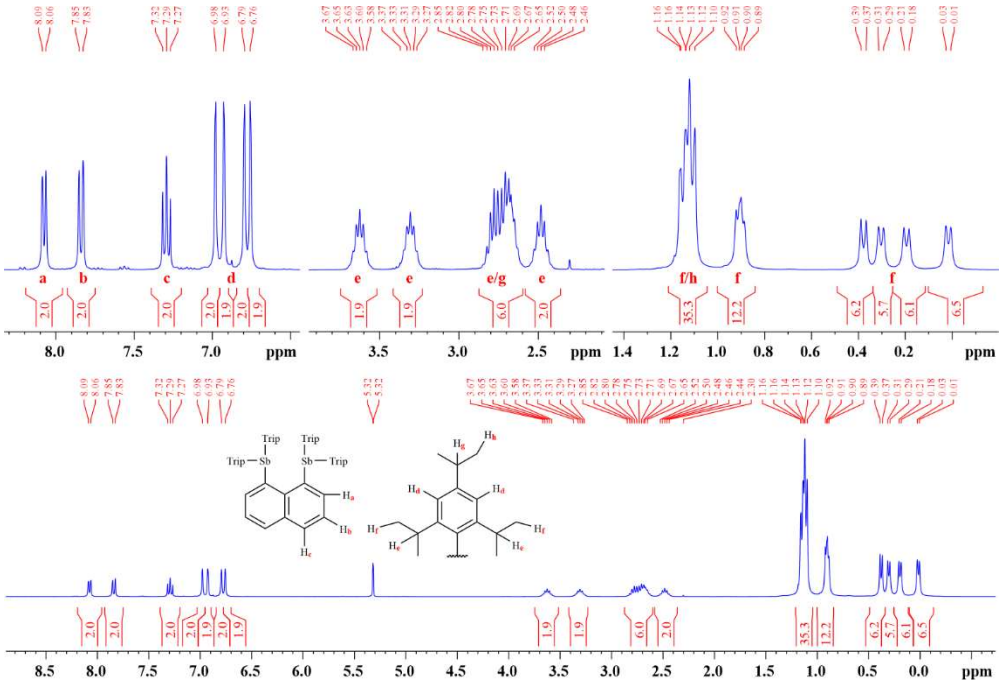


Figure S2. ^{1}H NMR spectrum of $(Trip_2Sb)_2Naph$ (**1**) in CD_2Cl_2 recorded at –40 °C**.**

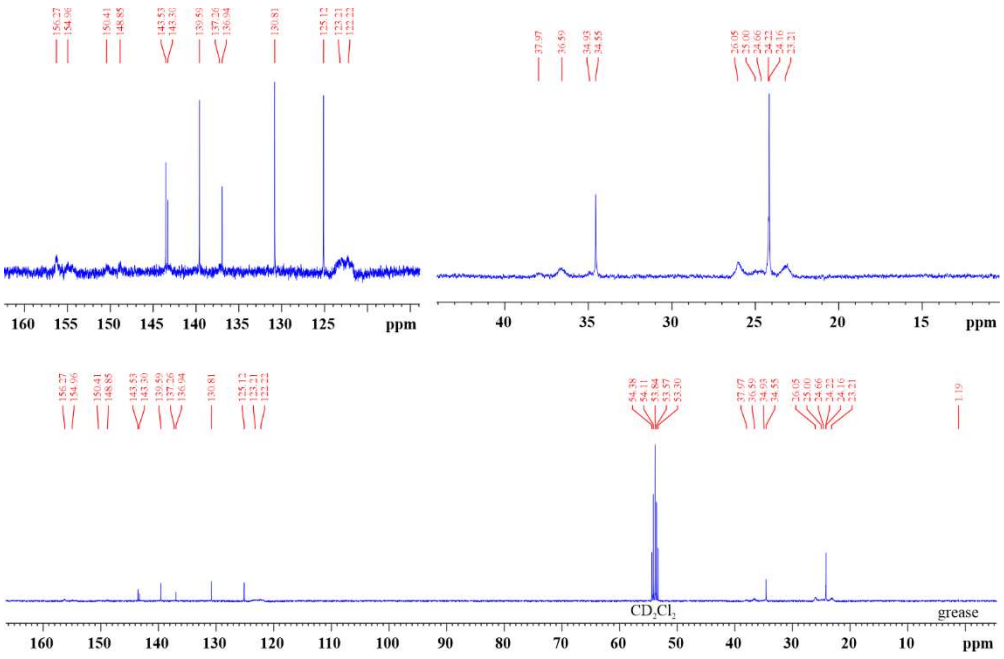


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of $(Trip_2Sb)_2Naph$ (**1**) in CD_2Cl_2.

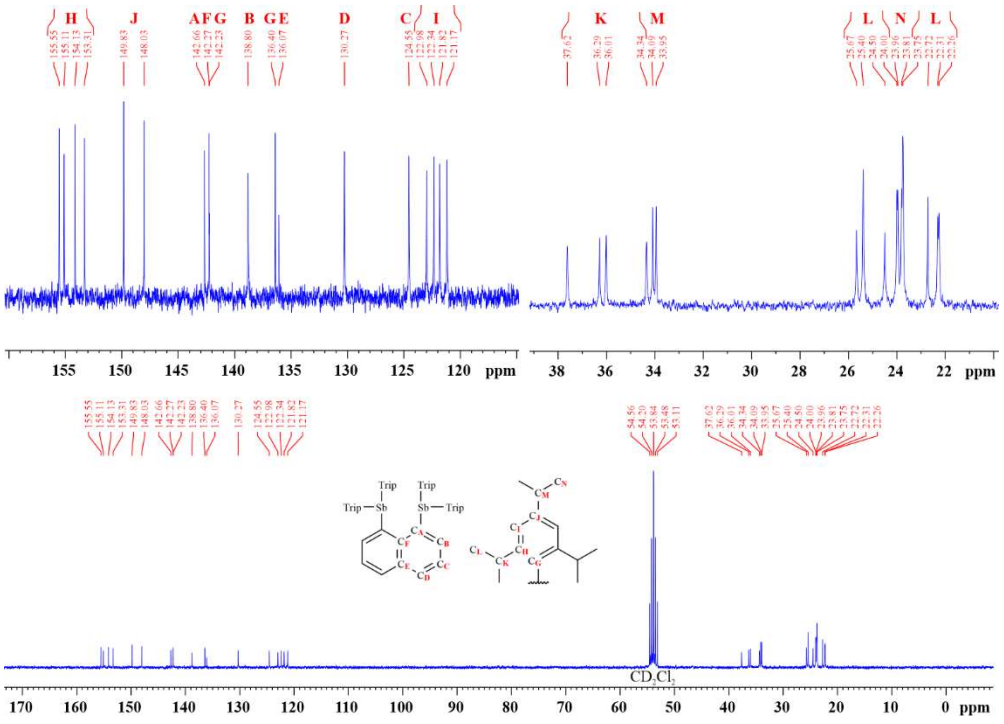


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $(Trip_2Sb)_2Naph$ (**1**) in CD_2Cl_2 recorded at –40 °C.

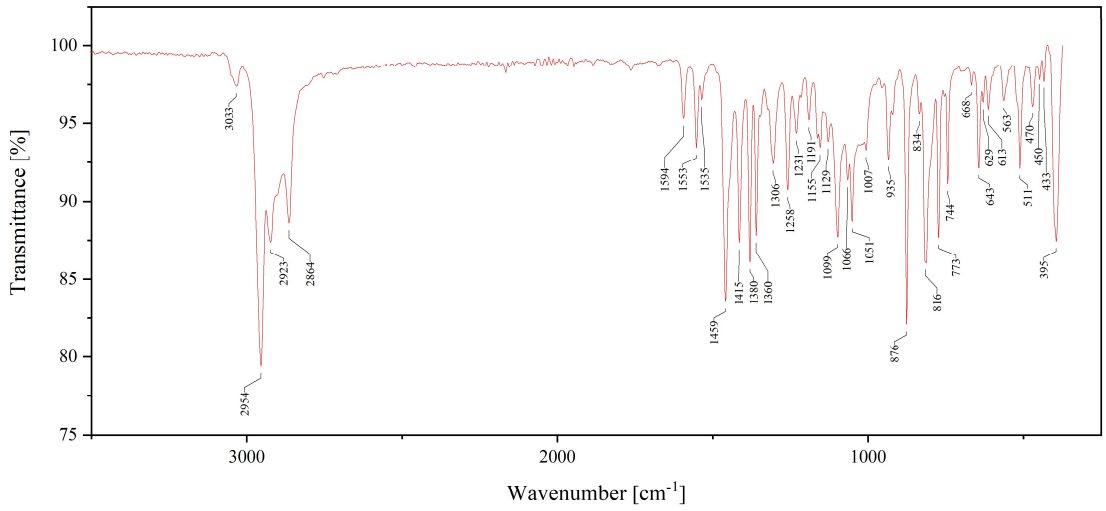


Figure S5. IR spectrum of neat $(Trip_2Sb)_2Naph$ (**1**).

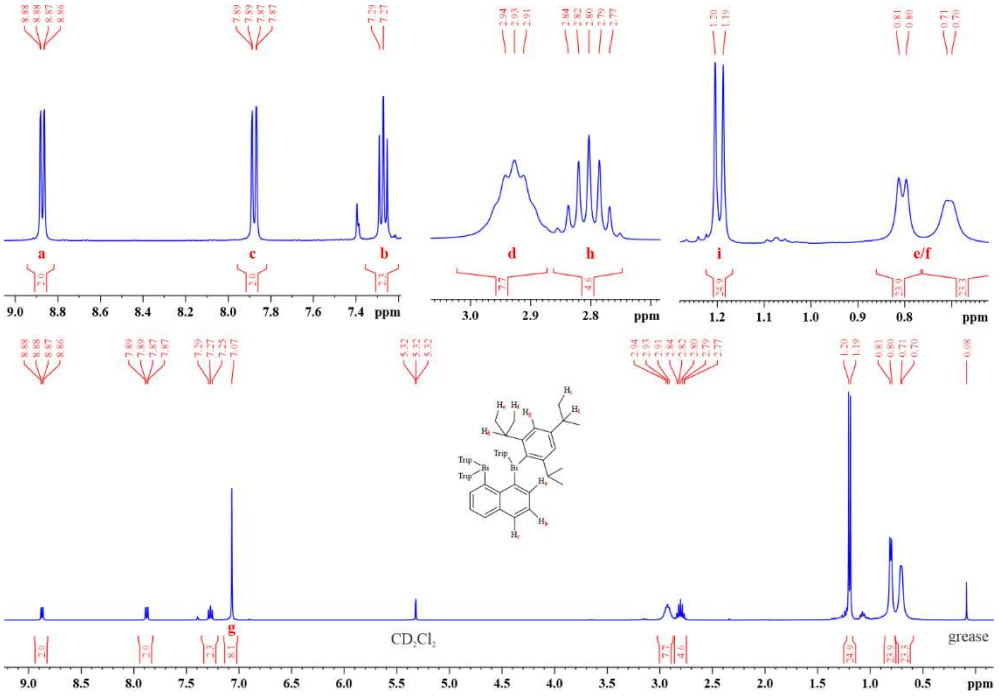


Figure S6. ^1H NMR spectrum of $(Trip_2Bi)_2Naph$ (**2**) in CD_2Cl_2.

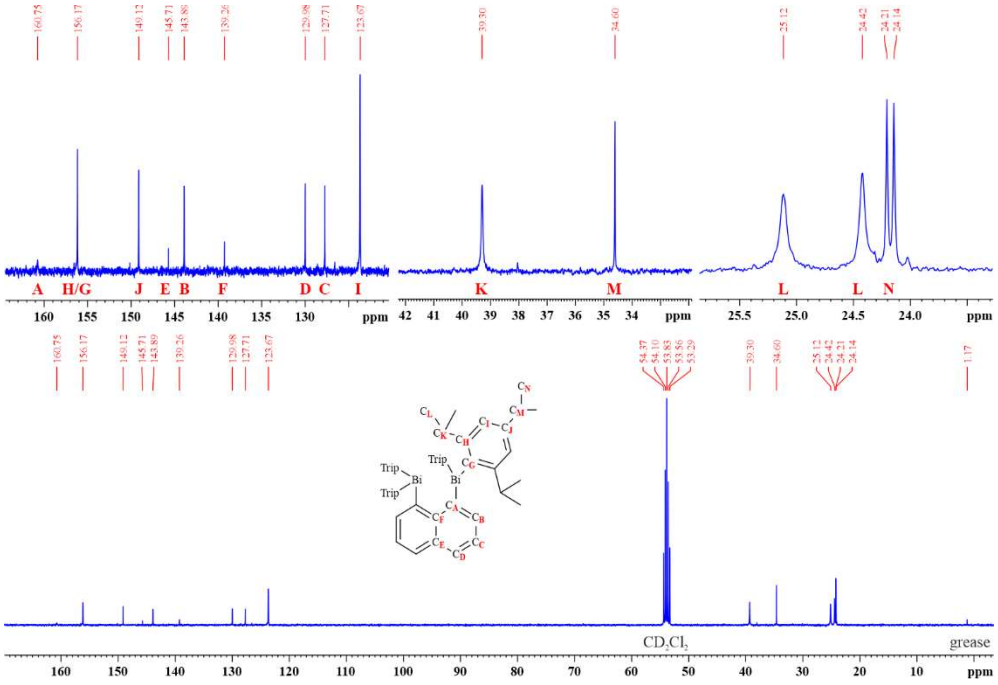


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of $(Trip_2Bi)_2Naph$ (**2**) in CD_2Cl_2.

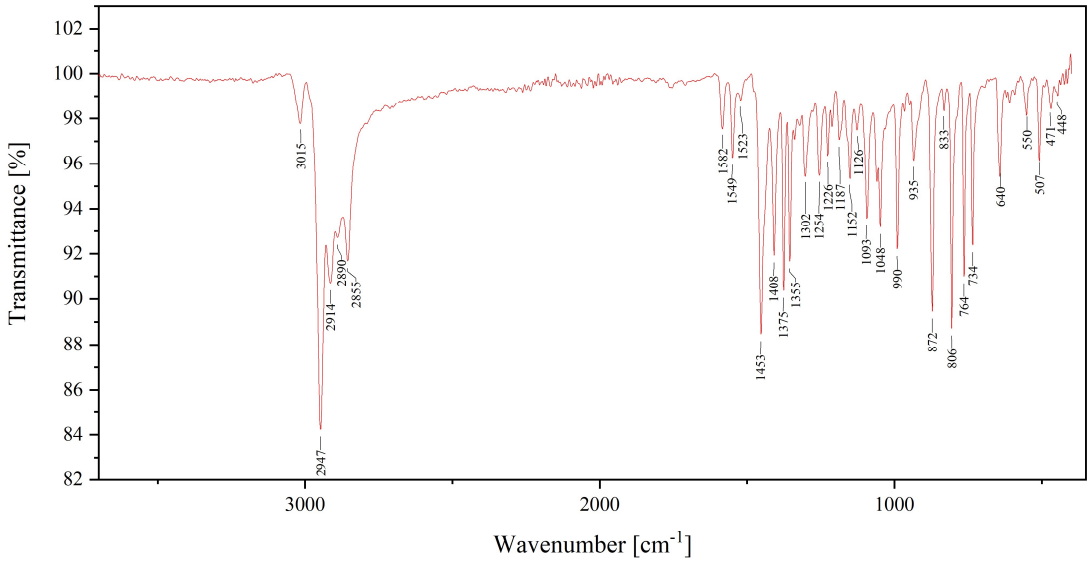


Figure S8. IR spectrum of neat $(Trip_2Bi)_2Naph$ (**2**).

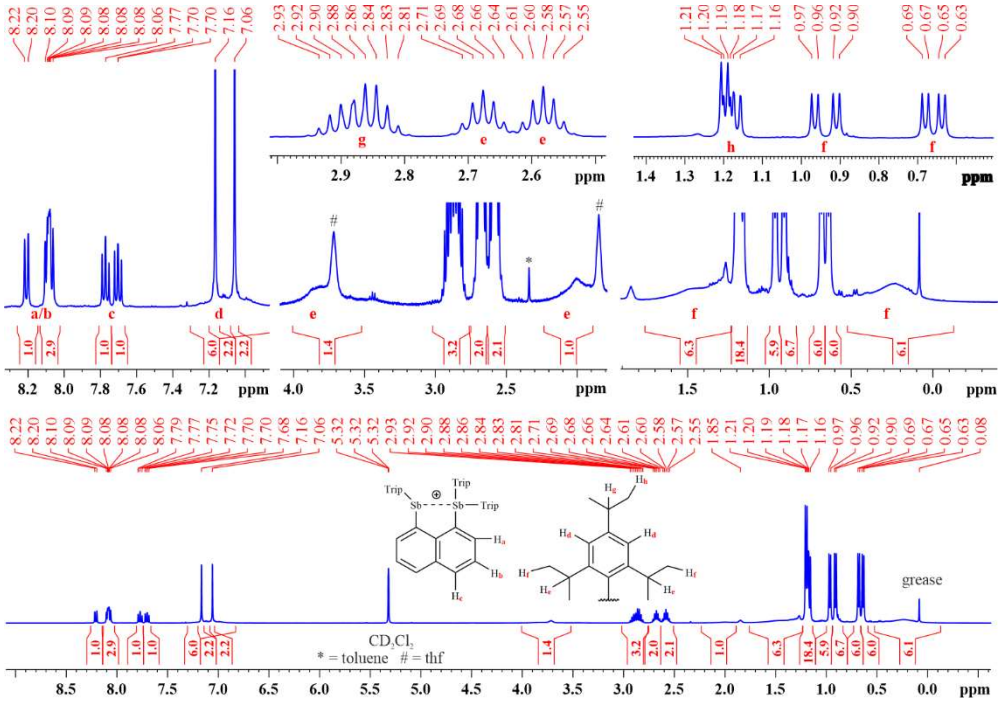


Figure S9. ^{1}H NMR spectrum of [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**) in CD_2Cl_2. Due to overlap of signals and lack of crosspeaks in 2D NMR spectra, no exact assignment of ^{1}H NMR signals to the corresponding protons was possible.

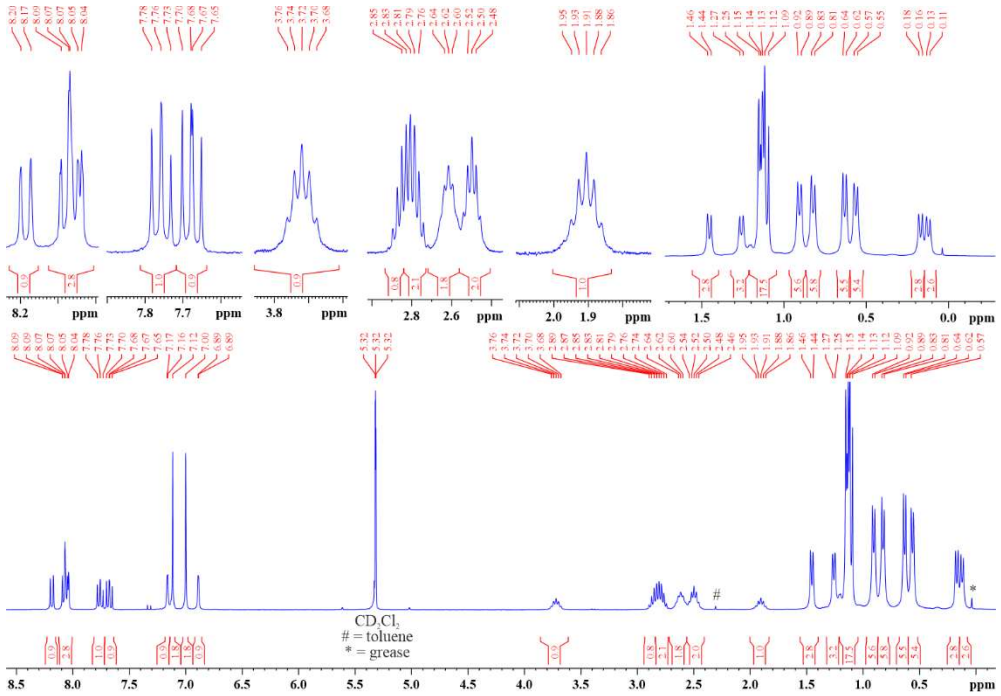


Figure S10. ^{1}H NMR spectrum of [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**) in CD_2Cl_2 at –30 °C. Due to low intensity in ^{13}C{^{1}H} NMR spectra, no complete assignment of ^{1}H NMR to the corresponding protons was possible.

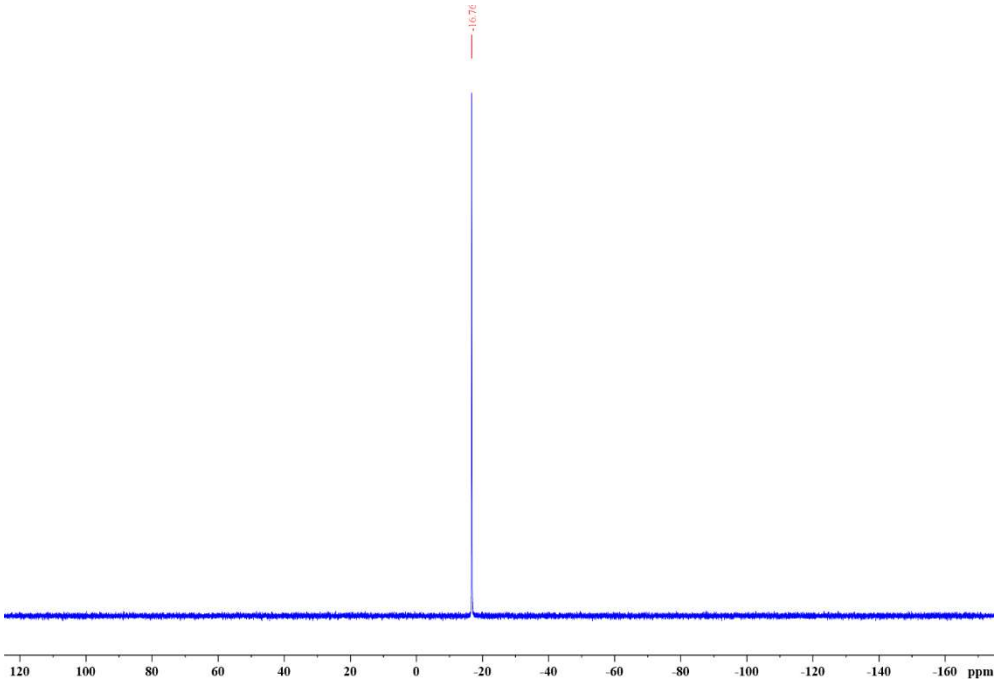


Figure S11. ^{11}B NMR spectrum of [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**) in CD_2Cl_2.

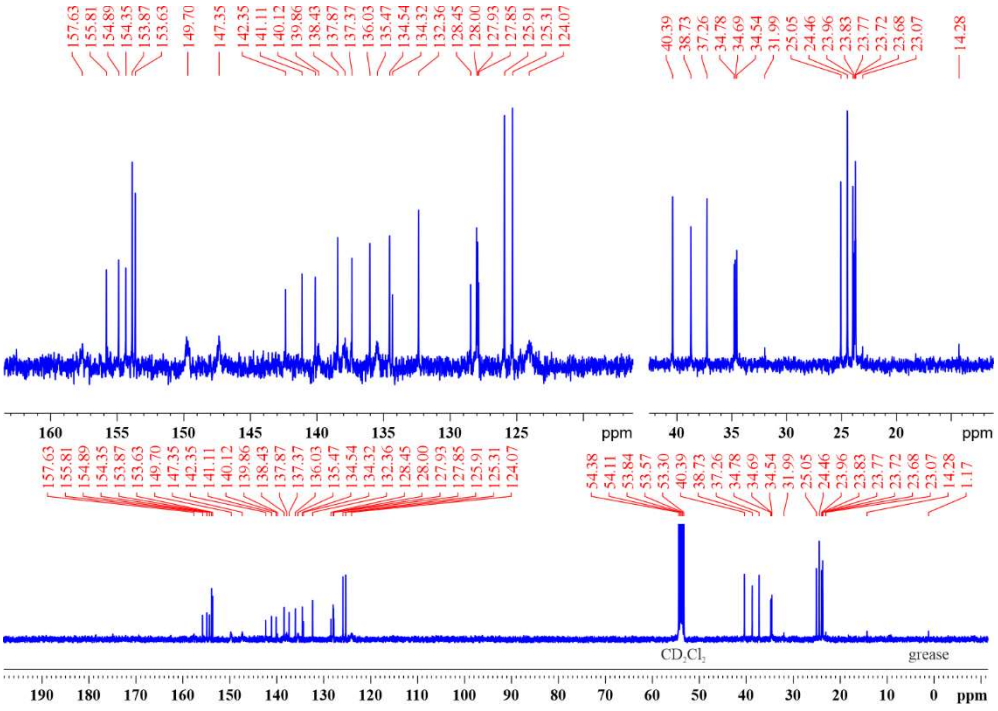


Figure S12. $^{13}C\{^1H\}$ NMR spectrum of [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**) in CD_2Cl_2**.** Due to a lack of crosspeaks in 2D NMR spectra, no exact assignment of ^{13}C NMR signals to the corresponding carbon atoms was possible.

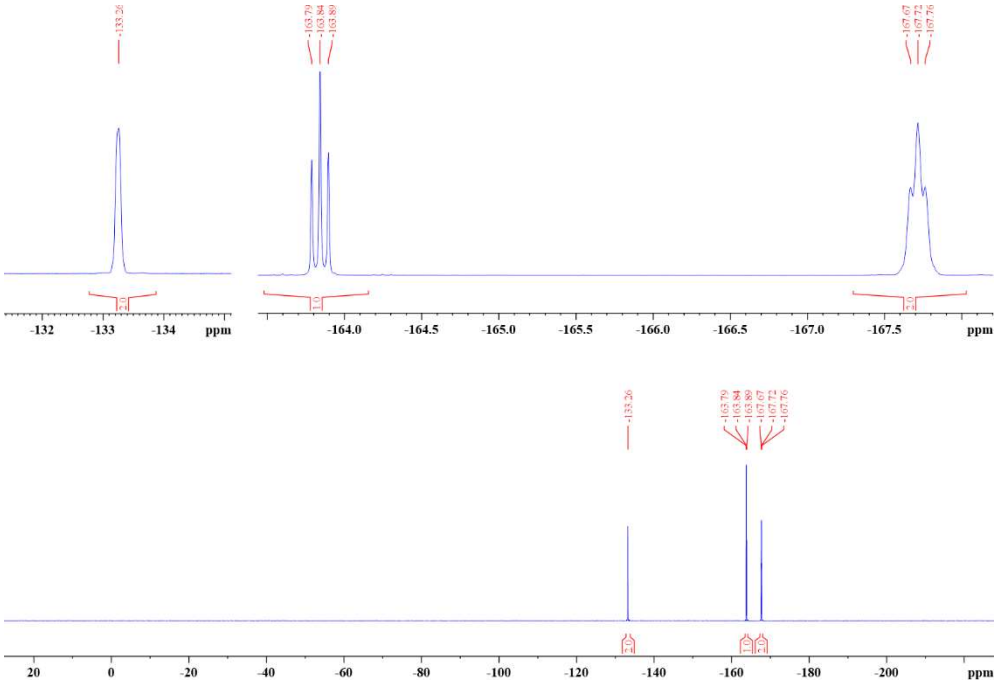


Figure S13. ^{19}F NMR spectrum of [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**) in CD_2Cl_2.

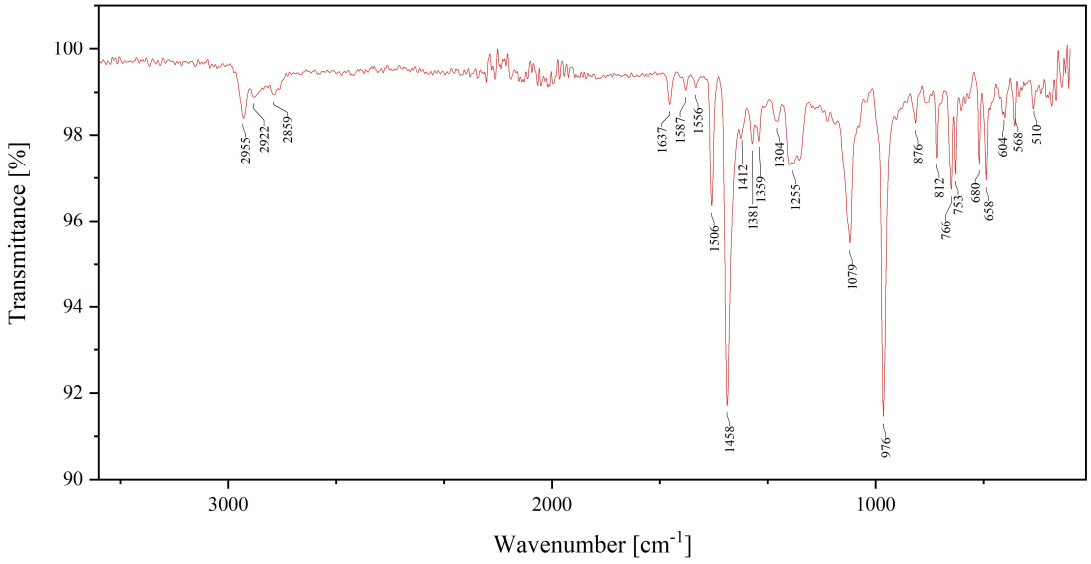


Figure S14. IR spectrum of neat [(Trip$_2$Sb)(TripSb)Naph][BAr$^{F\text{-}20}$] (**3**).

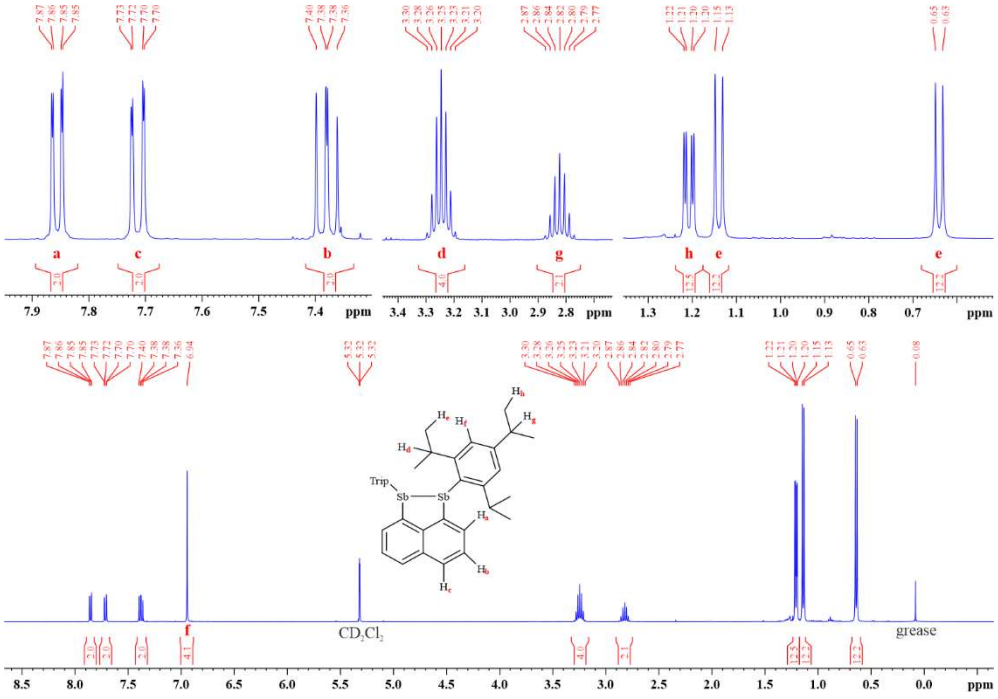


Figure S15. ^{1}H NMR spectrum of $(TripSb)_2Naph$ (**4**) in CD_2Cl_2.

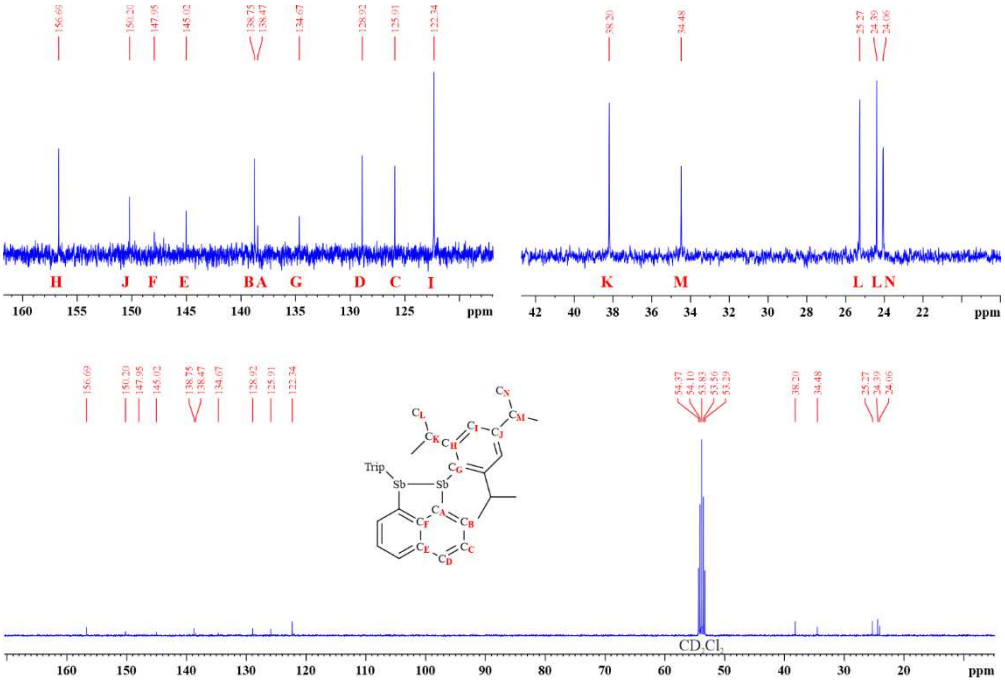


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of $(TripSb)_2Naph$ (**4**) in CD_2Cl_2**.**

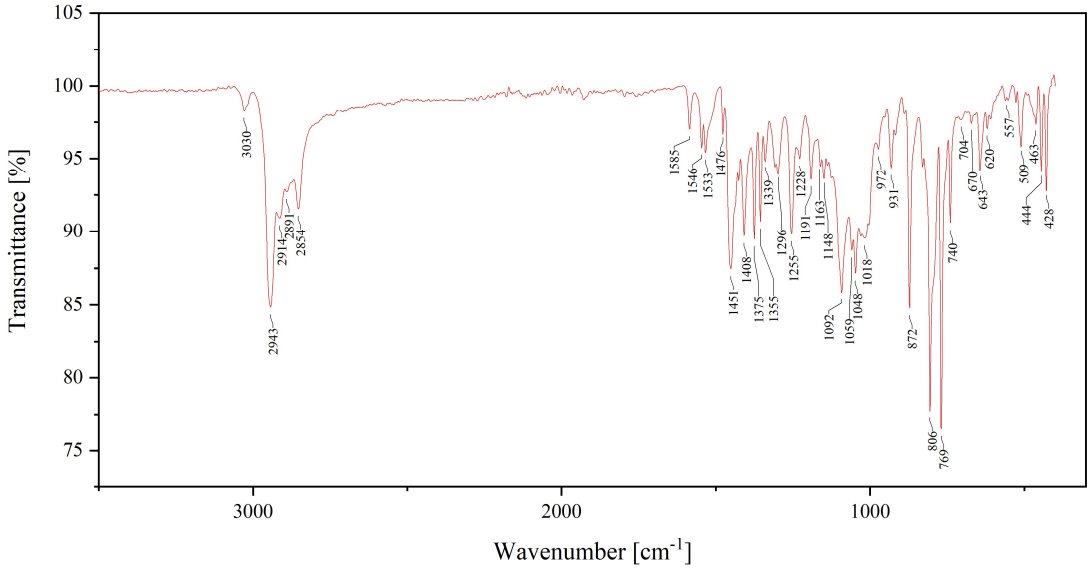


Figure S17. IR spectrum of neat $(TripSb)_2Naph$ (**4**).

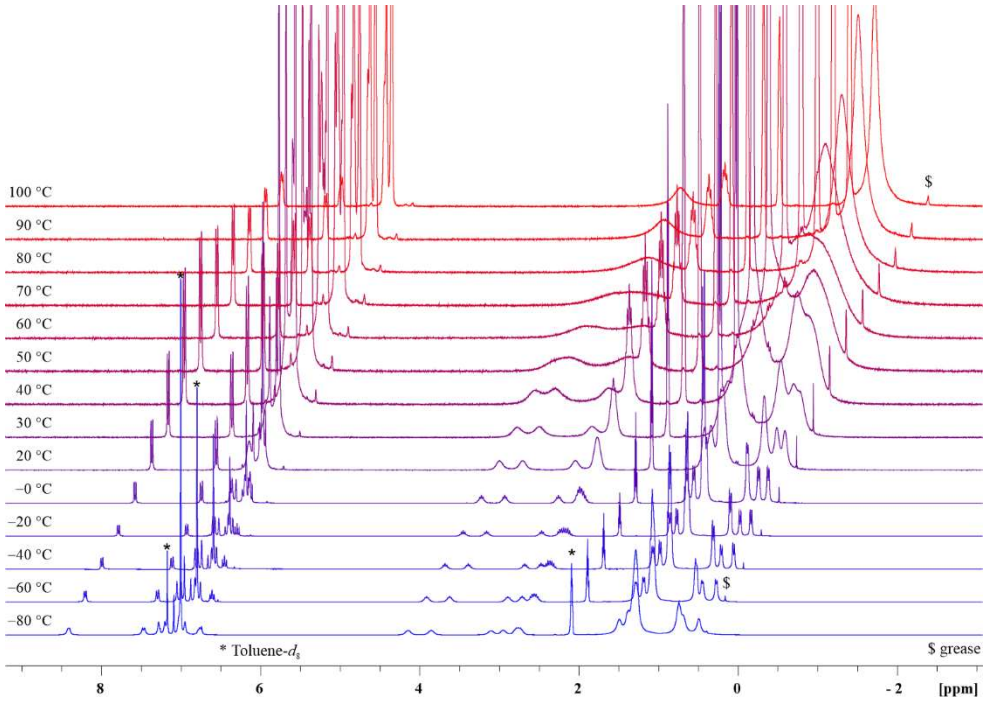


Figure S18. ^1H VT-NMR spectrum of $(Trip_2Sb)_2Naph$ (**1**) in toluene-d_8.

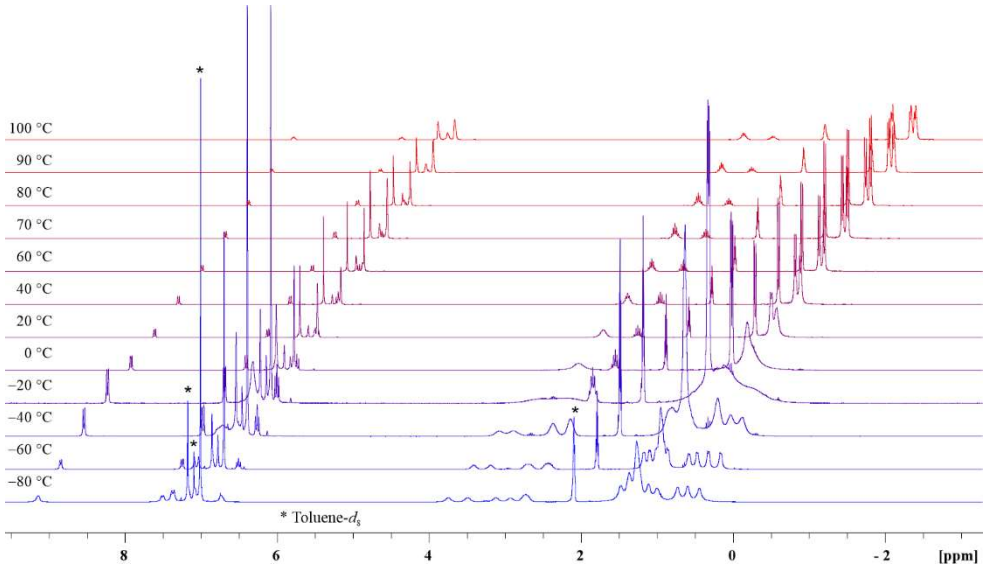


Figure S19. ^{1}H VT-NMR spectrum of $(Trip_2Bi)_2Naph$ (**2**) in toluene-d_8.

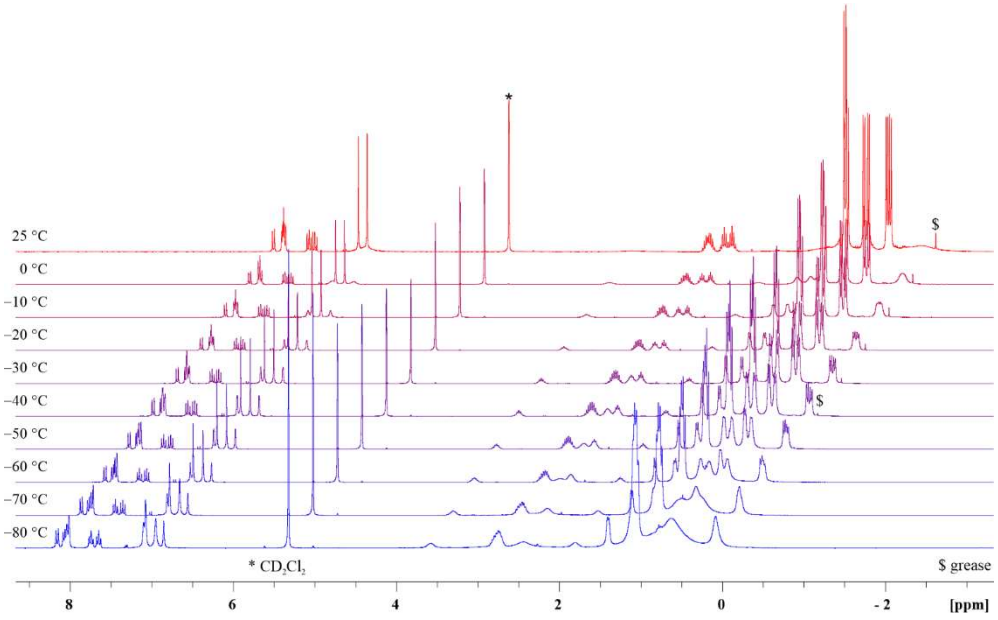


Figure S20. ^{1}H VT-NMR spectrum of $[(Trip_2Sb)(TripSb)Naph][BAr^{F\text{-}20}]$ (**3**) in CD_2Cl_2.

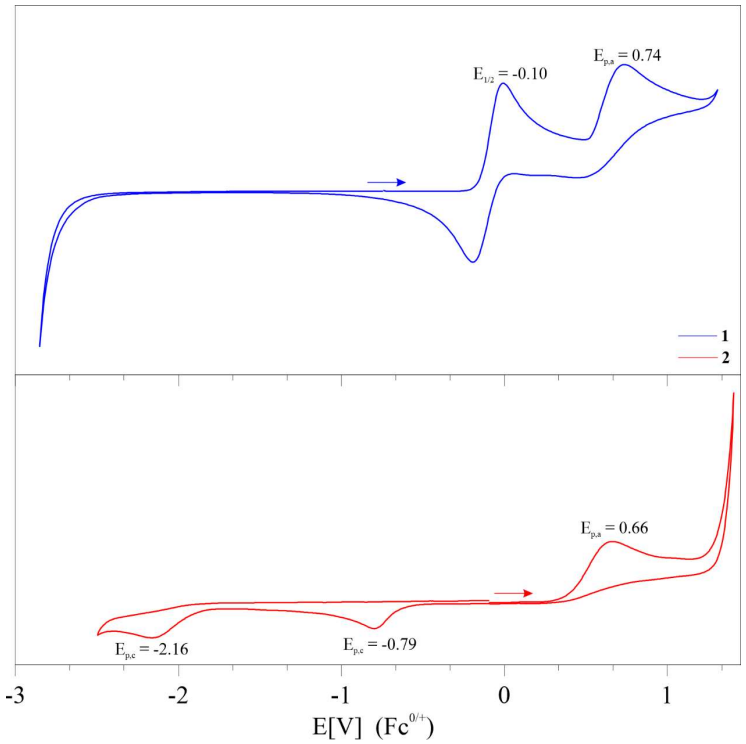


Figure S21. Cyclic voltammograms of solutions (1 mM) in DCM with [^{n}Bu$_4$N][B(3,5-(CF$_3$)$_2$-C$_6$H$_3$)$_4$] (100 mM) as the electrolyte. **1** shows two oxidation events, while one is observed for **2**.

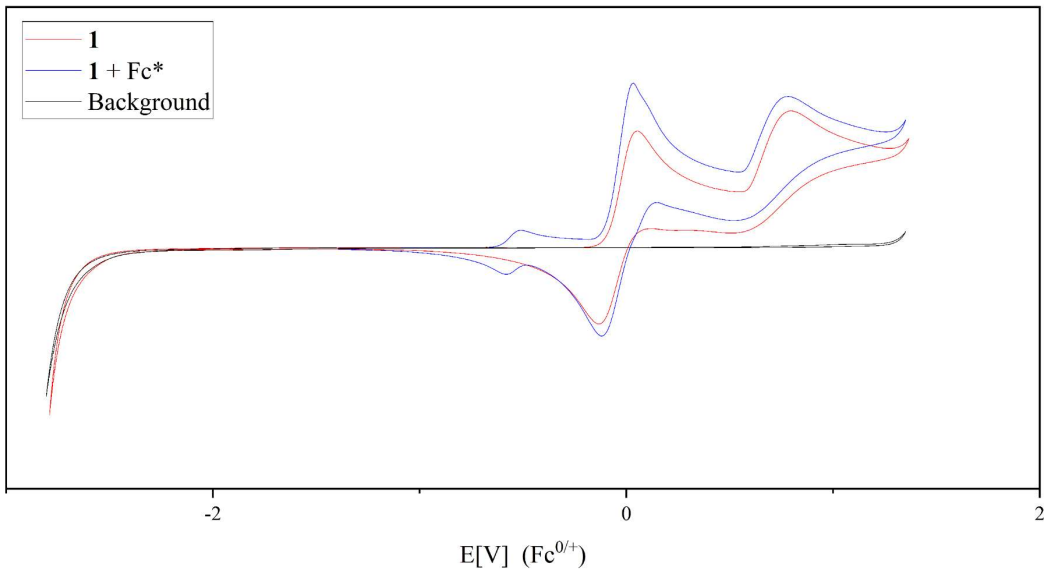


Figure S22. Cyclic voltammogram of (Trip$_2$Sb)$_2$Naph (**1**) in DCM solution (1 mM) at ambient temperature containing [^{n}Bu$_4$N][B(3,5-(CF$_3$)$_2$-C$_6$H$_3$)$_4$] (50 mM) as electrolyte and Fc* as the internal standard ($E_{1/2}$ –0.545 V vs Fc$^{0/+}$).[5]

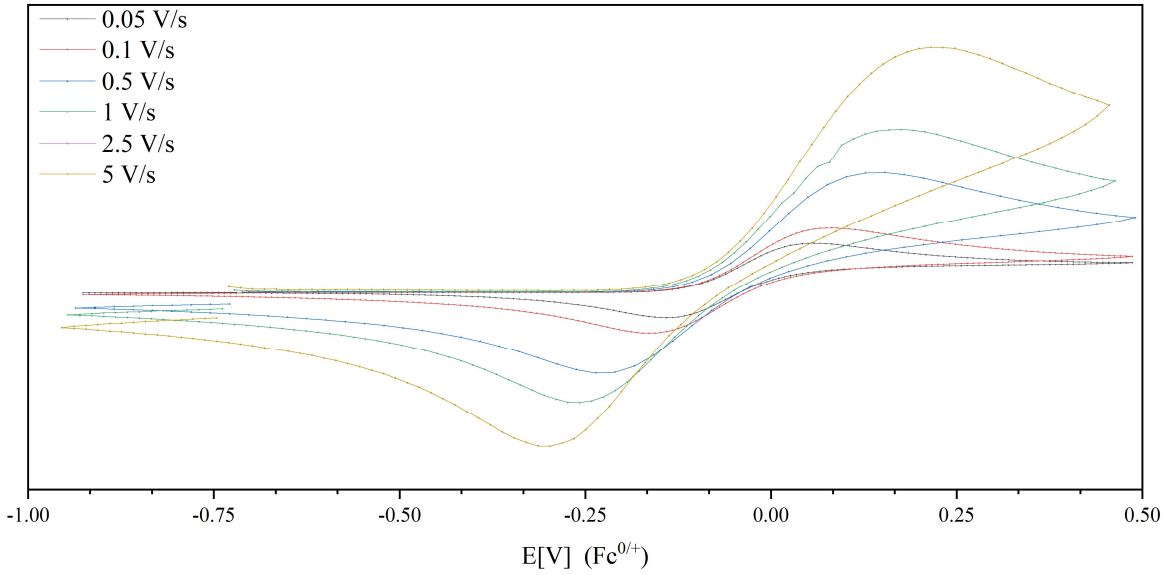


Figure S23. Cyclic voltammogram of $(Trip_2Sb)_2Naph$ (**1**) in DCM solution (1 mM) at ambient temperature containing $[^nBu_4N][B(3,5\text{-}(CF_3)_2\text{-}C_6H_3)_4]$ (50 mM) as electrolyte at varying scan rate showing the pseudoreversible oxidation event. Values are referenced to Fc. Fc* was used as the internal standard ($E_{1/2}$ –0.545 V vs $Fc^{0/+}$).[5]

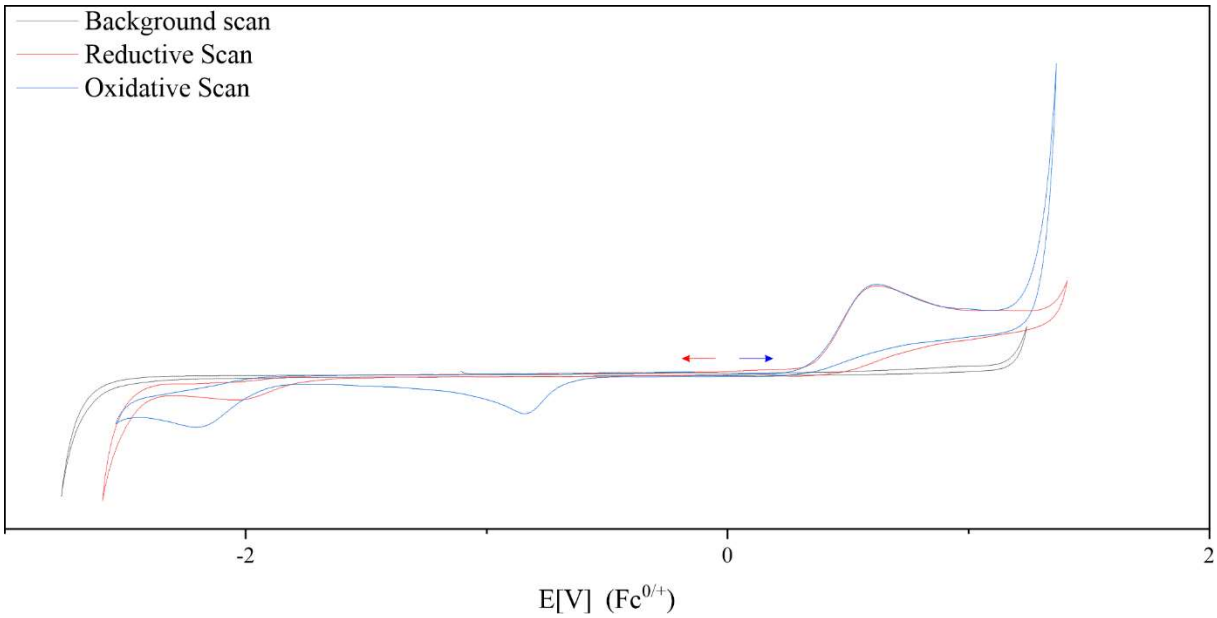


Figure S24. Cyclic voltammogram of $(Trip_2Bi)_2Naph$ (**2**) in DCM solution (1 mM) at ambient temperature containing $[^nBu_4N][B(3,5\text{-}(CF_3)_2\text{-}C_6H_3)_4]$ (50 mM) as electrolyte. The blue graph shows the scan in oxidative direction, while the red graph was performed in reductive direction. Values are referenced to Fc.

II. Crystallographic Details

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data of **1** (alf_116_d) and **3** (alf_121_d) were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) those of **2** (alf_155) and **4** (alf_146_b) on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, micro-focus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-2013)[6] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[7,8]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups. In **2** (alf_155) an isopropyl group is disordered over two positions. Its bond lengths and angles were restrained to be equal (SADI). The atoms were refined with common displacement parameters (EADP) to which RIGU restraints were applied. In **3** (alf_121_d) an isopropyl group is disordered over two positions. Its bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints were applied to its anisotropic displacement parameters. The high residual electron density in **2** and **4** is likely caused by absorption. Several methods and parameters were tried to improve the absorption correction, however, the residual density could not be reduced any further. The highest residual density maxima in **3** are a straight line with the heavy atoms and evenly spaced thus they are likely artifacts caused by Fourier series truncation.

CCDC-2157418 (**1**, alf_116_D), -2157419 (**2**, alf_155), -2157420 (**3**, alf_121_d), and -2157421 (**4**, alf_146_b) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3. Single crystal X-ray diffraction data of **1**-**4**.

Compound (Identification code)	**1 (alf_116_Dm)**	**2 (alf_155m)**	**3 (alf_121_dm)**	**4 (alf_146_bm)**
Empirical formula	$C_{70}H_{98}Sb_2$	$C_{70}H_{98}Bi_2$	$C_{79}H_{75}BF_{20}Sb_2$	$C_{40}H_{52}Sb_2$
M [g/mol]	1182.98	1357.44	1658.70	776.31
Crystal size [mm]	0.422 x 0.356 x 0.184	0.416 × 0.155 × 0.118	0.428 × 0.417 × 0.250	0.312 × 0.230 × 0.104
T [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	orthorhombic	monoclinic	triclinic	orthorhombic
Space group	$P2_12_12$	$C2/c$	$P\bar{1}$	$Pbca$
a [Å]	15.8867(7)	34.169(3)	14.118(3)	15.8584(15)
b [Å]	14.0109(7)	10.4618(8)	15.623(3)	17.1790(15)
c [Å]	14.5536(7)	18.2971(14)	17.104(3)	26.761(2)
α [°]	90	90	82.723(8)	90
β [°]	90	110.0432(19)	80.545(8)	90
γ [°]	90	90	78.391(8)	90
V [Å^3]	3239.4(3)	6144.4(8)	3627.9(12)	7290.6(11)
Z	2	4	2	8
D_{calc} [g·cm^{-3}]	1.213	1.467	1.518	1.415
μ(MoK_α [mm^{-1}])	0.871	11.390 (CuK_α)	0.840	11.920
Transmissions	0.75/0.66	0.75/0.44	0.75/0.62	0.75/0.35
F(000)	1240	2736	1672	3152
Index ranges	$-26 \le h \le 26$	$-42 \le h \le 42$	$-21 \le h \le 21$	$-16 \le h \le 19$
	$-23 \le k \le 23$	$-13 \le k \le 13$	$-24 \le k \le 24$	$-21 \le k \le 21$
	$-24 \le l \le 24$	$-20 \le l \le 22$	$-26 \le l \le 26$	$-34 \le l \le 33$
Θ_{max} [°]	36.632	80.540	33.920	80.951
Reflections collected	172477	70130	230758	100079
Independent reflections	16019	6421	28346	7676
R_{int}	0.0225	0.0607	0.0494	0.0652
Refined parameters	338	338	958	401
R_1 [$I > 2\sigma(I)$]	0.0162	0.0491	0.0324	0.0610
wR_2 [all data]	0.0422	0.1341	0.0769	0.1613
X(Flack)	–0.0183(19)	-	-	-
GooF	1.087	1.102	1.125	1.135
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.980/–0.558	6.445/–2.252	2.988/–1.085	3.216/–1.648

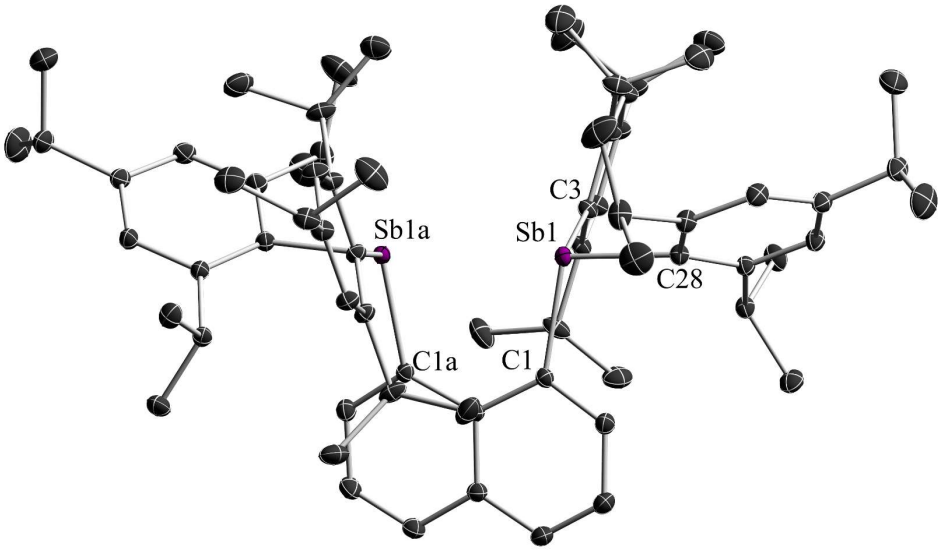


Figure S25. Solid-state structure of **1**. Displacement ellipsoids drawn at 50 % probability levels. The H atoms are omitted for clarity.

Table S4. Bond lengths [Å] of **1**.

Sb1-C1	2.1769(11)	C12-C34	1.5240(15)
Sb1-C28	2.1902(10)	C13-C30	1.527(2)
Sb1-C3	2.2019(11)	C13-C29	1.531(2)
Sb1-Sb1#1	3.2327(2)	C14-C15	1.4007(15)
C1-C2	1.3805(16)	C14-C19	1.5205(16)
C1-C4	1.4447(12)	C15-C16	1.3927(17)
C2-C7	1.4119(17)	C16-C17	1.3908(16)
C3-C14	1.4118(15)	C16-C22	1.5147(16)
C3-C18	1.4167(16)	C17-C18	1.3991(16)
C4-C5	1.433(2)	C18-C25	1.5255(16)
C5-C6	1.4206(14)	C19-C20	1.534(2)
C5-C6#1	1.4207(14)	C19-C21	1.534(2)
C6-C7	1.3676(18)	C22-C24	1.527(2)
C8-C9	1.3991(17)	C22-C23	1.535(2)
C8-C28	1.4179(15)	C25-C27	1.532(2)
C8-C13	1.5252(17)	C25-C26	1.533(2)
C9-C10	1.3905(17)	C31-C32	1.526(2)
C10-C11	1.3918(16)	C31-C33	1.534(2)
C10-C31	1.5169(17)	C34-C36	1.5350(17)
C11-C12	1.4004(15)	C34-C35	1.5374(17)
C12-C28	1.4094(15)		

Table S5. Bond angles [°] of **1**.

C1-Sb1-C28	101.51(4)	C9-C8-C13	117.29(10)	C17-C18-C25	116.13(10)
C1-Sb1-C3	106.84(4)	C28-C8-C13	123.22(10)	C3-C18-C25	124.08(10)
C28-Sb1-C3	97.64(4)	C10-C9-C8	122.02(10)	C14-C19-C20	113.12(11)
C1-Sb1-Sb1#1	80.89(3)	C9-C10-C11	117.67(10)	C14-C19-C21	111.38(11)
C28-Sb1-Sb1#1	167.59(3)	C9-C10-C31	121.32(10)	C20-C19-C21	109.90(10)
C3-Sb1-Sb1#1	93.23(3)	C11-C10-C31	121.00(11)	C16-C22-C24	110.37(11)
C2-C1-C4	119.58(10)	C10-C11-C12	122.43(10)	C16-C22-C23	112.29(11)
C2-C1-Sb1	115.24(8)	C11-C12-C28	119.18(9)	C24-C22-C23	110.96(12)
C4-C1-Sb1	125.19(8)	C11-C12-C34	117.61(10)	C18-C25-C27	111.30(11)
C1-C2-C7	122.32(11)	C28-C12-C34	123.19(9)	C18-C25-C26	111.81(11)
C14-C3-C18	118.65(10)	C8-C13-C30	112.63(12)	C27-C25-C26	111.60(11)
C14-C3-Sb1	127.81(8)	C8-C13-C29	110.79(12)	C12-C28-C8	118.95(10)
C18-C3-Sb1	113.47(8)	C30-C13-C29	110.87(13)	C12-C28-Sb1	125.01(7)
C5-C4-C1#1	117.12(7)	C15-C14-C3	119.38(10)	C8-C28-Sb1	114.17(8)
C5-C4-C1	117.12(7)	C15-C14-C19	116.10(10)	C10-C31-C32	112.22(12)
C1#1-C4-C1	125.75(13)	C3-C14-C19	124.51(10)	C10-C31-C33	110.77(11)
C6-C5-C6#1	119.07(15)	C16-C15-C14	122.53(10)	C32-C31-C33	110.86(13)
C6-C5-C4	120.46(7)	C17-C16-C15	117.51(10)	C12-C34-C36	112.51(9)
C6#1-C5-C4	120.46(7)	C17-C16-C22	121.86(10)	C12-C34-C35	111.29(9)
C7-C6-C5	120.92(11)	C15-C16-C22	120.59(10)	C36-C34-C35	109.40(10)
C6-C7-C2	119.09(11)	C16-C17-C18	122.13(10)		
C9-C8-C28	119.47(10)	C17-C18-C3	119.78(10)		

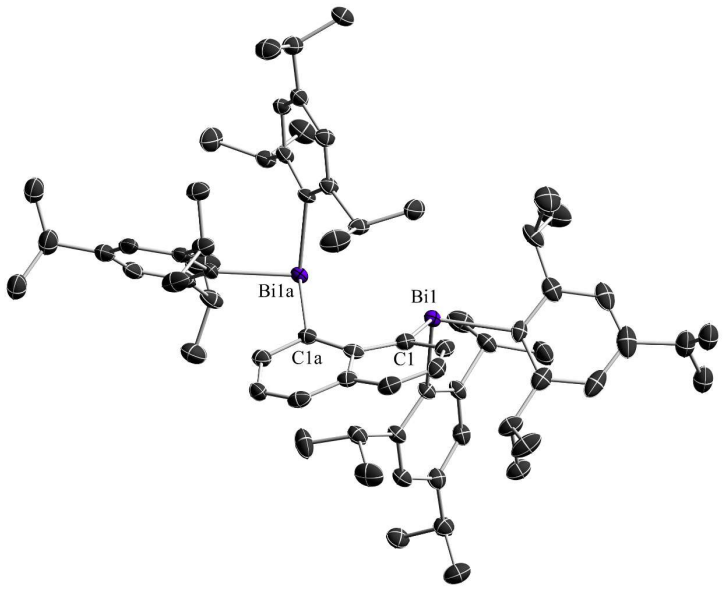


Figure S26. Solid-state structure of **2**. Displacement ellipsoids are drawn at a 50 % probability level. The H atoms are omitted for clarity.

Table S4. Bond lengths [Å] of **2**.

Bi1-C11	2.318(4)	C102-C112	1.533(8)
Bi1-C12	2.326(5)	C132-C152	1.526(7)
Bi1-C13	2.326(5)	C132-C142	1.528(7)
Bi1-Bi1#1	3.6742(4)	C13-C23	1.409(8)
C11-C21	1.380(6)	C13-C63	1.417(8)
C11-C61	1.441(5)	C23-C33	1.414(7)
C21-C31	1.411(7)	C23-C73	1.522(8)
C31-C41	1.356(8)	C33-C43	1.396(10)
C41-C51	1.416(7)	C43-C53	1.346(11)
C51-C61	1.435(9)	C43-C103	1.537(11)
C12-C62	1.403(7)	C43-C10'3	1.66(2)
C12-C22	1.408(7)	C53-C63	1.390(8)
C22-C32	1.394(7)	C63-C133	1.514(8)
C22-C72	1.515(6)	C73-C83	1.539(7)
C32-C42	1.409(7)	C73-C93	1.546(7)
C42-C52	1.371(7)	C103-C123	1.432(10)
C42-C102	1.521(7)	C103-C113	1.471(10)
C52-C62	1.405(7)	C10'3-C12'3	1.429(16)
C62-C132	1.524(6)	C10'3-C11'3	1.440(15)
C72-C82	1.525(8)	C133-C143	1.532(7)
C72-C92	1.532(7)	C133-C153	1.537(8)
C102-C122	1.520(7)		

Table S5. Bond angles [°] of **2**.

C11-Bi1-C12	107.53(16)	C22-C32-C42	121.8(4)	C43-C33-C23	121.4(6)
C11-Bi1-C13	96.72(17)	C52-C42-C32	117.4(4)	C53-C43-C33	118.3(6)
C12-Bi1-C13	92.31(19)	C52-C42-C102	121.1(4)	C53-C43-C103	116.4(7)
C11-Bi1-Bi1#1	74.73(11)	C32-C42-C102	121.5(4)	C33-C43-C103	125.3(7)
C12-Bi1-Bi1#1	102.87(13)	C42-C52-C62	122.7(4)	C53-C43-C10'3	145.7(10)
C13-Bi1-Bi1#1	164.20(13)	C12-C62-C52	119.1(4)	C33-C43-C10'3	95.2(10)
C21-C11-C61	119.2(4)	C12-C62-C132	123.9(4)	C43-C53-C63	123.2(6)
C21-C11-Bi1	113.3(3)	C52-C62-C132	117.0(4)	C53-C63-C13	119.5(5)
C61-C11-Bi1	127.5(3)	C22-C72-C82	113.4(4)	C53-C63-C133	116.3(5)
C11-C21-C31	121.7(5)	C22-C72-C92	110.5(4)	C13-C63-C133	124.1(5)
C41-C31-C21	119.8(5)	C82-C72-C92	110.4(5)	C23-C73-C83	111.7(4)
C31-C41-C51	120.5(5)	C122-C102-C42	112.2(4)	C23-C73-C93	110.2(5)
C41#1-C51-C41	119.8(7)	C122-C102-C112	110.4(4)	C83-C73-C93	108.8(4)
C41#1-C51-C61	120.1(3)	C42-C102-C112	112.1(4)	C123-C103-C113	124.6(8)
C41-C51-C61	120.1(3)	C62-C132-C152	113.2(4)	C123-C103-C43	112.9(7)
C51-C61-C11	116.9(3)	C62-C132-C142	109.7(4)	C113-C103-C43	110.3(7)
C51-C61-C11#1	116.9(3)	C152-C132-C142	111.3(5)	C12'3-C10'3-C11'3	120.4(17)
C11-C61-C11#1	126.3(6)	C23-C13-C63	118.4(5)	C12'3-C10'3-C43	117.3(15)
C62-C12-C22	119.2(4)	C23-C13-Bi1	124.4(4)	C11'3-C10'3-C43	120.0(15)
C62-C12-Bi1	115.3(3)	C63-C13-Bi1	116.7(4)	C63-C133-C143	111.1(5)
C32-C22-C12	119.4(4)	C13-C23-C33	119.1(5)	C63-C133-C153	112.5(5)
C32-C22-C72	118.4(4)	C13-C23-C73	123.4(5)	C143-C133-C153	109.5(5)
C12-C22-C72	122.2(4)	C33-C23-C73	117.4(5)		

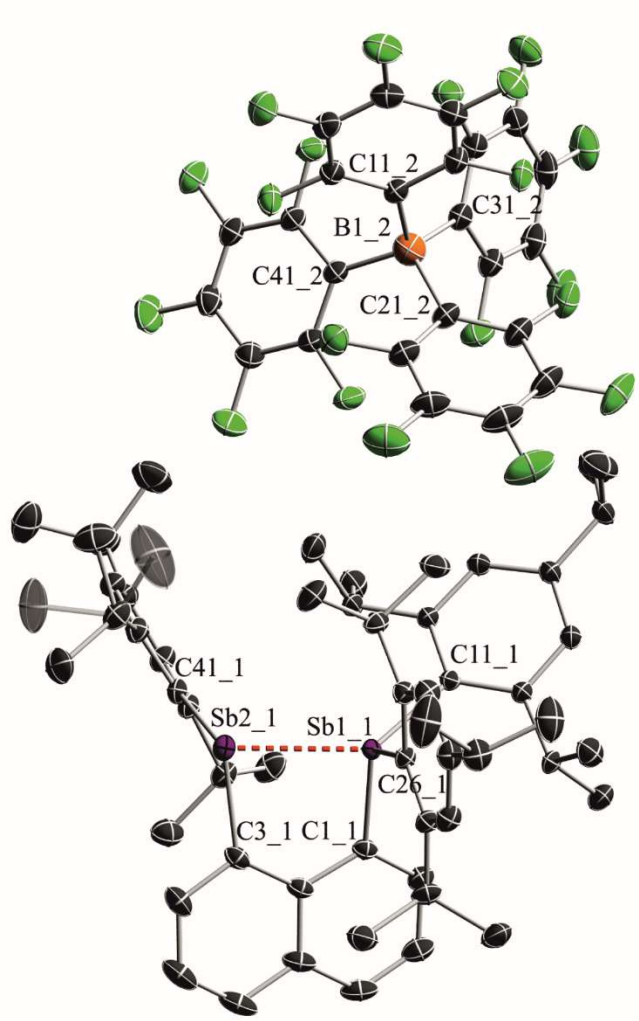


Figure S27. Solid-state structure of **3**. Displacement ellipsoids drawn at 50 % probability levels. The hydrogen atoms are omitted for clarity.

Table S6. Bond lengths [Å] of **3**.

Sb11-C11	2.1170(15)	C291-C351	1.518(2)	F332-C342	1.345(2)
Sb11-C111	2.1367(15)	C301-C311	1.397(2)	F342-C352	1.345(2)
Sb11-C261	2.1465(15)	C311-C381	1.517(2)	F352-C362	1.348(2)
Sb11-Sb21	2.7980(4)	C321-C341	1.532(2)	F412-C422	1.349(2)
Sb21-C31	2.1647(17)	C321-C331	1.534(3)	F422-C432	1.345(2)
Sb21-C411	2.1708(16)	C351-C361	1.506(3)	F432-C442	1.344(2)
C11-C101	1.375(2)	C351-C371	1.512(3)	F442-C452	1.341(2)
C11-C21	1.428(2)	C381-C401	1.531(3)	F452-C462	1.347(2)
C21-C71	1.430(2)	C381-C391	1.536(3)	C112-C162	1.390(2)
C21-C31	1.433(2)	C411-C461	1.407(2)	C112-C122	1.397(2)
C31-C41	1.381(2)	C411-C421	1.421(2)	C112-B12	1.651(3)
C41-C51	1.411(3)	C421-C431	1.391(2)	C122-C132	1.381(2)
C51-C61	1.362(3)	C421-C471	1.524(2)	C132-C142	1.375(3)
C61-C71	1.419(3)	C431-C441	1.391(2)	C142-C152	1.376(3)

C71-C81	1.415(3)	C441-C451	1.388(2)	C152-C162	1.390(2)
C81-C91	1.366(3)	C441-C501	1.517(2)	C212-C222	1.390(2)
C91-C101	1.410(2)	C451-C461	1.397(2)	C212-C262	1.391(3)
C111-C121	1.405(2)	C461-C531	1.512(2)	C212-B12	1.651(3)
C111-C161	1.411(2)	C471-C49'1	1.468(14)	C222-C232	1.385(3)
C121-C131	1.396(2)	C471-C481	1.507(3)	C232-C242	1.366(4)
C121-C171	1.519(2)	C471-C491	1.536(3)	C242-C252	1.381(3)
C131-C141	1.393(2)	C471-C48'1	1.581(13)	C252-C262	1.380(3)
C141-C151	1.389(2)	C501-C521	1.516(3)	C312-C322	1.387(3)
C141-C201	1.515(2)	C501-C511	1.524(3)	C312-C362	1.392(2)
C151-C161	1.400(2)	C531-C551	1.530(3)	C312-B12	1.652(3)
C161-C231	1.522(2)	C531-C541	1.538(3)	C322-C332	1.388(3)
C171-C181	1.527(3)	F122-C122	1.3471(19)	C332-C342	1.372(3)
C171-C191	1.529(3)	F132-C132	1.341(2)	C342-C352	1.372(3)
C201-C221	1.525(3)	F142-C142	1.342(2)	C352-C362	1.383(3)
C201-C211	1.528(3)	F152-C152	1.339(2)	C412-C462	1.389(2)
C231-C251	1.522(2)	F162-C162	1.347(2)	C412-C422	1.395(2)
C231-C241	1.532(2)	F212-C222	1.346(2)	C412-B12	1.653(3)
C261-C311	1.406(2)	F222-C232	1.350(3)	C422-C432	1.381(2)
C261-C271	1.412(2)	F232-C242	1.343(2)	C432-C442	1.374(3)
C271-C281	1.392(2)	F242-C252	1.340(3)	C442-C452	1.375(3)
C271-C321	1.519(2)	F252-C262	1.350(2)	C452-C462	1.386(3)
C281-C291	1.388(2)	F312-C322	1.348(2)		
C291-C301	1.385(2)	F322-C332	1.343(2)		

Table S7. Bond angles [°] of **3**.

C11-Sb11-C111	113.07(6)	C281-C291-C351	121.84(16)	C222-C212-B12	126.72(17)
C11-Sb11-C261	113.33(6)	C291-C301-C311	122.66(15)	C262-C212-B12	118.79(15)
C111-Sb11-C261	102.86(6)	C301-C311-C261	117.67(14)	F212-C222-C232	114.62(17)
C11-Sb11-Sb21	91.26(4)	C301-C311-C381	117.72(14)	F212-C222-C212	121.95(17)
C111-Sb11-Sb21	137.25(4)	C261-C311-C381	124.57(14)	C232-C222-C212	123.4(2)
C261-Sb11-Sb21	98.29(4)	C271-C321-C341	112.48(14)	F222-C232-C242	120.67(19)
C31-Sb21-C411	107.08(6)	C271-C321-C331	111.18(15)	F222-C232-C222	119.2(2)
C31-Sb21-Sb11	80.51(4)	C341-C321-C331	111.43(15)	C242-C232-C222	120.1(2)
C411-Sb21-Sb11	106.31(4)	C361-C351-C371	110.98(19)	F232-C242-C232	120.9(2)
C101-C11-C21	121.81(14)	C361-C351-C291	113.21(16)	F232-C242-C252	119.9(2)
C101-C11-Sb11	122.65(12)	C371-C351-C291	110.91(16)	C232-C242-C252	119.23(18)
C21-C11-Sb11	115.24(11)	C311-C381-C401	113.30(15)	F242-C252-C262	120.8(2)
C11-C21-C71	116.93(15)	C311-C381-C391	110.32(15)	F242-C252-C242	120.19(19)
C11-C21-C31	124.35(14)	C401-C381-C391	110.94(15)	C262-C252-C242	119.0(2)
C71-C21-C31	118.72(14)	C461-C411-C421	120.11(14)	F252-C262-C252	115.97(18)
C41-C31-C21	119.49(15)	C461-C411-Sb21	126.25(11)	F252-C262-C212	119.62(16)
C41-C31-Sb21	114.95(13)	C421-C411-Sb21	113.47(11)	C252-C262-C212	124.40(19)

C21-C31-Sb21	125.54(11)	C431-C421-C411	118.42(15)	C322-C312-C362	113.49(16)
C31-C41-C51	121.21(18)	C431-C421-C471	119.20(15)	C322-C312-B12	126.62(15)
C61-C51-C41	120.26(17)	C411-C421-C471	122.33(15)	C362-C312-B12	119.73(16)
C51-C61-C71	120.91(17)	C441-C431-C421	122.29(15)	F312-C322-C312	121.37(16)
C81-C71-C61	121.29(16)	C451-C441-C431	118.18(15)	F312-C322-C332	114.89(17)
C81-C71-C21	119.49(16)	C451-C441-C501	120.58(15)	C312-C322-C332	123.74(17)
C61-C71-C21	119.22(17)	C431-C441-C501	121.21(15)	F322-C332-C342	120.02(18)
C91-C81-C71	121.71(16)	C441-C451-C461	122.19(15)	F322-C332-C322	120.04(19)
C81-C91-C101	119.52(17)	C451-C461-C411	118.61(14)	C342-C332-C322	119.94(19)
C11-C101-C91	120.20(16)	C451-C461-C531	119.11(14)	F332-C342-C332	120.7(2)
C121-C111-C161	121.53(13)	C411-C461-C531	122.19(14)	F332-C342-C352	120.3(2)
C121-C111-Sb11	119.49(10)	C49'1-C471-C421	119.2(13)	C332-C342-C352	118.98(18)
C161-C111-Sb11	117.86(10)	C481-C471-C421	110.66(16)	F342-C352-C342	119.99(18)
C131-C121-C111	117.90(14)	C481-C471-C491	109.91(19)	F342-C352-C362	120.6(2)
C131-C121-C171	118.45(14)	C421-C471-C491	114.42(16)	C342-C352-C362	119.36(18)
C111-C121-C171	123.63(13)	C49'1-C471-C48'1	110.0(14)	F352-C362-C352	116.45(17)
C141-C131-C121	122.31(15)	C421-C471-C48'1	107.9(8)	F352-C362-C312	119.15(16)
C151-C141-C131	118.04(14)	C521-C501-C441	109.80(17)	C352-C362-C312	124.39(19)
C151-C141-C201	120.11(14)	C521-C501-C511	110.6(2)	C462-C412-C422	112.74(15)
C131-C141-C201	121.81(15)	C441-C501-C511	113.11(16)	C462-C412-B12	127.53(15)
C141-C151-C161	122.53(14)	C461-C531-C551	115.00(15)	C422-C412-B12	119.55(15)
C151-C161-C111	117.45(13)	C461-C531-C541	109.91(14	F412-C422-C432	116.00(15)
C151-C161-C231	117.79(13)	C551-C531-C541	109.85(15)	F412-C422-C412	119.25(15)
C111-C161-C231	124.69(13)	C162-C112-C122	113.55(15)	C432-C422-C412	124.74(16)
C121-C171-C181	112.18(14)	C162-C112-B12	127.48(15)	F422-C432-C442	119.49(16)
C121-C171-C191	111.04(14)	C122-C112-B12	118.69(14)	F422-C432-C422	120.88(17)
C181-C171-C191	109.83(15)	F122-C122-C132	116.09(15)	C442-C432-C422	119.63(17)
C141-C201-C221	113.24(16)	F122-C122-C112	119.08(15)	F432-C442-C432	120.57(18)
C141-C201-C211	109.45(17)	C132-C122-C112	124.82(16)	F432-C442-C452	120.88(18)
C221-C201-C211	110.68(18)	F132-C132-C142	119.95(17)	C432-C442-C452	118.54(17)
C161-C231-C251	112.69(14)	F132-C132-C122	121.23(17)	F442-C452-C442	119.20(18)
C161-C231-C241	109.82(14)	C142-C132-C122	118.80(17)	F442-C452-C462	120.84(19)
C251-C231-C241	110.89(14)	F142-C142-C132	120.21(18)	C442-C452-C462	119.95(18)
C311-C261-C271	121.05(13)	F142-C142-C152	120.36(17)	F452-C462-C452	114.77(16)
C311-C261-Sb11	124.31(11)	C132-C142-C152	119.42(16)	F452-C462-C412	120.95(16)
C271-C261-Sb11	114.64(10)	F152-C152-C142	119.78(16)	C452-C462-C412	124.28(17)
C281-C271-C261	118.27(14)	F152-C152-C162	120.27(17)	C112-B12-C212	100.46(13)
C281-C271-C321	117.59(14)	C142-C152-C162	119.95(16)	C112-B12-C312	112.42(14)
C261-C271-C321	124.14(13)	F162-C162-C152	115.47(15)	C212-B12-C312	113.81(13)
C291-C281-C271	122.00(15)	F162-C162-C112	121.15(15)	C112-B12-C412	114.02(13)
C301-C291-C281	118.30(15)	C152-C162-C112	123.38(16)	C212-B12-C412	113.65(14)
C301-C291-C351	119.85(16)	C222-C212-C262	113.82(17)	C312-B12-C412	102.97(13)

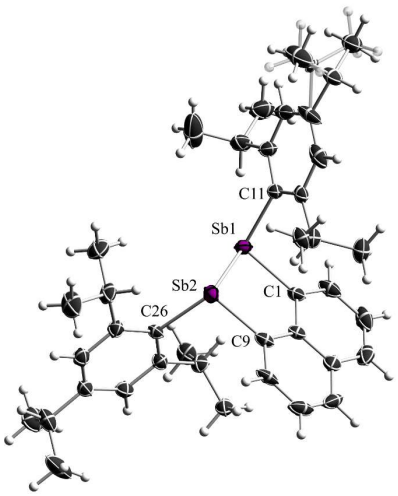


Figure S28. Solid-state structure of **4**. Displacement ellipsoids are drawn at a 50 % probability levels.

Table S8. Bond lengths [Å] of **4**.

Sb1-C1	2.149(6)	C16-C23	1.511(9)
Sb1-C11	2.196(6)	C17-C19	1.520(11)
Sb1-Sb2	2.7991(6)	C17-C18	1.526(13)
Sb2-C9	2.153(6)	C20-C21	1.487(10)
Sb2-C26	2.192(6)	C20-C22	1.508(10)
C1-C2	1.391(9)	C20'-C22	1.447(14)
C1-C10	1.440(8)	C20'-C21	1.480(14)
C2-C3	1.393(10)	C23-C24	1.530(9)
C3-C4	1.349(12)	C23-C25	1.534(9)
C4-C5	1.424(10)	C26-C27	1.408(8)
C5-C6	1.411(10)	C26-C31	1.411(8)
C5-C10	1.422(8)	C27-C28	1.390(8)
C6-C7	1.373(12)	C27-C32	1.525(8)
C7-C8	1.401(10)	C28-C29	1.380(9)
C8-C9	1.392(8)	C29-C30	1.397(9)
C9-C10	1.426(8)	C29-C35	1.520(9)
C11-C16	1.409(9)	C30-C31	1.387(9)
C11-C12	1.411(9)	C31-C38	1.535(8)
C12-C13	1.391(10)	C32-C34	1.524(8)
C12-C17	1.539(10)	C32-C33	1.535(9)
C13-C14	1.391(12)	C35-C36	1.517(11)
C14-C15	1.369(11)	C35-C37	1.518(12)
C14-C20'	1.54(2)	C38-C40	1.520(10)
C14-C20	1.554(10)	C38-C39	1.530(9)
C15-C16	1.397(9)		

Table S9. Bond angles [°] of **4**.

C1-Sb1-C11	100.7(2)	C16-C11-Sb1	124.5(4)	C16-C23-C25	112.1(5)
C1-Sb1-Sb2	86.18(16)	C12-C11-Sb1	116.4(5)	C24-C23-C25	111.4(5)
C11-Sb1-Sb2	100.81(17)	C13-C12-C11	118.8(7)	C27-C26-C31	119.6(5)
C9-Sb2-C26	99.9(2)	C13-C12-C17	119.2(6)	C27-C26-Sb2	124.5(4)
C9-Sb2-Sb1	85.91(15)	C11-C12-C17	122.0(6)	C31-C26-Sb2	115.4(4)
C26-Sb2-Sb1	102.91(15)	C14-C13-C12	122.6(7)	C28-C27-C26	118.5(5)
C2-C1-C10	119.1(6)	C15-C14-C13	117.8(6)	C28-C27-C32	117.9(5)
C2-C1-Sb1	118.4(5)	C15-C14-C20’	143.2(11)	C26-C27-C32	123.6(5)
C10-C1-Sb1	122.3(4)	C13-C14-C20’	98.2(11)	C29-C28-C27	123.0(6)
C1-C2-C3	122.0(6)	C15-C14-C20	115.6(8)	C28-C29-C30	117.7(6)
C4-C3-C2	120.1(6)	C13-C14-C20	126.5(8)	C28-C29-C35	123.0(6)
C3-C4-C5	121.0(6)	C14-C15-C16	122.2(7)	C30-C29-C35	119.3(6)
C6-C5-C10	118.3(6)	C15-C16-C11	119.5(6)	C31-C30-C29	121.8(6)
C6-C5-C4	121.8(6)	C15-C16-C23	116.8(6)	C30-C31-C26	119.3(5)
C10-C5-C4	119.8(6)	C11-C16-C23	123.7(5)	C30-C31-C38	118.9(5)
C7-C6-C5	121.8(6)	C19-C17-C18	111.1(7)	C26-C31-C38	121.7(5)
C6-C7-C8	119.6(6)	C19-C17-C12	113.1(6)	C34-C32-C27	113.5(5)
C9-C8-C7	121.2(6)	C18-C17-C12	110.1(8)	C34-C32-C33	109.8(5)
C8-C9-C10	119.1(6)	C21-C20-C22	113.8(8)	C27-C32-C33	111.2(5)
C8-C9-Sb2	118.0(5)	C21-C20-C14	112.0(7)	C36-C35-C37	110.5(7)
C10-C9-Sb2	122.9(4)	C22-C20-C14	108.4(7)	C36-C35-C29	111.5(6)
C5-C10-C9	119.8(5)	C22-C20’-C21	118.0(13)	C37-C35-C29	112.1(6)
C5-C10-C1	117.9(5)	C22-C20’-C14	112.2(13)	C40-C38-C39	110.3(6)
C9-C10-C1	122.2(5)	C21-C20’-C14	113.0(12)	C40-C38-C31	110.1(6)
C16-C11-C12	119.0(6)	C16-C23-C24	112.3(5)	C39-C38-C31	114.7(6)

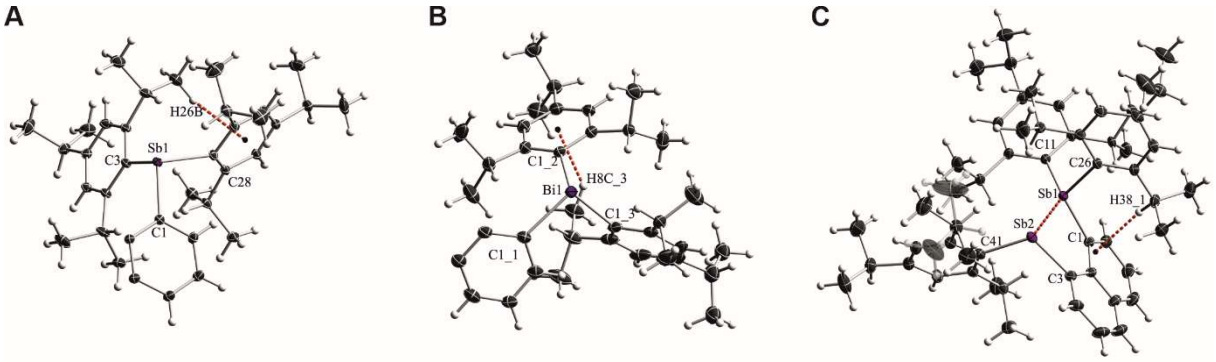


Figure S29. Observed intramolecular CH-π contacts in **1** (A), **2** (B) and **3** (C).

III. Computational Details

All calculations were performed by using the program packages Gaussian 16[9], Amsterdam Density Functional[10] (ADF) and AIMAll[11]. The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP[12] together with the dispersion correction with Becke-Johnson damping[13] (D3BJ) using Gaussian 16. The basis set def2-TZVP was applied. For all structures C1 symmetry was applied. Frequency calculations were carried out at each of the stationary points to verify the nature of the stationary point. It turned out that all stationary states except of **1** have none imaginary frequency. However, the negative frequency in **1** has a mode below 1.6 cm^{-1}. Natural bond orbital analysis was performed using the NBO[14] version 3.1 implemented in Gaussian 16. The bond energy analysis calculations[15] (B3LYP-D3BJ/TZP) were carried out using Amsterdam Density Functional (ADF). Quantum theory of atoms in molecules (QTAIM)[16] analyses (B3LYP-D3BJ/TZP and B3LYP-D3BJ/def2-TZVP) were performed using Amsterdam Density Functional (ADF) and AIMAll. Interacting quantum atoms (IQA)[17] calculations were carried out using ADF.

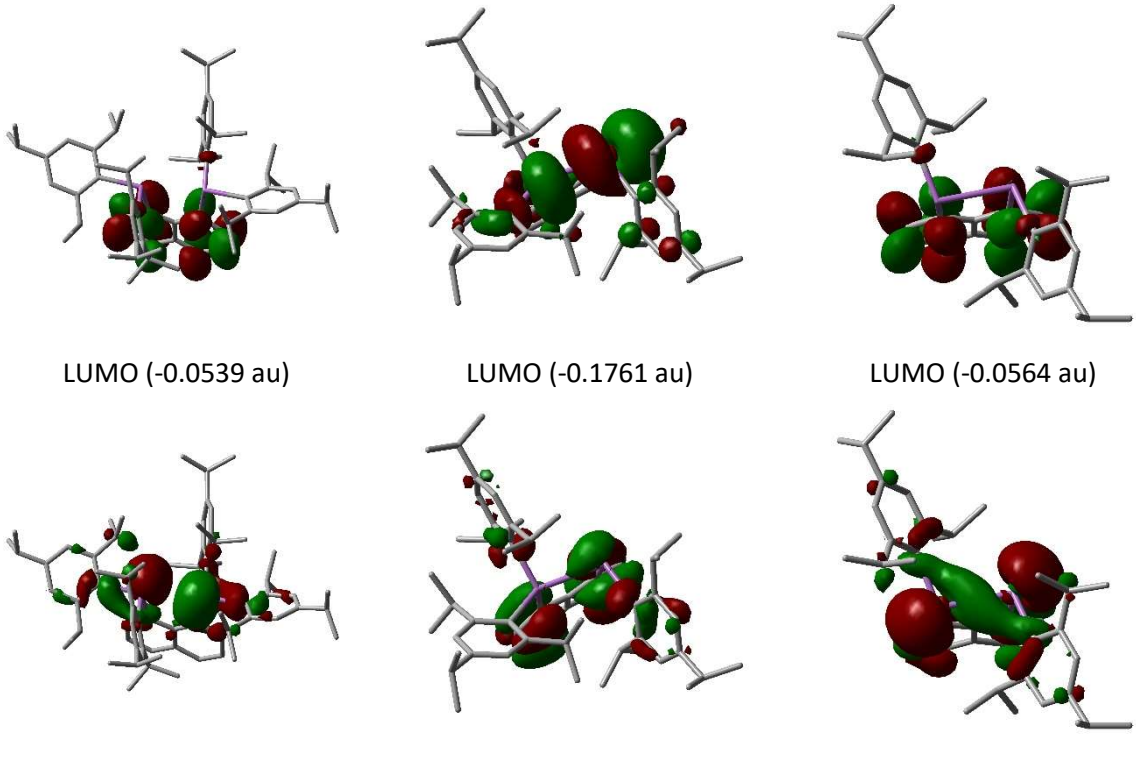
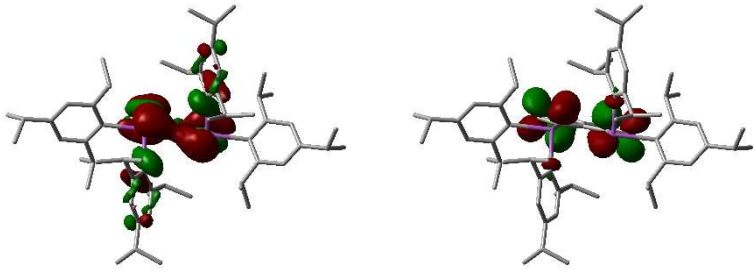
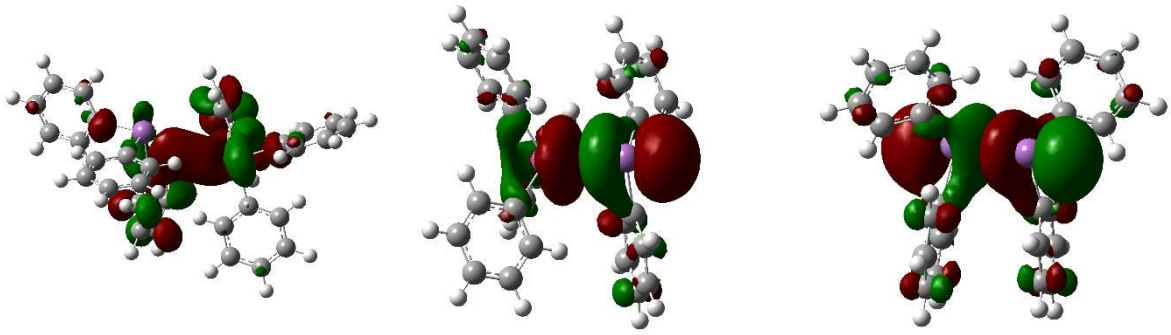


Figure S30. Selected orbitals of **1** (left), **3** (middle), and **4** (right) calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03). Hydrogen atoms are omitted for clarity.

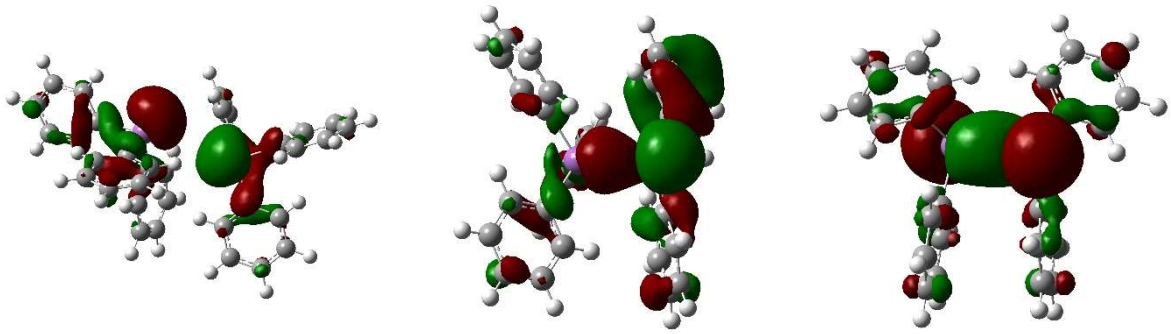


HOMO (-0.2103 au) LUMO (-0.0511 au)

Figure S31. Selected orbitals of **2** calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03).



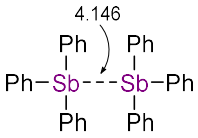
LUMO (-0.0391 au) LUMO (-0.1918 au) LUMO (-0.0573 au)



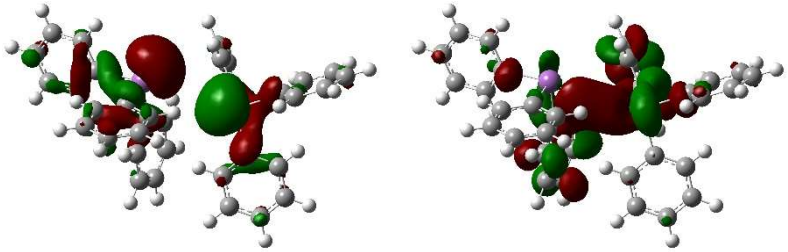
HOMO (-0.2234 au) HOMO (-0.3492 au) HOMO (-0.2086 au)

S1 **S3** **S4**

Figure S32. Selected orbitals of **S1** (left), **S3** (middle), and **S4** (right) calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03).

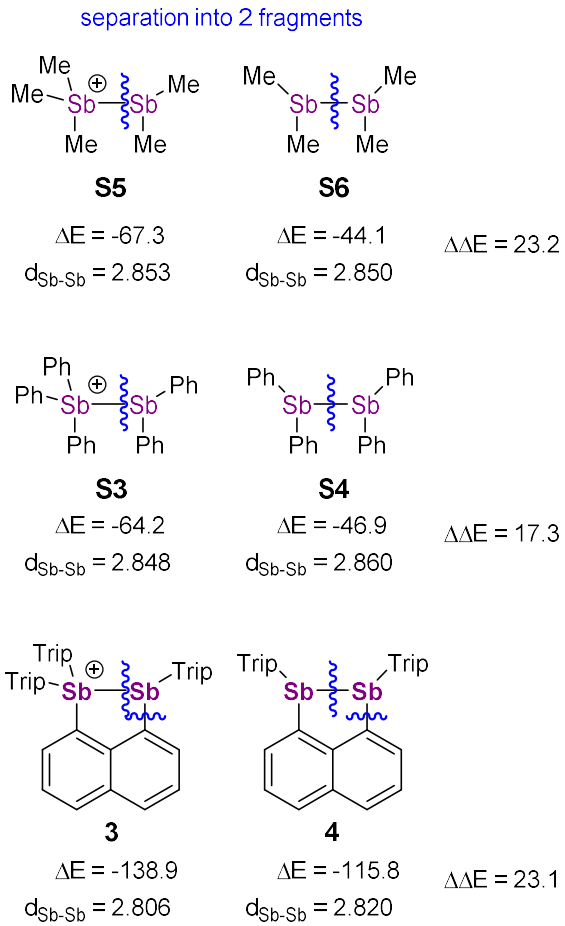


S2



HOMO (-0.2234 au) LUMO (-0.0391 au)

Figure S33. Selected orbitals of **S2** calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03).



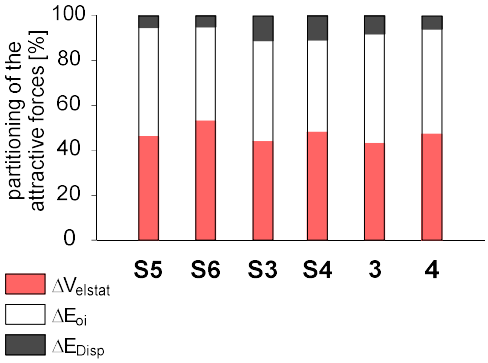
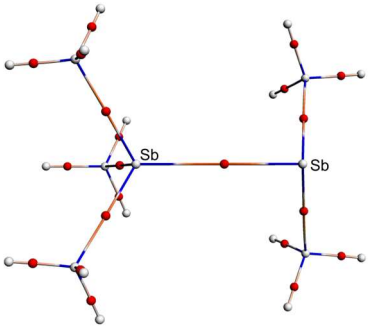


Figure S34. Calculated (B3LYP-D3BJ/def2-TZVP) Sb···Sb distances [Å] for **S3**-**S6**, **3** and **4**. The percentage contributions of the attractive forces (ΔV_{elstat}, ΔE_{oi} and ΔE_{Disp}) and the total binding energies (ΔE in kcal mol^{-1}) between the pictured fragments stem from bond energy analysis calculations (B3LYP-D3BJ/TZP).

a)



b)

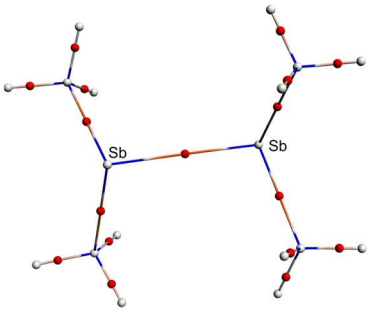
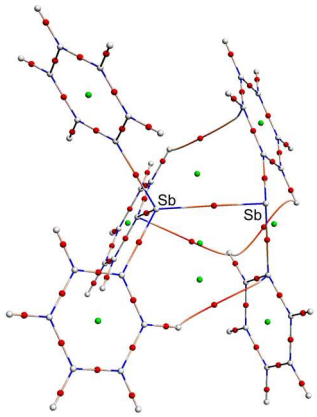


Figure S35. Molecular graphs of **S5** (a) and **S6** (b) showing the bond paths (lines) and the different critical points: nuclear (white dots) and bond (red dots) critical points (B3LYP-D3BJ/TZP).

a)



b)

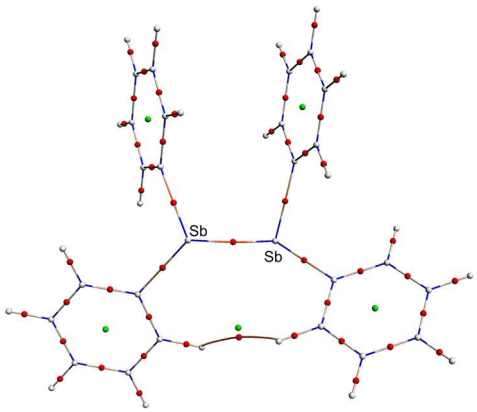
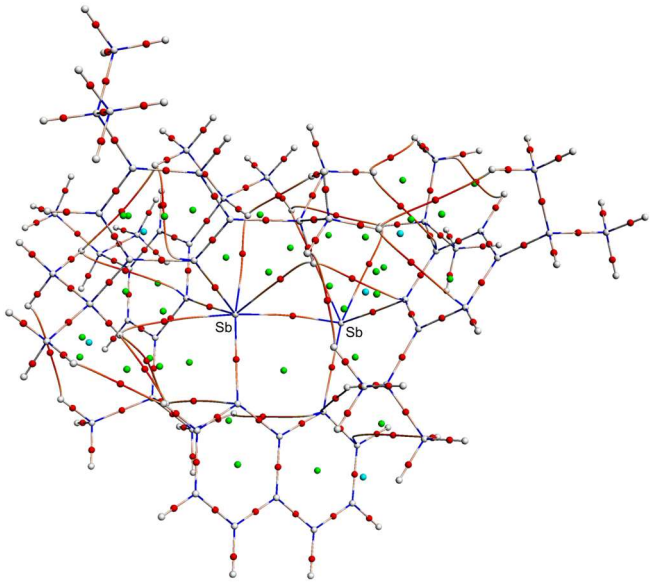


Figure S36. Molecular graphs of **S3** (a) and **S4** (b) showing the bond paths (lines) and the different critical points: nuclear (white dots), bond (red dots) and ring (green dots) critical points (B3LYP-D3BJ/TZP).

a)



b)

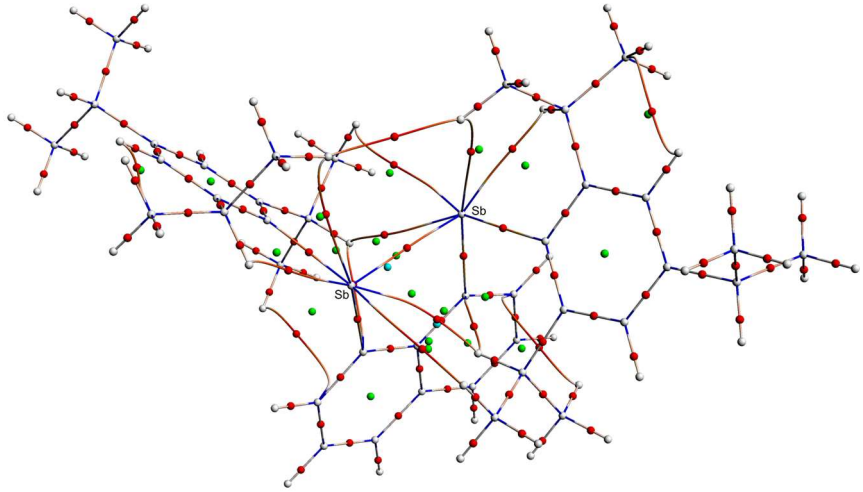


Figure S37. Molecular graphs of **3** (a) and **4** (b) showing the bond paths (lines) as well as the nuclear (white dots), bond (red dots), ring (green dots) and cage (blue dots) critical points (B3LYP-D3BJ/TZP).

Table S10. Sb···Sb distances [Å] and distances [Å] between the bond critical points (BCP) of the Sb--Sb interaction and the Sb atoms in **S3**-**S6**, **3** and **4** (B3LYP-D3BJ/TZP).

	$d_{(Sb1\text{-}Sb2)}$ [Å]	$d_{(Sb1\text{-}BCP)}$ [Å]	$d_{(BCP\text{-}Sb2)}$ [Å]	$\alpha_{(Sb1\text{-}BCP\text{-}Sb2)}$ [°]
S5	2.853	1.360	1.497	174
S6	2.850	1.425	1.425	179
S3	2.848	1.134	1.767	157
S4	2.860	1.440	1.440	167
3	2.806	1.114	1.771	152
4	2.820	1.395	1.425	179

Table S11. Topological and energetic properties of the electron density $\rho(\mathbf{r})$ calculated at the bond critical points of the Sb--Sb interaction for **S3**-**S6**, **3** and **4**. The electron density (ρ_{CP}), the Laplacian of the electron density ($\nabla^2\rho_{CP}$), the electron kinetic (G_{CP}), potential (V_{CP}) and total (H_{CP}) energy densities at the critical points are given in a.u. (B3LYP-D3BJ/TZP).

	ρ_{CP}	$\nabla^2\rho_{CP}$	G_{CP}	V_{CP}	H_{CP}
S5	0.05676898	-0.00116968	0.02388120	-0.04805483	-0.02417362
S6	0.05943471	-0.01539731	0.02342353	-0.05069639	-0.02727286
S3	0.05742284	-0.00369247	0.02392469	-0.04877250	-0.02484781
S4	0.05804408	-0.01390003	0.02266751	-0.04881002	-0.02614252
3	0.06050129	-0.00762143	0.02550149	-0.05290833	-0.02740684
4	0.06116809	-0.01641720	0.02452909	-0.05316248	-0.02863339

Table S12. Interaction energies ($V_{inter(Total)}$) between the two Sb atoms in **S3**-**S6**, **3** and **4** as well as the covalent and ionic part (B3LYP-D3BJ/TZP). The values are given in kcal mol^{-1}.

	$V_{inter(Total)}$	ionic part	covalent part
S5	28.40	118.27	-89.87
S6	-37.86	60.33	-98.19
S3	48.70	135.42	-86.72
S4	-18.56	73.76	-92.31
3	40.47	128.61	-88.13
4	-21.33	74.88	-96.21

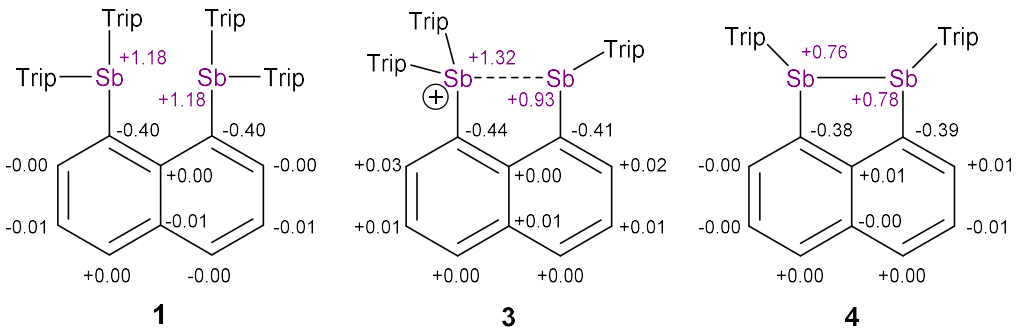


Figure S38. Atomic charges calculated using AIM analysis (B3LYP-D3BJ/TZP).

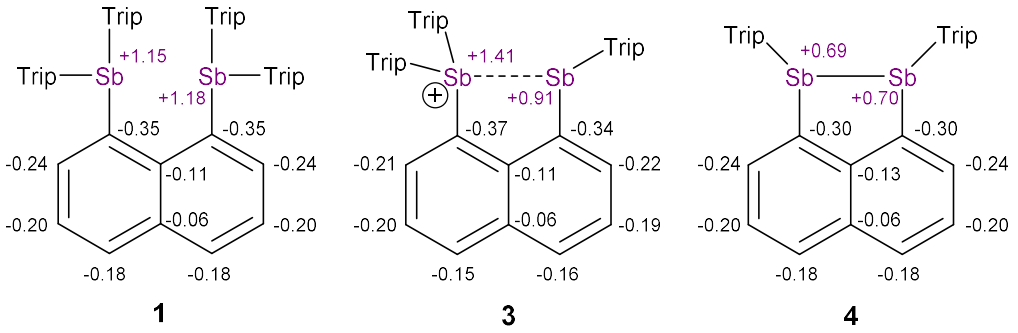


Figure S39. Atomic charges calculated using NBO analysis (B3LYP-D3BJ/def2-TZVP).

IV. Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S13. Absolute energies [au] calculated by means B3LYP-D3BJ/def2-TZVP.

	E
1	-3208.620120
2	-3157.355407
3	-2622.668353
4	-2037.105805
S1	-1871.236600
S2	-1819.966979
S3	-1639.278526
S4	-1407.739882
S5	-680.145643
S6	-640.445580

Cartesian coordinates of the optimized geometry for **1** at B3LYP-D3BJ/def2-TZVP level of theory:

Sb	1.58866500	0.05952800	0.28240300
C	1.27493100	0.13711400	2.44820500
C	2.40489800	0.38681100	3.19390100
H	3.35143500	0.52372400	2.69188600
C	1.63911600	-2.07269700	-0.28915400
C	0.00267700	0.00604300	3.10113700
C	0.00329800	0.00792800	4.53924000
C	1.20095000	0.24121000	5.25584100
H	1.15931200	0.25058000	6.33826400
C	2.37706100	0.45753300	4.59773300
H	3.29052900	0.65483900	5.14436200
C	4.01139300	1.80154200	-0.40141000
C	5.32240700	2.09705600	-0.76194000
H	5.53302300	3.04548700	-1.23983500
C	6.36821000	1.21063700	-0.52740500
C	6.07620400	0.01864400	0.11923000
H	6.88812500	-0.66698200	0.33222100
C	4.77741400	-0.32582900	0.49667600
C	2.93955200	2.84673600	-0.68992300
H	2.02760900	2.55134000	-0.17158200
C	1.37167600	-3.18034800	0.53575000
C	1.31900500	-4.45481700	-0.03098900
H	1.10293600	-5.30275000	0.60816300
C	1.53754400	-4.68273700	-1.37922900
C	1.80815100	-3.58060900	-2.17955700
H	1.98661700	-3.73039000	-3.23611800
C	1.84875100	-2.28597600	-1.66981300
C	1.12211900	-3.09189000	2.02978300
H	1.29480800	-2.06761200	2.33470500
C	2.08501300	-3.96187800	2.84626500
H	1.92802600	-5.02559000	2.65846300
H	1.92970800	-3.78653900	3.91266000
H	3.12364700	-3.73216700	2.61432400
C	-0.33031800	-3.43751900	2.37721600
H	-1.02877100	-2.83193900	1.80432400
H	-0.52504500	-3.25493000	3.43558300
H	-0.54492500	-4.48727500	2.16590300
C	1.46245300	-6.08018100	-1.95587200
H	1.30172000	-6.76359400	-1.11663100
C	2.77026800	-6.48754600	-2.64307400
H	2.71722400	-7.52131700	-2.99102800
H	3.61598800	-6.39768500	-1.95980800
H	2.97314800	-5.85543400	-3.50996900
C	0.26892800	-6.22455200	-2.90820900
H	0.37352000	-5.55929900	-3.76792600
H	-0.66620000	-5.97353800	-2.40523600

H	0.19250200	-7.24774100	-3.28249100
C	2.14785900	-1.16497700	-2.65607900
H	1.88170300	-0.21680800	-2.18422200
C	3.63905600	-1.09466300	-3.00513200
H	3.96358800	-2.02030900	-3.48580100
H	4.24969500	-0.93923500	-2.11793100
H	3.83059200	-0.26912600	-3.69389700
C	1.29305100	-1.25655700	-3.92387300
H	1.42196000	-0.35870700	-4.53019700
H	0.23596300	-1.35507600	-3.67806000
H	1.57695100	-2.10980500	-4.54165500
C	3.72628100	0.55826200	0.20359100
C	3.30271400	4.23175100	-0.14682400
H	4.15726300	4.66554300	-0.66915700
H	3.54577400	4.18357300	0.91551200
H	2.45724100	4.91105700	-0.27187300
C	2.59202200	2.90807500	-2.18123100
H	3.45377400	3.22891800	-2.77055200
H	1.77342800	3.60880200	-2.35538200
H	2.28057700	1.93094300	-2.55162200
C	7.78409900	1.53547600	-0.95377800
H	8.41172600	0.69426900	-0.64483800
C	8.31495600	2.79283300	-0.25572400
H	9.35605100	2.97567600	-0.53021900
H	8.25850800	2.69239700	0.82917000
H	7.73564400	3.67374200	-0.53974300
C	7.89328800	1.66221700	-2.47799900
H	7.29530300	2.49927800	-2.84438800
H	7.53769000	0.75713300	-2.97255100
H	8.92909800	1.83443300	-2.77825400
C	4.57937200	-1.63967500	1.23173200
H	3.52742200	-1.71288600	1.49707400
C	5.38192400	-1.67828600	2.53909300
H	6.45616500	-1.67259400	2.34652900
H	5.15007200	-2.58604300	3.09939100
H	5.15194400	-0.82275500	3.17433300
C	4.92221800	-2.84946400	0.35532100
H	4.31596000	-2.86911200	-0.54768500
H	4.74053400	-3.77824100	0.89882700
H	5.97406700	-2.83288200	0.06280500
C	-1.27011300	-0.12711200	2.44974400
C	-2.39930300	-0.37554700	3.19699800
H	-3.34607300	-0.51472500	2.69610500
C	-1.19369400	-0.22364900	5.25747800
H	-1.15113200	-0.23005500	6.33988700
C	-2.37027700	-0.44235700	4.60096900
H	-3.28317200	-0.63865100	5.14891800
Sb	-1.58473000	-0.05430100	0.28400900
C	-1.64380800	2.07653700	-0.29105100
C	-4.00078400	-1.80605300	-0.39735900
C	-5.31097300	-2.10722700	-0.75618100
H	-5.51823800	-3.05699600	-1.23287800
C	-6.36008600	-1.22472300	-0.52161600
C	-6.07224500	-0.03072500	0.12319900
H	-6.88668500	0.65197300	0.33597500
C	-4.77450200	0.31940000	0.49906800
C	-2.92484200	-2.84682800	-0.68672100
H	-2.01361900	-2.54769200	-0.16931700
C	-1.37954100	3.18643500	0.53177700
C	-1.33387200	4.46037100	-0.03670300
H	-1.12017300	5.31013000	0.60082000
C	-1.55605500	4.68540600	-1.38485600
C	-1.82315800	3.58098300	-2.18317100
H	-2.00418100	3.72847400	-3.23962900
C	-1.85691500	2.28688900	-1.67158400
C	-1.12552200	3.10047000	2.02513500
H	-1.29509300	2.07620400	2.33177200
C	-2.08804200	3.96905400	2.84348800
H	-1.93406600	5.03298700	2.65444800

H	-1.92950300	3.79493600	3.90960400
H	-3.12680100	3.73667400	2.61448600
C	0.32739500	3.44925400	2.36743700
H	1.02498500	2.84373000	1.79330700
H	0.52584100	3.26896900	3.42551400
H	0.53954700	4.49897100	2.15339700
C	-1.48757500	6.08221900	-1.96378100
H	-1.32847500	6.76764300	-1.12587100
C	-2.79786500	6.48324000	-2.64997000
H	-2.74934600	7.51661200	-2.99976800
H	-3.64233700	6.39124100	-1.96544600
H	-2.99940200	5.84885900	-3.51552200
C	-0.29579900	6.22963200	-2.91786900
H	-0.39922300	5.56297500	-3.77663500
H	0.64078400	5.98233500	-2.41573000
H	-0.22334600	7.25263100	-3.29346200
C	-2.15212300	1.16321500	-2.65593300
H	-1.88340900	0.21671200	-2.18225200
C	-3.64283000	1.08765900	-3.00587300
H	-3.96993300	2.01128900	-3.48866500
H	-4.25356000	0.93218200	-2.11873200
H	-3.83137900	0.26012700	-3.69306200
C	-1.29653200	1.25528000	-3.92317200
H	-1.42322000	0.35667400	-4.52883800
H	-0.23982000	1.35605000	-3.67655300
H	-1.58154000	2.10750000	-4.54184900
C	-3.72019500	-0.56101100	0.20619600
C	-3.28140300	-4.23347600	-0.14348100
H	-4.13406500	-4.67129200	-0.66555100
H	-3.52427500	-4.18648600	0.91894300
H	-2.43269000	-4.90868000	-0.26882400
C	-2.57838000	-2.90671500	-2.17834600
H	-3.43881400	-3.23283200	-2.76671000
H	-1.75580700	-3.60258700	-2.35287500
H	-2.27305700	-1.92795800	-2.54945400
C	-7.77506200	-1.55573700	-0.94626600
H	-8.40580100	-0.71676900	-0.63757600
C	-8.30013500	-2.81452700	-0.24642300
H	-9.34074100	-3.00187900	-0.51973200
H	-8.24306000	-2.71275200	0.83831300
H	-7.71752100	-3.69336600	-0.53010000
C	-7.88520200	-1.68447500	-2.47025500
H	-7.28420900	-2.51950300	-2.83636100
H	-7.53371200	-0.77847900	-2.96607300
H	-8.92059800	-1.86115600	-2.76934000
C	-4.58100900	1.63522500	1.23192500
H	-3.52924300	1.71281800	1.49679000
C	-5.38335200	1.67344100	2.53943000
H	-6.45761600	1.66429000	2.34712800
H	-5.15404800	2.58280800	3.09817500
H	-5.15078700	0.81964600	3.17605000
C	-4.92851700	2.84236600	0.35368500
H	-4.32306400	2.86257600	-0.54982900
H	-4.74945200	3.77260500	0.89557400
H	-5.98054500	2.82179400	0.06203700

Cartesian coordinates of the optimized geometry for **2** at B3LYP-D3BJ/def2-TZVP level of theory:

Bi	1.61862000	0.42118300	0.09063800
C	1.22137000	0.38407300	2.36473200
C	2.27833700	0.85015300	3.11044400
H	3.18089500	1.17350100	2.61150700
C	2.23745500	0.91109700	4.51645000
H	3.09422200	1.28297000	5.06414000
C	1.12728200	0.46573500	5.17235100
H	1.08398800	0.46391800	6.25482500
C	0.00003000	-0.00028700	4.45447000

C	0.00001200	-0.00024800	3.01507900
C	2.08281200	-1.75899500	-0.53469400
C	1.83613100	-2.91796600	0.22211400
C	2.20039300	-4.15817800	-0.29663500
H	2.02159300	-5.04261000	0.30267100
C	2.77944200	-4.29721900	-1.55196000
C	2.97412800	-3.14696500	-2.30138100
H	3.40997500	-3.23879600	-3.28955600
C	2.63738300	-1.88057800	-1.82007100
C	1.16884400	-2.89562600	1.58325900
H	0.88641900	-1.87173500	1.78795300
C	2.10155300	-3.33027000	2.71802300
H	2.42987200	-4.36370100	2.58765200
H	1.58270400	-3.25816600	3.67599900
H	2.98639200	-2.69949100	2.77082400
C	-0.11762000	-3.72713600	1.60368100
H	0.09058400	-4.79413500	1.50354000
H	-0.77979500	-3.44493800	0.78685600
H	-0.65241600	-3.57210000	2.54184300
C	3.18520500	-5.65376200	-2.08720500
H	3.58983000	-5.49371100	-3.09114400
C	4.29353700	-6.28149200	-1.23345200
H	3.94098800	-6.47667500	-0.21850300
H	5.15662800	-5.61790600	-1.16362000
H	4.62214800	-7.23079300	-1.66207000
C	1.98435300	-6.59801800	-2.21488500
H	2.28602300	-7.54939700	-2.65829400
H	1.20585600	-6.15899600	-2.84080000
H	1.54640400	-6.81000100	-1.23733400
C	2.88727600	-0.69869400	-2.74603900
H	2.59580800	0.21669100	-2.23268600
C	2.00975600	-0.77910200	-4.00029300
H	2.26554100	-1.64858300	-4.60821900
H	2.14040300	0.11214100	-4.61807700
H	0.95498600	-0.85824800	-3.73222000
C	4.36915300	-0.53188600	-3.09611200
H	4.97031200	-0.41243200	-2.19565900
H	4.51494400	0.35307300	-3.71858100
H	4.74521900	-1.39532600	-3.64779000
C	3.83369700	1.08965800	0.11488200
C	4.89686300	0.29545900	0.58481000
C	6.20583900	0.68293500	0.30612200
H	7.01786600	0.06103900	0.66191200
C	6.50278700	1.83139100	-0.41797400
C	5.44338200	2.61903800	-0.84092300
H	5.65983400	3.52772600	-1.39071300
C	4.11457300	2.27539100	-0.58609000
C	4.70504000	-0.96860200	1.40347700
H	3.63660300	-1.10635200	1.54919400
C	5.24125500	-2.21124600	0.68374800
H	5.02321500	-3.10900600	1.26433000
H	6.32416300	-2.14973500	0.55717900
H	4.78882800	-2.32961200	-0.29766000
C	5.34872300	-0.84669200	2.79121100
H	5.10496400	-1.72004300	3.39957400
H	5.00252200	0.03980600	3.32076700
H	6.43613300	-0.78840800	2.71657700
C	7.93215600	2.21037100	-0.74203500
H	7.89591000	3.15757000	-1.28856300
C	8.76504400	2.43593900	0.52475300
C	8.58890300	1.16974200	-1.65721800
C	3.04259100	3.23130800	-1.09083400
H	2.06864100	2.84933200	-0.78525100
C	3.17978200	4.62030600	-0.45756500
H	3.17584400	4.55375900	0.63105100
H	2.35011000	5.26090800	-0.76306300
H	4.10875000	5.10625500	-0.76081100
C	3.01583800	3.31746900	-2.62083300
H	2.86593900	2.33458700	-3.06862700

H	3.95217500	3.72086100	-3.01057100
H	2.20408700	3.96817600	-2.95206000
C	-1.22137100	-0.38449500	2.36474400
C	-2.27834300	-0.85057300	3.11045700
H	-3.18093900	-1.17382800	2.61152500
C	-2.23741800	-0.91161500	4.51645600
H	-3.09418400	-1.28348700	5.06414900
C	-1.12721000	-0.46633400	5.17235300
H	-1.08388400	-0.46458900	6.25482600
Bi	-1.61874500	-0.42145800	0.09067800
C	-2.08264700	1.75881900	-0.53453000
C	-1.83579600	2.91775100	0.22228700
C	-2.19983000	4.15802200	-0.29648600
H	-2.02091300	5.04242600	0.30282600
C	-2.77882600	4.29715600	-1.55182300
C	-2.97372200	3.14692800	-2.30123200
H	-3.40954900	3.23882600	-3.28940900
C	-2.63720000	1.88048800	-1.81990700
C	-1.16862400	2.89531700	1.58349100
H	-0.88637400	1.87138500	1.78820900
C	-2.10136600	3.33009800	2.71817700
H	-2.42962300	4.36353700	2.58771800
H	-1.58256600	3.25803200	3.67618200
H	-2.98624100	2.69937000	2.77098900
C	0.11796300	3.72663500	1.60406100
H	-0.09005700	4.79366200	1.50383700
H	0.78022900	3.44429900	0.78736300
H	0.65258700	3.57155900	2.54231200
C	-3.18434600	5.65376600	-2.08708300
H	-3.58888700	5.49379200	-3.09106900
C	-4.29268300	6.28161800	-1.23342600
H	-3.94021000	6.47670600	-0.21843100
H	-5.15587200	5.61814800	-1.16371200
H	-4.62111700	7.23098300	-1.66203800
C	-1.98336000	6.59787000	-2.21461800
H	-2.28486100	7.54928900	-2.65805600
H	-1.20484700	6.15875500	-2.84044800
H	-1.54549400	6.80979700	-1.23701800
C	-2.88728400	0.69863500	-2.74586500
H	-2.59596800	-0.21679400	-2.23250600
C	-2.00975000	0.77889000	-4.00011600
H	-2.26538000	1.64841200	-4.60804800
H	-2.14054400	-0.11233200	-4.61789800
H	-0.95496600	0.85785700	-3.73203800
C	-4.36919000	0.53204800	-3.09592600
H	-4.97036100	0.41272200	-2.19546400
H	-4.51512000	-0.35291600	-3.71835500
H	-4.74512600	1.39552300	-3.64763900
C	-3.83393900	-1.08956400	0.11496700
C	-4.89695400	-0.29516500	0.58489900
C	-6.20600200	-0.68235700	0.30618100
H	-7.01790500	-0.06030100	0.66196700
C	-6.50317500	-1.83072600	-0.41796200
C	-5.44392700	-2.61857900	-0.84091700
H	-5.66055000	-3.52719700	-1.39075300
C	-4.11504700	-2.27521300	-0.58604800
C	-4.70484900	0.96881400	1.40361900
H	-3.63637200	1.10637900	1.54921900
C	-5.24094600	2.21159200	0.68403600
H	-5.02270600	3.10927600	1.26466000
H	-6.32387700	2.15026200	0.55757400
H	-4.78859900	2.32995800	-0.29741000
C	-5.34837800	0.84689100	2.79142200
H	-5.10446100	1.72018300	3.39980600
H	-5.00219500	-0.03967300	3.32088200
H	-6.43580300	0.78871200	2.71691300
C	-7.93261000	-2.20930400	-0.74219400
H	-7.89658200	-3.15672600	-1.28835100
C	-8.76598800	-2.43403300	0.52441800

H	-8.85453100	-1.51341100	1.10482100
H	-8.30935800	-3.18966400	1.16535300
H	-9.77486900	-2.76461500	0.26846400
C	-8.58864700	-1.16874700	-1.65797700
H	-8.00761500	-1.02884700	-2.57072500
H	-8.66197300	-0.20043900	-1.15856400
H	-9.59795800	-1.47956900	-1.93626700
C	-3.04326200	-3.23135200	-1.09077500
H	-2.06922900	-2.84948900	-0.78532200
C	-3.18061700	-4.62023900	-0.45729700
H	-3.17644800	-4.55354100	0.63130900
H	-2.35114300	-5.26105900	-0.76287400
H	-4.10975100	-5.10603100	-0.76029000
C	-3.01665400	-3.31770500	-2.62076400
H	-2.86667800	-2.33489100	-3.06869000
H	-3.95306800	-3.72103500	-3.01037800
H	-2.20500700	-3.96854700	-2.95198600
H	8.00806600	1.02907200	-2.56997200
H	9.59807000	1.48101300	-1.93552900
H	8.66275100	0.20170900	-1.15735000
H	8.30808800	3.19192400	1.16504100
H	8.85339200	1.51566600	1.10574200
H	9.77399800	2.76645000	0.26898900

Cartesian coordinates of the optimized geometry for **3** at B3LYP-D3BJ/def2-TZVP level of theory:

Sb	0.69892300	-0.19792900	-0.46221400
C	0.44651200	-1.58513800	-2.05666800
Sb	-1.11916200	-1.62859700	1.12532900
C	0.90898600	-1.33036500	-3.32358000
H	1.34560300	-0.37192300	-3.56580700
C	0.85176000	-2.32881300	-4.31391400
H	1.22017100	-2.11813400	-5.30881200
C	0.35720900	-3.56751900	-4.00245500
H	0.34069900	-4.35264500	-4.74789100
C	-0.70186100	-5.12230100	-2.41116900
H	-0.67483300	-5.89312700	-3.17084600
C	-1.25286800	-5.37162700	-1.18575900
H	-1.66062900	-6.34658100	-0.95489700
C	-1.32497700	-4.34215300	-0.22458100
H	-1.81520400	-4.55663900	0.71812800
C	-0.81402300	-3.09048900	-0.47263200
C	-0.16581400	-2.82486100	-1.71845900
C	-0.16366700	-3.84900500	-2.71694600
C	-3.03877700	-0.67156400	0.72722400
C	-3.69716500	-0.61321700	-0.51398700
C	-4.93654700	0.02084700	-0.58416400
H	-5.44902400	0.06599800	-1.53684600
C	-5.53757400	0.60348200	0.52143700
C	-4.86491000	0.53947300	1.73875500
H	-5.31617600	0.99555100	2.60803200
C	-3.62873200	-0.08012900	1.86986100
C	-3.14336200	-1.24156300	-1.77390300
H	-2.10254100	-1.46737800	-1.58709100
C	-3.85301200	-2.56763500	-2.07278600
H	-4.89972400	-2.39540200	-2.33002600
H	-3.82455500	-3.23399400	-1.21144300
H	-3.37530200	-3.07539100	-2.91228800
C	-3.16314900	-0.32454800	-2.99889800
H	-4.17657300	-0.06403400	-3.30572900
H	-2.68563200	-0.83088100	-3.83937400
H	-2.62010400	0.60042800	-2.81274100
C	-6.86846300	1.31131900	0.39899400
H	-7.21026200	1.17461700	-0.63070200
C	-6.71371900	2.81814800	0.64347700
H	-5.98276300	3.25635000	-0.03801300
H	-6.38303000	3.01736700	1.66491900

H	-7.66623800	3.32926000	0.49550100
C	-7.92638900	0.70449800	1.32729900
H	-8.89203200	1.18702800	1.16923100
H	-7.65722900	0.83941500	2.37670100
H	-8.04498900	-0.36439200	1.14528600
C	-2.97927500	-0.12735200	3.24846600
H	-1.89411700	-0.13551800	3.11242600
C	-3.36777000	-1.41860700	3.98078600
H	-4.44611500	-1.44887000	4.14538600
H	-2.87053300	-1.47921700	4.95025400
H	-3.09972300	-2.30769300	3.40660900
C	-3.27160400	1.09162900	4.12731700
H	-3.05929300	2.02491700	3.60617500
H	-2.65006900	1.05282300	5.02282800
H	-4.31005600	1.11573400	4.45928300
C	0.90502800	1.80945000	-1.18038500
C	-0.12701200	2.73595200	-0.96205400
C	0.14719800	4.07881700	-1.19669000
H	-0.63484900	4.80505700	-1.02191300
C	1.38818400	4.51629300	-1.64876500
C	2.36481800	3.56253200	-1.90149800
H	3.32303400	3.88931900	-2.28510600
C	2.15808600	2.20259200	-1.67632100
C	-1.51717900	2.35161600	-0.49287600
H	-1.61602300	1.26530700	-0.56783800
C	-1.75947500	2.73904900	0.96964900
H	-1.59978100	3.80865400	1.11411900
H	-1.09383200	2.20953500	1.65011000
H	-2.78382700	2.50253400	1.25147000
C	1.66741100	5.98706400	-1.86508700
H	2.69148400	6.06703600	-2.23973400
C	0.73476000	6.59212100	-2.92072900
H	0.80117200	6.04974400	-3.86479200
H	0.99800400	7.63433200	-3.10662600
H	-0.30557500	6.56689200	-2.59051300
C	1.59115000	6.76275300	-0.54406100
H	1.85880400	7.80863000	-0.70087800
H	2.27039900	6.34405100	0.19993300
H	0.58095100	6.73628700	-0.13040200
C	3.28650800	1.24383800	-2.01199900
H	2.94636800	0.22472600	-1.81736800
C	3.64835000	1.30811700	-3.50188300
H	2.76986900	1.18735500	-4.13685900
H	4.36331000	0.52219000	-3.74974300
H	4.10544000	2.26522800	-3.75482500
C	4.52427900	1.48348300	-1.14069200
H	4.93910200	2.47538800	-1.32465900
H	5.29808600	0.75097300	-1.37227200
H	4.28971300	1.40281400	-0.08132600
C	2.47611500	-0.54475200	0.70669500
C	3.45822900	-1.49857400	0.40259000
C	4.56472700	-1.58592800	1.24553400
H	5.33114800	-2.31801200	1.02687600
C	4.72896800	-0.76578500	2.35369000
C	3.72888300	0.15912400	2.63327100
H	3.83212200	0.80554700	3.49481600
C	2.59551800	0.28349500	1.83789300
C	3.35842400	-2.46099700	-0.76342800
H	2.60803600	-2.07940200	-1.44810400
C	4.65403400	-2.57938200	-1.57099900
H	4.47932500	-3.18558500	-2.46102400
H	5.45078300	-3.05917000	-1.00185000
H	5.01329200	-1.60100800	-1.89190500
C	2.87524000	-3.83650200	-0.28462300
H	1.93412300	-3.75961100	0.26025100
H	3.61075500	-4.29412900	0.37937800
H	2.71918400	-4.50399700	-1.13353900
C	5.96205700	-0.87435800	3.22305300
H	6.57238600	-1.68344900	2.81266000

C	5.60619300	-1.24405500	4.66762000
H	5.01678300	-0.45753000	5.14317300
H	6.51260700	-1.38156700	5.25898500
H	5.02850000	-2.16848000	4.70823800
C	6.79393500	0.41296100	3.16699800
H	7.06573800	0.66308900	2.14049700
H	7.71185400	0.29928300	3.74559400
H	6.24032500	1.25703600	3.58350100
C	1.55437700	1.31359200	2.23814900
H	0.71240700	1.24385700	1.54620700
C	0.97741500	1.02963900	3.62900900
H	0.16294700	1.72128700	3.85144200
H	1.73509500	1.15052400	4.40369200
H	0.59477700	0.01001600	3.69529800
C	2.08134000	2.74680800	2.11969100
H	2.42739100	2.95639200	1.10826000
H	2.91300600	2.91330800	2.80559800
H	1.29467900	3.46183900	2.36429000
C	-2.61116000	2.95588200	-1.38079400
H	-2.41202900	2.78373400	-2.43810500
H	-2.69473700	4.03254300	-1.22738500
H	-3.57318000	2.50846400	-1.13281200

Cartesian coordinates of the optimized geometry for **4** at B3LYP-D3BJ/def2-TZVP level of theory:

Sb	0.72627500	-0.00964000	1.17206200
C	0.65884800	2.16024000	1.00233300
Sb	-0.71822100	-0.03651200	-1.24942300
C	1.32590300	2.89790600	1.95129500
H	1.90605600	2.39769100	2.71797100
C	1.28113000	4.30693900	1.95156100
H	1.82853100	4.86033400	2.70395000
C	0.54059500	4.96525000	1.00885700
H	0.48961600	6.04732000	1.00385000
C	-0.95800400	4.92895900	-0.94410200
H	-0.99981200	6.01083500	-0.90810000
C	-1.64139500	4.23689800	-1.90563800
H	-2.23560800	4.76268400	-2.64214500
C	-1.56550500	2.82982500	-1.94561400
H	-2.10239700	2.30378600	-2.72638200
C	-0.83562700	2.12526500	-1.01793600
C	-0.11726400	2.81868900	0.00178400
C	-0.17862600	4.24937900	0.02226900
C	2.74319000	-0.44617500	0.40069800
C	3.43050500	-1.50718800	1.03618700
C	4.73568400	-1.79830400	0.65484700
H	5.25776300	-2.60899700	1.14319400
C	5.39444000	-1.07680900	-0.33636000
C	4.69784900	-0.05780500	-0.96325800
H	5.19220400	0.50290900	-1.74801200
C	3.38202500	0.26752800	-0.62637300
C	2.75455900	-2.39230400	2.07518800
H	2.08964900	-1.75886300	2.66744100
C	1.88299000	-3.45027200	1.38298400
H	2.50359100	-4.11498200	0.77811000
H	1.14752100	-2.99511300	0.71774000
H	1.34516600	-4.05350200	2.11746400
C	3.71004200	-3.05748300	3.06726500
H	3.13723600	-3.54497700	3.85808200
H	4.37689400	-2.32871900	3.53026000
H	4.32335600	-3.82648600	2.59374400
C	7.78766100	-1.19383100	0.44608000
H	7.56330500	-1.88188100	1.26380800
H	7.71894100	-0.17762800	0.83704200
H	8.81844100	-1.37257000	0.13253400
C	2.71738900	1.37249100	-1.42207200
H	1.69028500	1.44655300	-1.08727300

C	2.67116600	1.05380700	-2.92068700
H	2.20420400	0.08466600	-3.10021900
H	3.67018500	1.03379400	-3.35993000
H	2.08920000	1.81392700	-3.44600000
C	3.35889200	2.73935000	-1.16466500
H	4.39148400	2.76379600	-1.51921700
H	3.35822800	2.97597500	-0.10131100
H	2.80337100	3.52187600	-1.68528600
C	-2.69439600	-0.65795800	-0.50065900
C	-3.38784000	-0.03325500	0.55237900
C	-4.67001200	-0.47221400	0.87812500
H	-5.19735100	0.02390500	1.68347600
C	-5.28474200	-1.52361200	0.21410900
C	-4.57415000	-2.15208200	-0.80036800
H	-5.03930500	-2.98349200	-1.31287000
C	-3.29486900	-1.74479700	-1.17321000
C	-2.81036700	1.09235800	1.38682800
H	-1.79320500	1.25994300	1.05548400
C	-3.55914000	2.41203000	1.17792200
H	-3.58014000	2.68538000	0.12363500
H	-3.06669100	3.21751600	1.72625900
H	-4.58957900	2.34128700	1.53256400
C	-2.73524500	0.72483100	2.87298300
H	-2.19481300	-0.21147100	3.01718900
H	-3.72847100	0.61201800	3.31145900
H	-2.21207800	1.50801300	3.42554500
C	-6.67869000	-1.98427600	0.58443700
H	-6.92659200	-2.81833400	-0.07893900
C	-7.71793000	-0.88111200	0.35281400
H	-7.69328900	-0.52970800	-0.67973200
H	-7.52922500	-0.02328000	1.00155500
H	-8.72418700	-1.24739800	0.56744000
C	-6.73817500	-2.50326600	2.02597500
H	-7.73394300	-2.88778700	2.25697900
H	-6.51426400	-1.70676700	2.73854100
H	-6.01508200	-3.30470900	2.18439000
C	-2.55590200	-2.53620000	-2.24428800
H	-1.93838300	-1.83282500	-2.80810600
C	-3.46006200	-3.22809600	-3.26586500
H	-2.85279500	-3.64047100	-4.07356900
H	-4.17743300	-2.53119700	-3.70160900
H	-4.01678300	-4.05762300	-2.82600900
C	-1.60967400	-3.55463200	-1.59209500
H	-2.17957300	-4.28573900	-1.01454500
H	-0.90848100	-3.07299500	-0.90872900
H	-1.03050500	-4.08833500	-2.34864200
C	6.82132900	-1.39926800	-0.72640500
H	7.10294600	-0.69597100	-1.51578100
C	6.94484700	-2.81562900	-1.30047800
H	6.27523300	-2.95376400	-2.15063200
H	6.69030200	-3.56643500	-0.54949300
H	7.96695500	-3.00951400	-1.63283600

Cartesian coordinates of the optimized geometry for **S1** at B3LYP-D3BJ/def2-TZVP level of theory:

C	-4.13243900	-0.70018900	-0.85686700
C	-4.73760500	-1.22033500	0.28628800
C	-4.86973900	-0.63698200	-2.04003100
C	-6.05676400	-1.66064600	0.24815700
H	-4.18323000	-1.28102500	1.21345800
C	-6.19046600	-1.07028700	-2.07880800
H	-4.41734900	-0.24305800	-2.94351000
C	-6.78610500	-1.58406200	-0.93265400
H	-6.51515200	-2.06235600	1.14341500
H	-6.75200000	-1.00979000	-3.00277200
H	-7.81303700	-1.92546200	-0.96061200
C	-1.62358600	-0.61410100	1.13089500

C	-1.91798300	0.16349000	2.25139100
C	-1.03337100	-1.86505000	1.31253300
C	-1.63486100	-0.30611800	3.52998000
H	-2.37050400	1.13890700	2.13067800
C	-0.74430600	-2.33196100	2.58963300
H	-0.78440100	-2.48180800	0.45892200
C	-1.04689300	-1.55446100	3.70068000
H	-1.86865900	0.30707300	4.39150600
H	-0.27385400	-3.29901400	2.71227000
H	-0.81783600	-1.91601600	4.69499100
C	-2.59827100	2.06121000	-0.31563100
C	-1.57187400	3.00478500	-0.24519400
C	-3.89908400	2.45466400	-0.00524100
C	-1.83805400	4.31320200	0.14223400
H	-0.55425000	2.71987300	-0.48487200
C	-4.16742800	3.76574800	0.37617400
H	-4.70888200	1.73849000	-0.05393500
C	-3.13791800	4.69617000	0.45334400
H	-1.03106000	5.03313300	0.19946200
H	-5.18229000	4.05845200	0.61571900
H	-3.34732500	5.71522200	0.75280800
C	3.88302600	0.66237200	-1.44467100
C	4.62427800	-0.46832500	-1.78529600
C	4.40517800	1.92378300	-1.73267000
C	5.86736100	-0.33863700	-2.39587100
H	4.23540700	-1.45555600	-1.57260200
C	5.65038800	2.05558100	-2.33764000
H	3.84271200	2.81659800	-1.48299200
C	6.38338200	0.92255800	-2.67083500
H	6.43360300	-1.22453300	-2.65558300
H	6.04550900	3.04087100	-2.55134700
H	7.35138500	1.02216300	-3.14509200
C	1.72006600	-1.59307700	-0.68265700
C	2.18390900	-2.50036500	0.26787300
C	1.01969400	-2.07238700	-1.78964400
C	1.94630500	-3.86220400	0.11728000
H	2.71810400	-2.14615600	1.13938100
C	0.78083700	-3.43393600	-1.94247600
H	0.63944400	-1.38367400	-2.53408200
C	1.24026800	-4.33124400	-0.98494400
H	2.30790800	-4.55693500	0.86532600
H	0.22944800	-3.79184600	-2.80285000
H	1.04805300	-5.39061300	-1.09725000
C	2.75285500	0.44108000	1.55165200
C	4.11846000	0.42568600	1.83044600
C	1.84198700	0.36605300	2.60553800
C	4.56541300	0.33062600	3.14475000
H	4.83896300	0.48084200	1.02482100
C	2.28865700	0.26229100	3.91739600
H	0.77783400	0.37392500	2.41156100
C	3.65195800	0.24627900	4.18949500
H	5.62851700	0.31873300	3.35126600
H	1.56908200	0.19333000	4.72335300
H	4.00170600	0.16896900	5.21120500
Sb	1.96366200	0.54234400	-0.45571500
Sb	-2.09447500	0.03283300	-0.88115400

Cartesian coordinates of the optimized geometry for **S2** at B3LYP-D3BJ/def2-TZVP level of theory:

C	-4.25745000	0.57402200	0.80609400
C	-4.77689500	1.34172700	-0.23376400
C	-5.09048500	0.21453500	1.86506600
C	-6.11095400	1.73872100	-0.21654500
H	-4.14676200	1.62994500	-1.06513200
C	-6.42516800	0.60688800	1.88170100
H	-4.70863500	-0.38239400	2.68633500
C	-6.93695700	1.37090100	0.83915500

H	-6.50470600	2.33465200	-1.03080800
H	-7.06333700	0.31698900	2.70734000
H	-7.97479000	1.67866300	0.85025800
C	-1.58473900	0.90313500	-1.10605900
C	-1.86755900	0.33194600	-2.34601100
C	-1.00933900	2.17203800	-1.05699600
C	-1.58697900	1.02508800	-3.51999400
H	-2.30984200	-0.65425900	-2.40290300
C	-0.72133800	2.86114000	-2.23045000
H	-0.76984600	2.63215400	-0.10705100
C	-1.01350600	2.29052200	-3.46320100
H	-1.81121800	0.57239800	-4.47805100
H	-0.26173400	3.83986600	-2.17781200
H	-0.78761400	2.82621800	-4.37635600
C	-2.58757600	-2.10089600	-0.18438700
C	-1.56781800	-3.03847400	-0.34643400
C	-3.85813900	-2.39128600	-0.67695700
C	-1.80986300	-4.24319000	-0.99881200
H	-0.57160700	-2.83512900	0.02947200
C	-4.10277500	-3.59773900	-1.32679400
H	-4.66282300	-1.67655700	-0.56078900
C	-3.07941700	-4.52413000	-1.49053900
H	-1.00802200	-4.96066700	-1.12274500
H	-5.09419800	-3.81216300	-1.70670100
H	-3.27028300	-5.46114500	-1.99801300
C	4.00198100	-0.84405400	1.24004100
C	4.68221700	0.23469300	1.80109900
C	4.59989200	-2.10354800	1.25263300
C	5.94315300	0.05622600	2.36212300
H	4.23402100	1.21998800	1.80025800
C	5.86221400	-2.28304300	1.81003500
H	4.08917600	-2.95848600	0.82285800
C	6.53534100	-1.20158700	2.36616000
H	6.46353400	0.90177800	2.79503700
H	6.31795500	-3.26549500	1.81046800
H	7.51688600	-1.33877900	2.80164600
C	1.69615700	1.52869800	0.93792000
C	2.15589300	2.59972600	0.17585000
C	0.98728900	1.78554600	2.11035400
C	1.90251000	3.90787700	0.57563600
H	2.69837400	2.41900400	-0.74286500
C	0.72868200	3.09330900	2.51037900
H	0.61990500	0.96834900	2.72012400
C	1.18289300	4.15716600	1.73919800
H	2.26130800	4.73329900	-0.02697400
H	0.17021500	3.28000800	3.41923500
H	0.97780200	5.17524600	2.04451500
C	2.81569700	-0.02436100	-1.73906800
C	4.18459900	0.07534000	-1.97588700
C	1.91905000	0.27875400	-2.76222100
C	4.65095500	0.47736100	-3.22439500
H	4.89300800	-0.15148000	-1.18940900
C	2.38583300	0.68635300	-4.00713400
H	0.85172200	0.21539900	-2.59748700
C	3.75282500	0.78469000	-4.24041800
H	5.71688600	0.55364700	-3.40101400
H	1.67845500	0.92877400	-4.79025300
H	4.11753500	1.10054900	-5.20967400
Bi	1.97188600	-0.61413000	0.26919900
Bi	-2.10758100	-0.13641100	0.83600800

Cartesian coordinates of the optimized geometry for **S3** at B3LYP-D3BJ/def2-TZVP level of theory:

C	-0.27663200	-0.02290700	1.96103000
C	0.54723900	0.61223000	2.88775200
C	-0.94225600	-1.20346300	2.29033000
C	0.69942200	0.06295300	4.15524600

H	1.06727700	1.52572900	2.63178100
C	-0.78155900	-1.74388800	3.55984700
H	-1.57568900	-1.70607400	1.57340400
C	0.03911400	-1.11414700	4.48937100
H	1.33338300	0.55584600	4.88034200
H	-1.29698600	-2.65898100	3.81936700
H	0.16253700	-1.54012600	5.47619700
C	0.64112300	2.59222500	0.04629200
C	-0.04459800	3.80425700	0.01020000
C	2.03508500	2.56120900	0.10653800
C	0.67269600	4.99459400	0.04216800
H	-1.12559300	3.82768400	-0.04075900
C	2.74058800	3.75750800	0.13988800
H	2.57271500	1.62257100	0.12980100
C	2.06108500	4.97058000	0.10733400
H	0.14575500	5.93911800	0.01657300
H	3.82124000	3.74051100	0.18933700
H	2.61518700	5.89943100	0.13155000
C	-2.47595800	1.25443000	-0.26675800
C	-2.94393700	1.55030500	-1.54646500
C	-3.34111100	1.26180500	0.82518000
C	-4.28458600	1.86448400	-1.73020200
H	-2.27593200	1.54206700	-2.39939300
C	-4.68155900	1.57531500	0.63118600
H	-2.98071600	1.02590800	1.81788700
C	-5.15120200	1.87574000	-0.64228900
H	-4.65162500	2.09849800	-2.72061000
H	-5.35752000	1.58482100	1.47587900
H	-6.19529500	2.11834800	-0.78835000
C	-0.49186300	-2.60150600	-0.91687800
C	0.15931700	-3.62401900	-0.23103500
C	-1.88791000	-2.58074000	-0.96399800
C	-0.58138000	-4.60367200	0.42240200
H	1.23939100	-3.66669000	-0.19868100
C	-2.62423900	-3.55661500	-0.30433700
H	-2.41330400	-1.80096100	-1.50396300
C	-1.97012400	-4.56664800	0.39413700
H	-0.07039300	-5.39666400	0.95257200
H	-3.70547400	-3.53060300	-0.33887100
H	-2.54285500	-5.32902000	0.90522300
C	2.43082200	-1.02125400	-0.89534100
C	3.54035000	-0.55687500	-1.60470700
C	2.56299400	-1.33444100	0.45931700
C	4.76715300	-0.40627600	-0.96741200
H	3.45660200	-0.30419000	-2.65500100
C	3.78841900	-1.17682900	1.09360500
H	1.71721400	-1.68763200	1.03113300
C	4.89020800	-0.71141100	0.38257700
H	5.62320900	-0.05085800	-1.52557300
H	3.88091000	-1.41534600	2.14507400
H	5.84348600	-0.59097400	0.87986800
Sb	0.55682000	-1.03427400	-1.95740400
Sb	-0.43658000	0.77388000	0.00652800

Cartesian coordinates of the optimized geometry for **S4** at B3LYP-D3BJ/def2-TZVP level of theory:

C	-1.59236000	1.53931200	0.56217100
C	-1.18961400	2.65318700	1.29759700
C	-2.36585900	1.72813500	-0.58346200
C	-1.55170200	3.93410300	0.89715200
H	-0.57286300	2.52982000	2.17945000
C	-2.73062500	3.00869000	-0.98262500
H	-2.68504600	0.87613600	-1.16990900
C	-2.32319700	4.11427500	-0.24370700
H	-1.22277800	4.79018100	1.47230100
H	-3.32935500	3.14307200	-1.87509000
H	-2.60404500	5.11127200	-0.55833100

C	-2.43617100	-1.56321000	0.26391700
C	-3.76919800	-1.22804200	0.50652500
C	-2.16031700	-2.70311200	-0.49120400
C	-4.80102300	-2.00723000	-0.00470500
H	-4.01129600	-0.34625900	1.08735000
C	-3.19017200	-3.48764200	-0.99900600
H	-1.13548400	-2.98622600	-0.70228800
C	-4.51389600	-3.13989200	-0.75796500
H	-5.83005200	-1.72920000	0.18650200
H	-2.95741900	-4.36583300	-1.58826300
H	-5.31693400	-3.74645600	-1.15641800
C	2.43616700	-1.56321600	-0.26391500
C	3.76919400	-1.22803700	-0.50650500
C	2.16031100	-2.70312800	0.49119000
C	4.80101800	-2.00722500	0.00472800
H	4.01129300	-0.34624500	-1.08731600
C	3.19016500	-3.48765800	0.99899300
H	1.13547700	-2.98625000	0.70225900
C	4.51388900	-3.13989700	0.75797100
H	5.83004700	-1.72918600	-0.18646500
H	2.95741000	-4.36585700	1.58823700
H	5.31692600	-3.74646100	1.15642600
C	1.59236300	1.53930700	-0.56217500
C	1.18959200	2.65318700	-1.29758000
C	2.36589300	1.72812300	0.58343800
C	1.55168400	3.93410100	-0.89713300
H	0.57281700	2.52982400	-2.17941800
C	2.73066300	3.00867600	0.98260300
H	2.68510100	0.87612000	1.16986800
C	2.32321000	4.11426600	0.24370700
H	1.22274000	4.79018200	-1.47226500
H	3.32941800	3.14305300	1.87505300
H	2.60406100	5.11126200	0.55833200
Sb	0.84170800	-0.39936800	-1.15584000
Sb	-0.84171000	-0.39936500	1.15583900

Cartesian coordinates of the optimized geometry for **S5** at B3LYP-D3BJ/def2-TZVP level of theory:

Sb	1.19631400	0.00001900	-0.00047000
C	1.72950600	0.00014800	2.07056700
Sb	-1.62044100	-0.00002900	-0.45141000
C	-1.90483600	1.60977300	0.98528700
C	2.19519200	1.69620800	-0.82939300
H	3.25841900	1.60747600	-0.61493600
H	2.03008300	1.71538700	-1.90411400
H	1.79717500	2.60085100	-0.37562400
C	2.19488200	-1.69642300	-0.82924600
H	2.03061200	-1.71501500	-1.90410900
H	3.25799000	-1.60842000	-0.61390900
H	1.79596800	-2.60104000	-0.37621600
C	-1.90455800	-1.60965300	0.98555800
H	-2.97972000	-1.71188500	1.13005200
H	-1.51548700	-2.54330600	0.58507700
H	-1.43704400	-1.37695900	1.93926600
H	-1.51630600	2.54351100	0.58448000
H	-2.98000600	1.71153900	1.13007400
H	1.32473700	-0.89125500	2.54376100
H	2.81551100	0.00036000	2.14282000
H	1.32439200	0.89142400	2.54370600
H	-1.43694800	1.37751700	1.93891700

Cartesian coordinates of the optimized geometry for **S6** at B3LYP-D3BJ/def2-TZVP level of theory:

Sb	1.33966400	0.04682800	-0.48518400
C	1.88115500	-1.71689000	0.69081600

Sb	-1.33968200	0.04681400	0.48516600
C	-1.88080500	-1.71714500	-0.69065700
C	2.07338800	1.47048900	1.00381400
H	3.16248800	1.47033600	0.98643900
H	1.71545700	2.46921900	0.75823500
H	1.72300600	1.19131300	1.99569900
C	-2.07364500	1.47026700	-1.00388400
H	-3.16275100	1.46955400	-0.98670900
H	-1.71628500	2.46913300	-0.75801800
H	-1.72295400	1.19149700	-1.99577400
H	-1.42662300	-2.60124700	-0.24609900
H	-2.96397200	-1.83031200	-0.67714200
H	2.96434100	-1.82985300	0.67697200
H	1.54008500	-1.60712800	1.71874700
H	-1.53942400	-1.60747700	-1.71849700
H	1.42698400	-2.60113100	0.24652700

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