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Electronic Supplementary Information

A general route to monoorganopnicogen(III) (M = Sb, Bi) compounds with a pincer (*N,C,N*) group and oxo ligands

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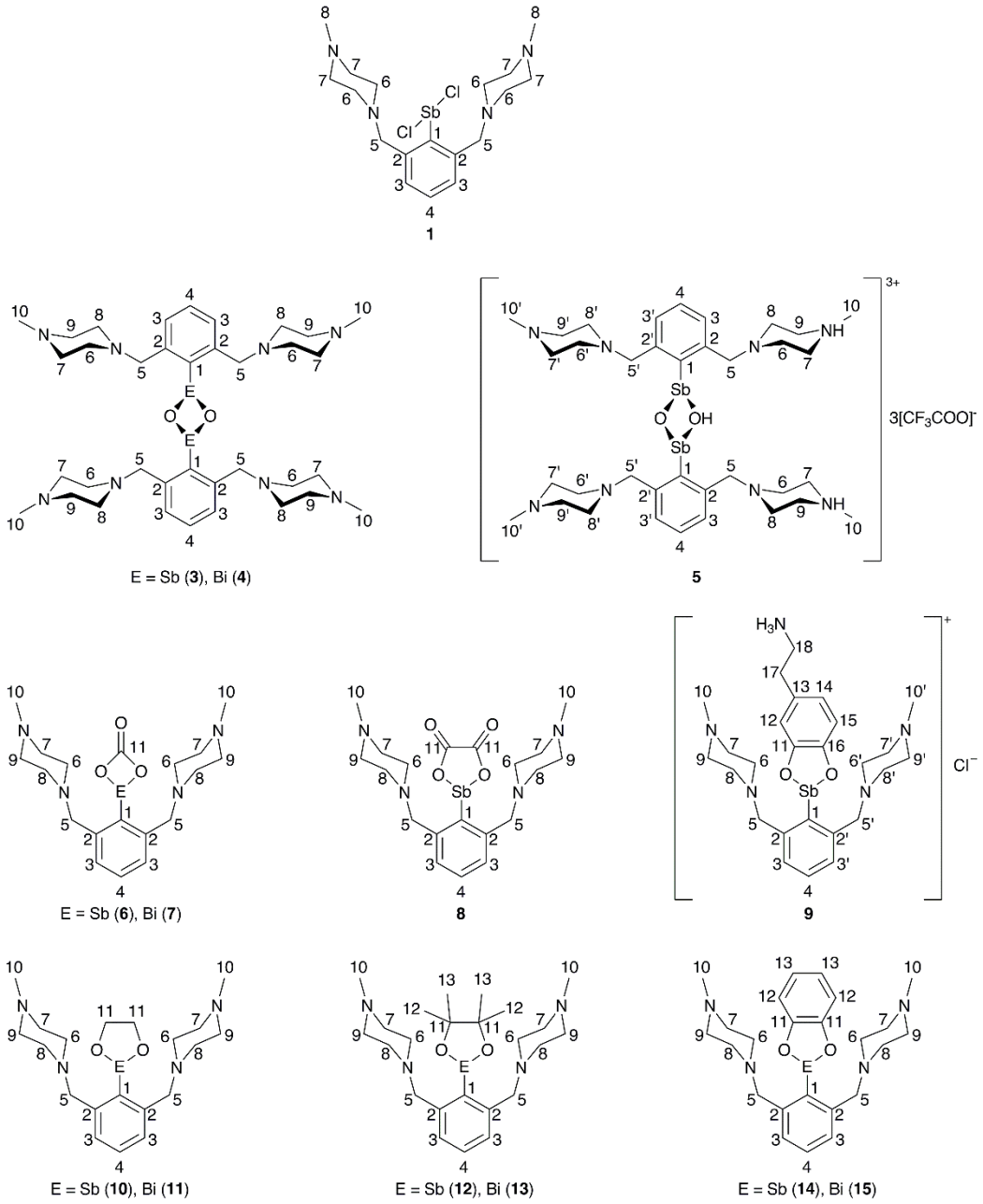
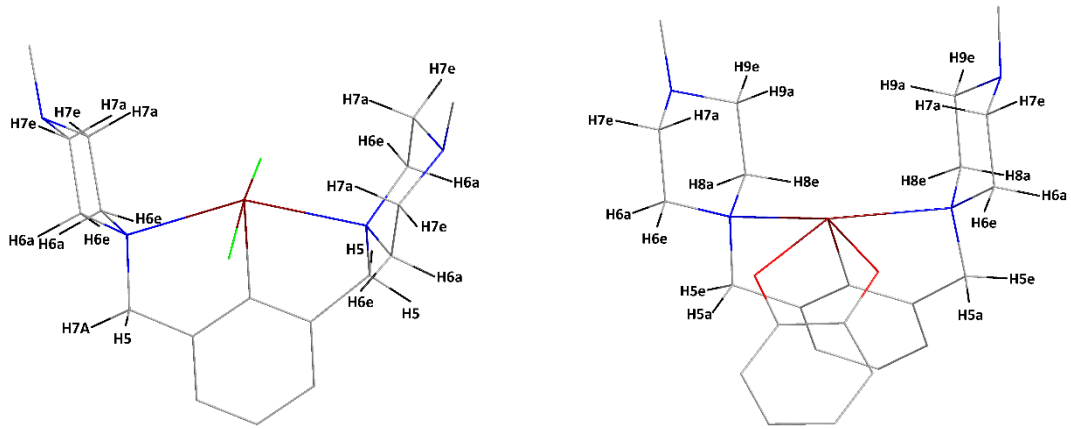
Content



Scheme S1. Full numbering scheme for NMR assignments.



Scheme S2. Numbering scheme of the protons in the pendant arms used for NMR assignments in species containing *trans* [*e.g.* $RSbCl_2$ (**1**), left] and *cis* [*e.g.* $RSb(O_2\text{-}1,2\text{-}C_6H_4)$ (**14**), right] coordinated nitrogen atoms.

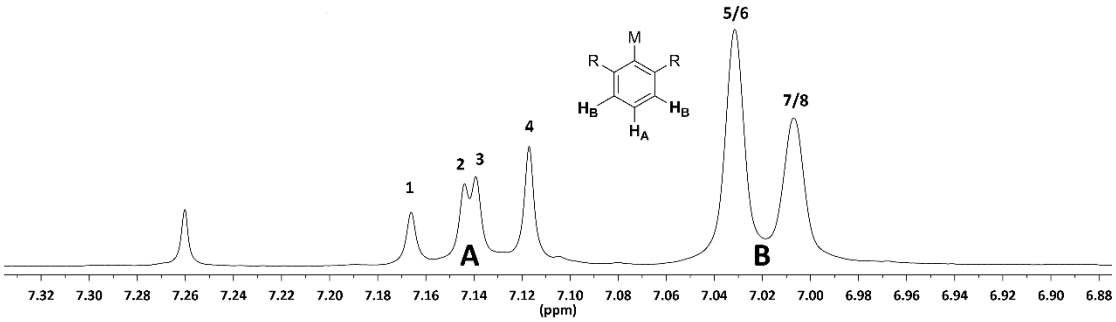


Figure S1. Assignment in AB_2 spin systems (example from ^1H NMR spectrum of **10** in $CDCl_3$ at 60 °C, 301 MHz).

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]SbCl$_2$ (1)

^{1}H NMR (301 MHz, $CDCl_3$, 213 K): δ 2.33 (s, 6H, H-8), 2.55 (dd, $^2J_{H\text{-}7a,H\text{-}7e} \approx {}^3J_{H\text{-}6a,H\text{-}7a}$ = 12.1 Hz, 4H, H-7a), 2.73 (dd, $^2J_{H\text{-}6a,H\text{-}6e} \approx {}^3J_{H\text{-}6a,H\text{-}7a}$ = 11.9 Hz, 4H, H-6a), 2.91 (d, $^2J_{H\text{-}7a,H\text{-}7e}$ = 12.2 Hz, 4H, H-7e), 3.72 (d, $^2J_{H\text{-}6a,H\text{-}6e}$ =11.6 Hz, 4H, H-6e), 4.14 (s, 2H, H-5), AB_2 spin system with B at δ 7.19 ppm (d, $^3J_{H\text{-}3,H\text{-}4}$ = 7.6 Hz, 2H, H-3) and A at δ 7.32 ppm (t, $^3J_{H\text{-}3,H\text{-}4}$ = 7.5 Hz, 1H, H-4).

^{13}C{^{1}H} NMR (76 MHz, $CDCl_3$, 213 K): δ 45.58 (C-8), 54.33 (C-6), 55.14 (C-7), 64.60 (C-5), 125.52 (C-3), 130.46 (C-4), 141.33 (C-2), 150.83 (C-1).

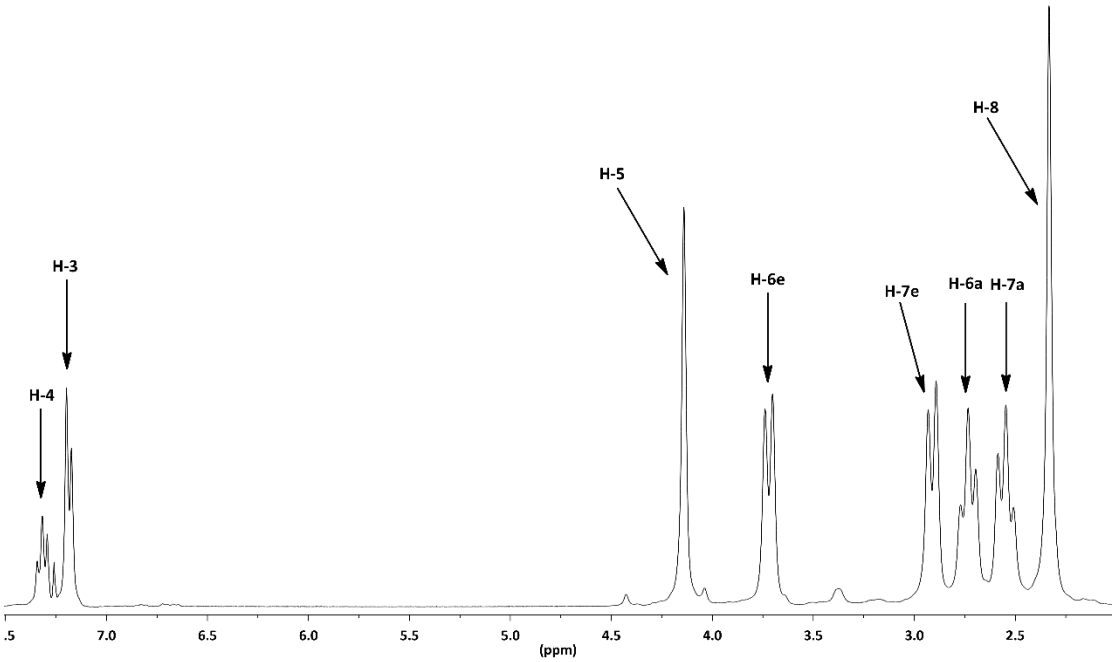


Figure S2. ^{1}H NMR (301 MHz, $CDCl_3$) spectrum of compound **1**, at -60 °C.

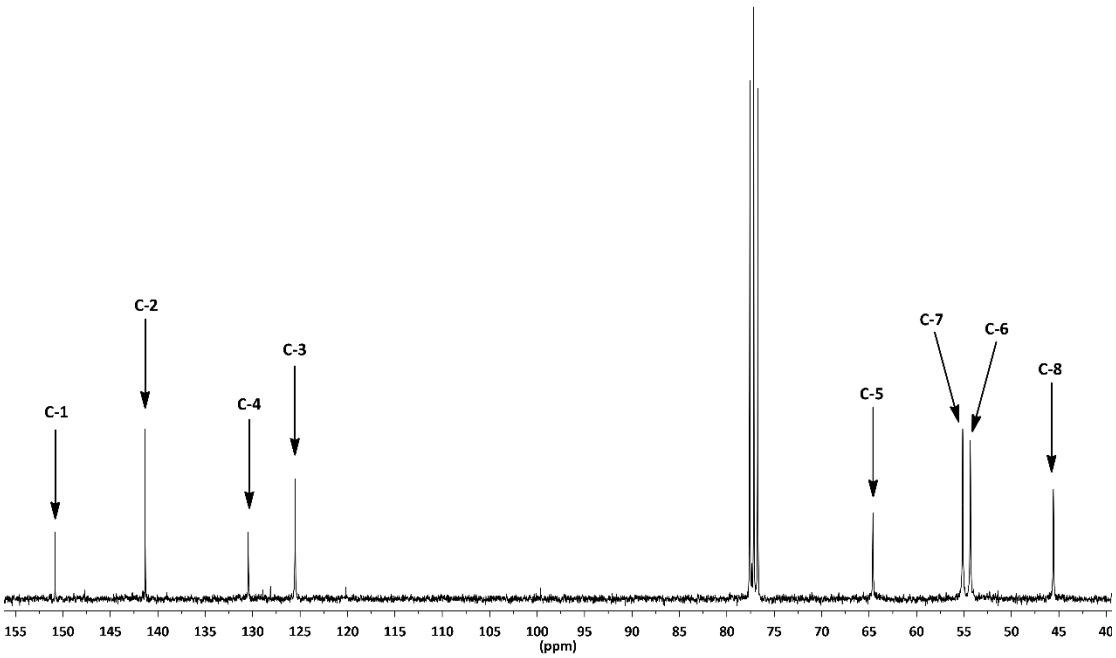


Figure S3. ^{13}C NMR (76 MHz, $CDCl_3$) spectrum of compound **1**, at -60 °C.

- the crystal contains a 1:1 mixture of (pS_{N1},pS_{N3})- and (pR_{N1},pR_{N3})-**1a** and (pS_{N5},pS_{N7})- and (pR_{N5},pR_{N7})-**1b** isomers

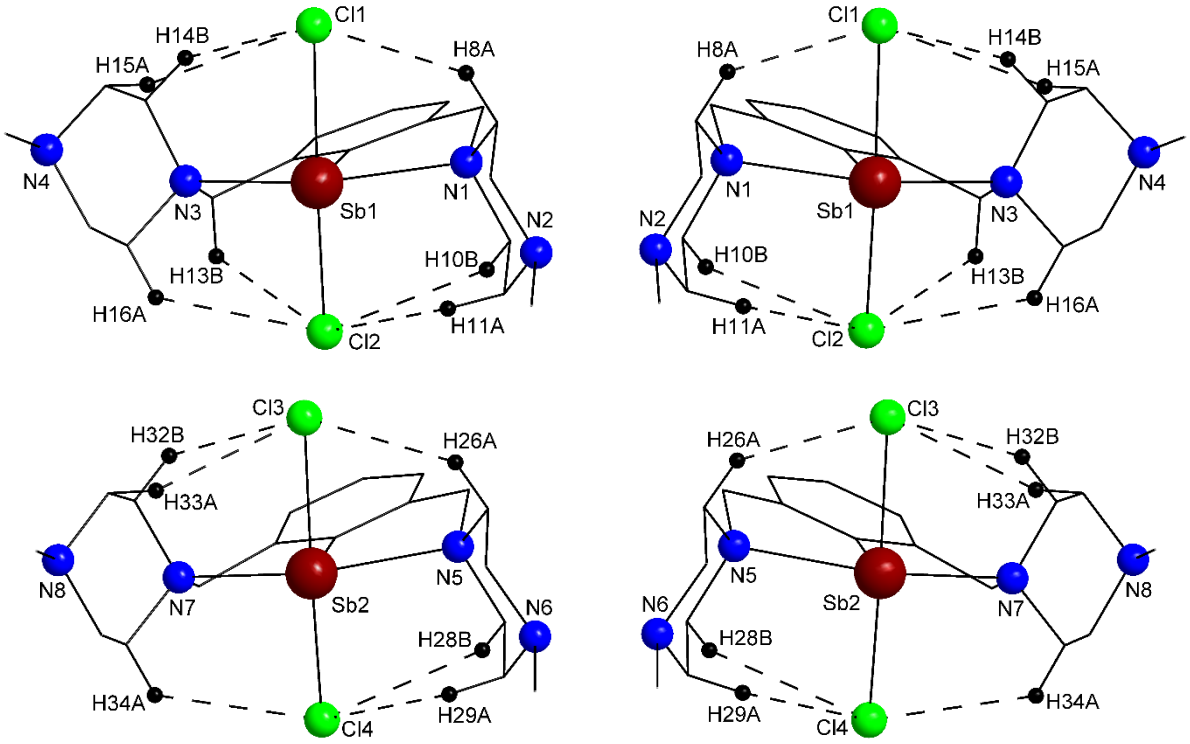


Figure S4. Molecular structure of isomers (pS_{N1},pS_{N3})-**1a** (*left, up*), (pR_{N1},pR_{N3})-**1a** (*right, up*), (pS_{N1},pS_{N3})-**1b** (*left, down*) and (pR_{N1},pR_{N3})-**1b** (*right, down*) in the crystal of **1**, showing the intramolecular Cl···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance

Cl(1)···H(8A)$_{methylene}$	2.78 Å	$\sum r_{vdW}$(Cl,H) 3.01 Å
Cl(1)···H(14B)$_{methylene}$	2.88 Å	
Cl(1)···H(15A)$_{methylene}$	2.92 Å	
Cl(2)···H(10B)$_{methylene}$	2.85 Å	
Cl(2)···H(11A)$_{methylene}$	2.94 Å	
Cl(2)···H(13B)$_{methylene}$	2.91 Å	
Cl(2)···H(16A)$_{methylene}$	2.83 Å	
Cl(3)···H(26A) $_{methylene}$	2.78 Å	
Cl(3)···H(32B) $_{methylene}$	2.81 Å	
Cl(3)···H(33A) $_{methylene}$	2.82 Å	
Cl(4)···H(28B) $_{methylene}$	2.91 Å	
Cl(4)···H(29A) $_{methylene}$	2.89 Å	
Cl(4)···H(34A) $_{methylene}$	2.81 Å	

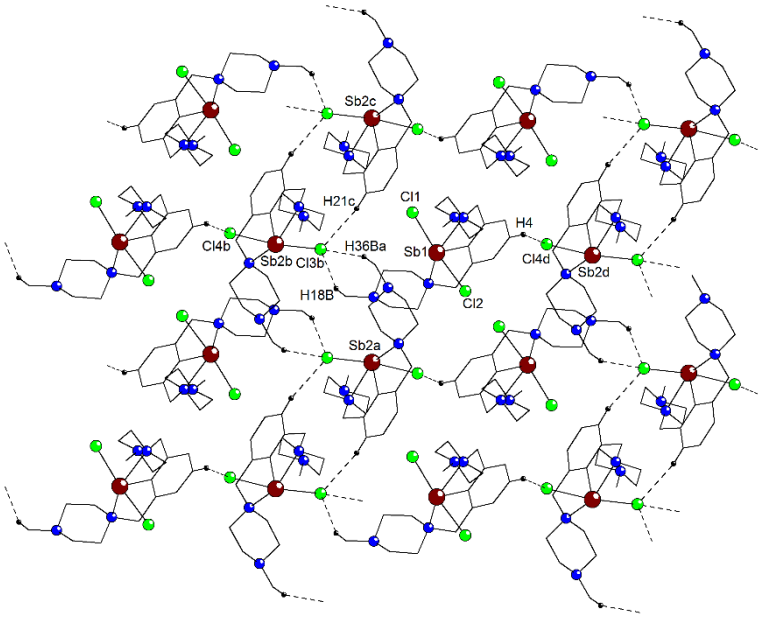


Figure S5. View along *a* axis of a layer based on Cl···H contacts in the crystal of **1** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*–1+x, y, z*), (*1–x, 1–y, 1–z*), (*–1+x, 1+y, z*) and (*1–x, 1–y, –z*) are given by "a", "b", "c" and "d", respectively].

-	intermolecular distance	Cl(3b)···H(21c)$_{aryl}$	2.95 Å	$\sum r_{vdW}$(Cl,H) 3.01 Å
		Cl(3b)···H(18B)$_{methyl}$	2.90 Å	
		Cl(3b)···H(36Ba)$_{methyl}$	2.87 Å	
		Cl(4d)···H(4)$_{aryl}$	2.92 Å	

- no further contacts between parallel layers in the crystal of **1**.

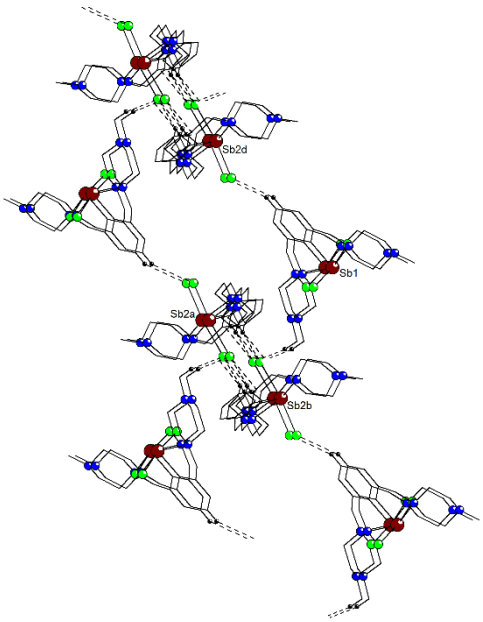


Figure S6. View along *b* axis of a layer based on Cl···H contacts in the crystal of **1** (only hydrogen atoms involved in intermolecular contacts are shown).

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]$_2$Sb$_2$O$_2$ (3)

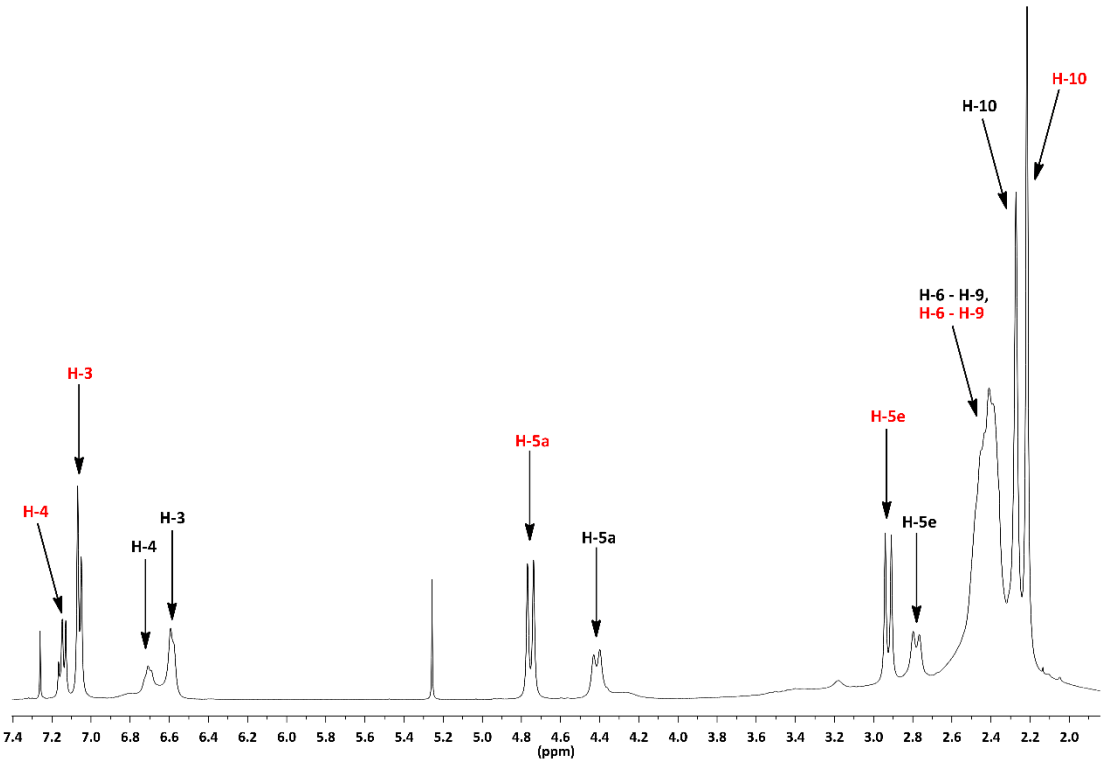


Figure S7. ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of compound **3**, at r.t. (isomer **3a** – black; isomer **3b** – red).

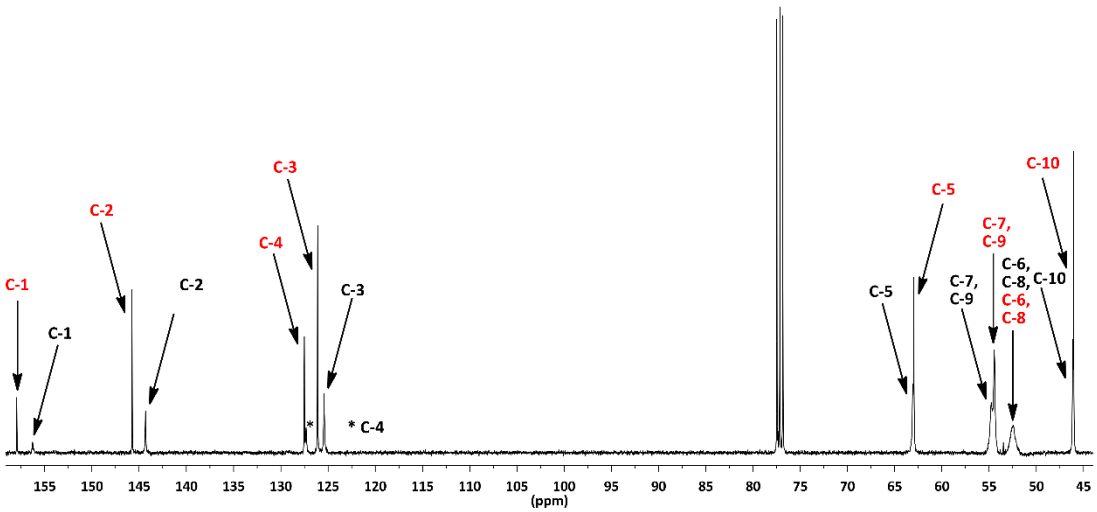


Figure S8. ^{13}C NMR (101 MHz, CDCl$_3$) spectrum of compound **3**, at r.t. (isomer **3a** – black; isomer **3b** – red).

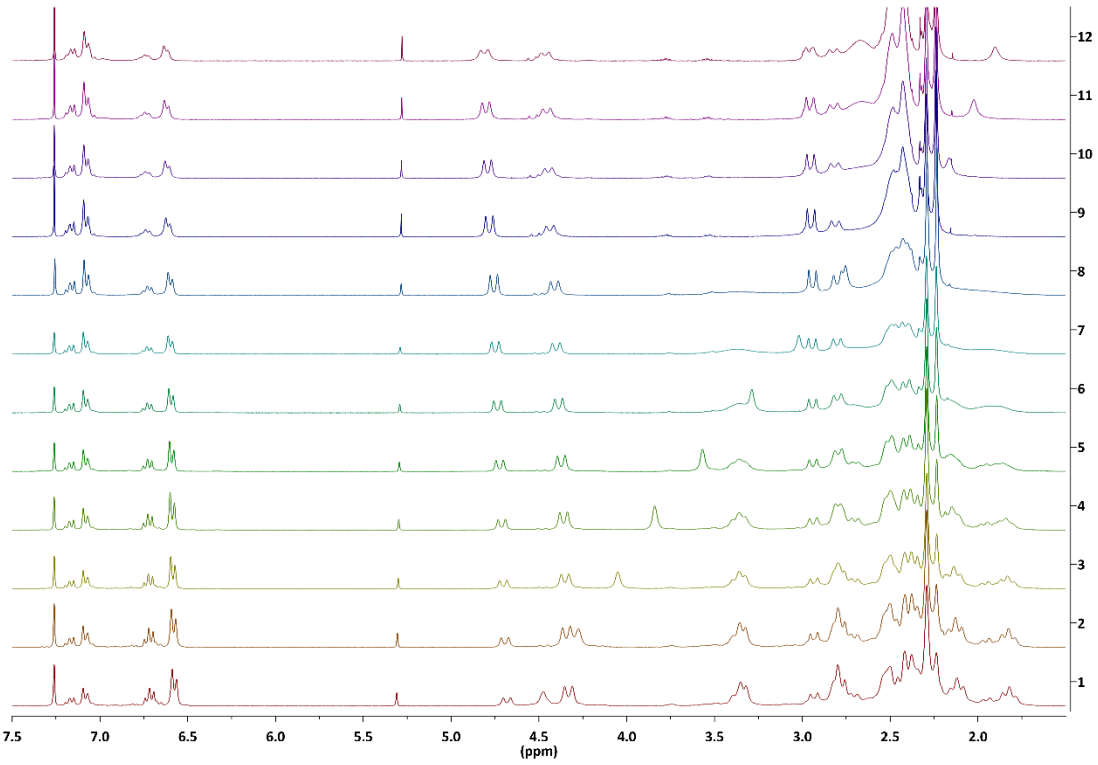


Figure S9. ^{1}H NMR (301 MHz, $CDCl_3$) spectra of compound **3** at temperatures ranging from -60 °C (down) to 60 °C (up); increments of 10 °C.

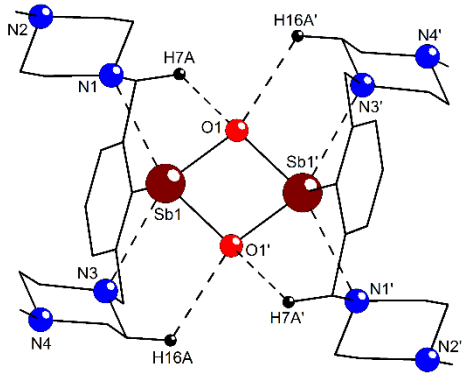


Figure S10. Molecular structure of **3**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown) [symmetry equivalent atoms (*1–x, 1–y, 2–z*) are given by "prime"].

- intramolecular distance $O(1)\cdots H(7A)_{methylene}$ 2.55 Å $\sum r_{vdW}(O,H)$ 2.60 Å
  $O(1)\cdots H(16A')_{methylene}$ 2.59 Å

- no further contacts between molecules in the crystal of **3**.

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]$_2$Bi$_2$O$_2$ (4)

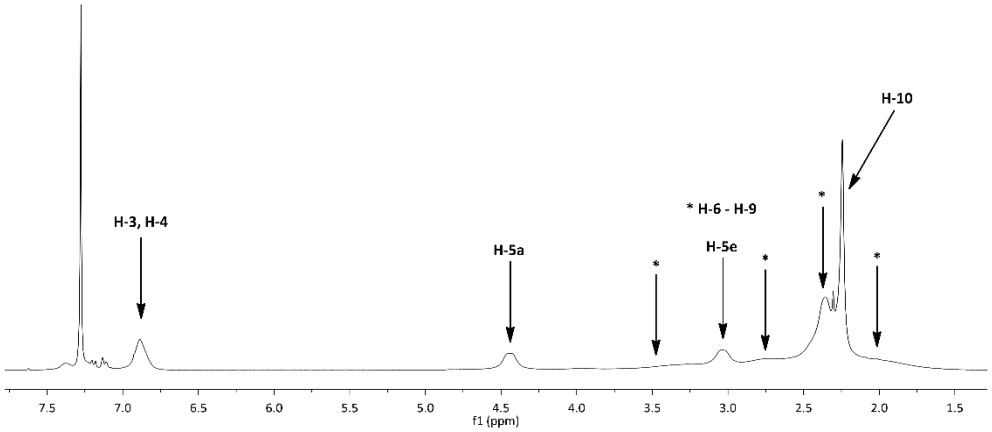


Figure S11. ^{1}H NMR (301 MHz, $CDCl_3$) spectrum of compound **4**, at r.t.

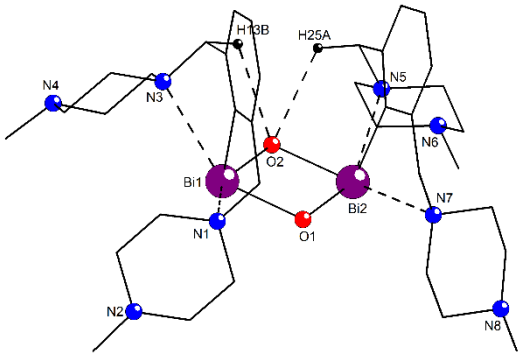


Figure S12. Molecular structure of **4**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

-	intramolecular distance	O(2)···H(13B)$_{methylene}$	2.59 Å	$\sum r_{vdW}$(O,H) 2.60 Å
		O(2)···H(25A)$_{methylene}$	2.54 Å	

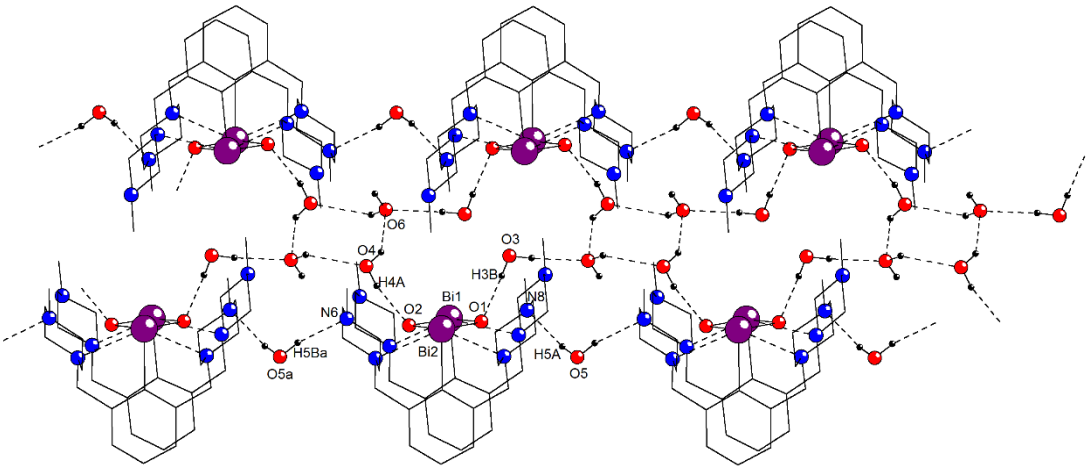


Figure S13. View of a chain polymer of dinuclear units of **4** and water molecules based on N···H and O···H hydrogen bonds in the crystal of **4**·4H$_2$O (only hydrogen atoms of water molecules are shown) [symmetry equivalent atoms (*–1+x, y, z*) are given by "a"].

-	intermolecular distance	N(6)···H(5Ba)$_{water}$	2.12 Å	$\sum r_{vdW}$(N,H) 2.74 Å
		N(8)···H(5A)$_{water}$	2.13 Å	
		O(1)···H(3B)$_{water}$	1.88 Å	$\sum r_{vdW}$(O,H) 2.64 Å
		O(2)···H(4A)$_{water}$	1.95 Å	

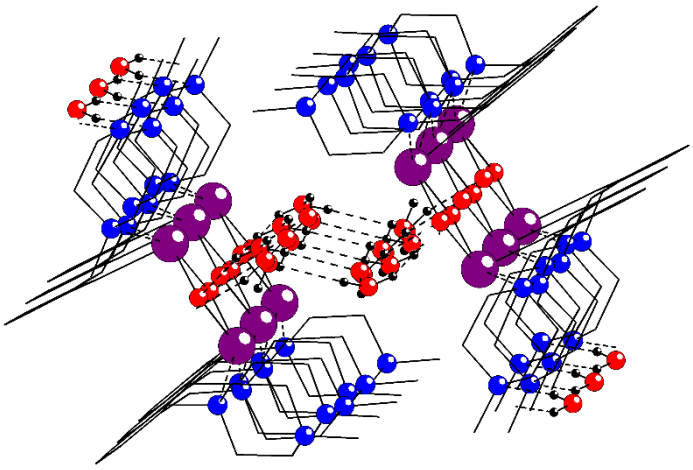


Figure S14. View along *a* axis of the chain polymer in the crystal of **4**·4H_2O (only hydrogen atoms of water molecules are shown).

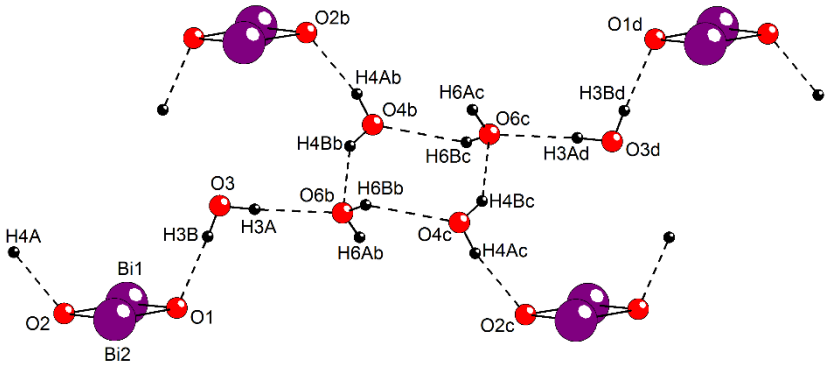


Figure S15. View of a hexameric cluster of water molecules connected to four dinuclear units of **4** through O···H hydrogen bonds in the crystal of **4**·4H_2O (only hydrogen atoms of water molecules are shown) [symmetry equivalent atoms (*1–x, 1–y, 1–z*), (*1+x, y, z*) and (*2–x, 1–y, 1–z*) are given by "b", "c" and "d", respectively].

-	intermolecular distance	$O(6b)\cdots H(3A)_{water}$	2.12 Å	$\sum r_{vdW}(O,H)$ 2.64 Å
		$O(6b)\cdots H(4Bb)_{water}$	2.11 Å	
		$O(4c)\cdots H(6Bb)_{water}$	2.30 Å	

[{2-(MeN(H){CH_2CH_2}$_2$NCH_2)-6-(MeN{CH_2CH_2}$_2$NCH_2)C_6H_3}$_2$$Sb_2$O(OH)](O$_2CCF_3$)$_3$ (5)

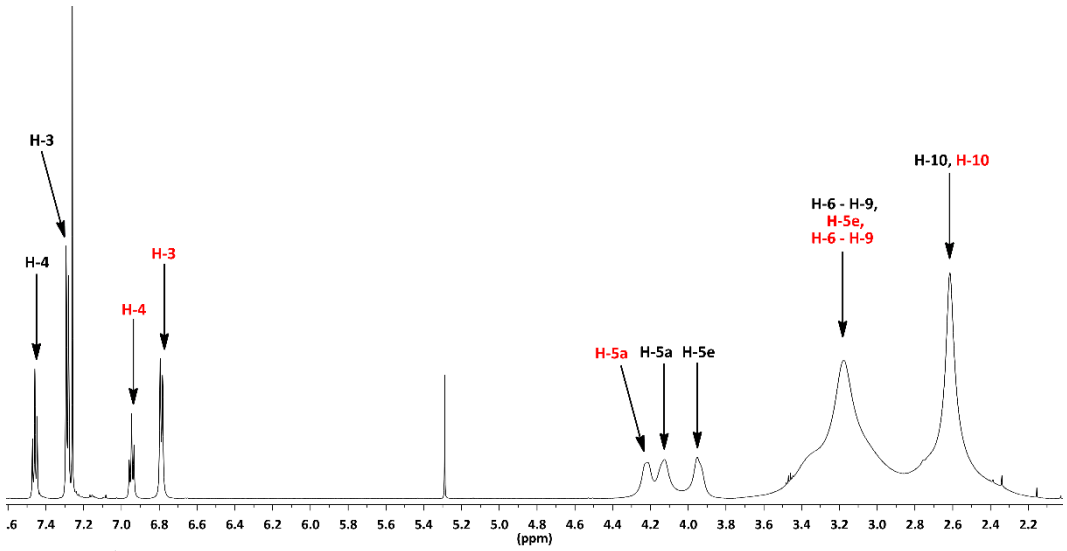


Figure S16. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **5**, at r.t. (isomer **5a** – black; isomer **5b** – red).

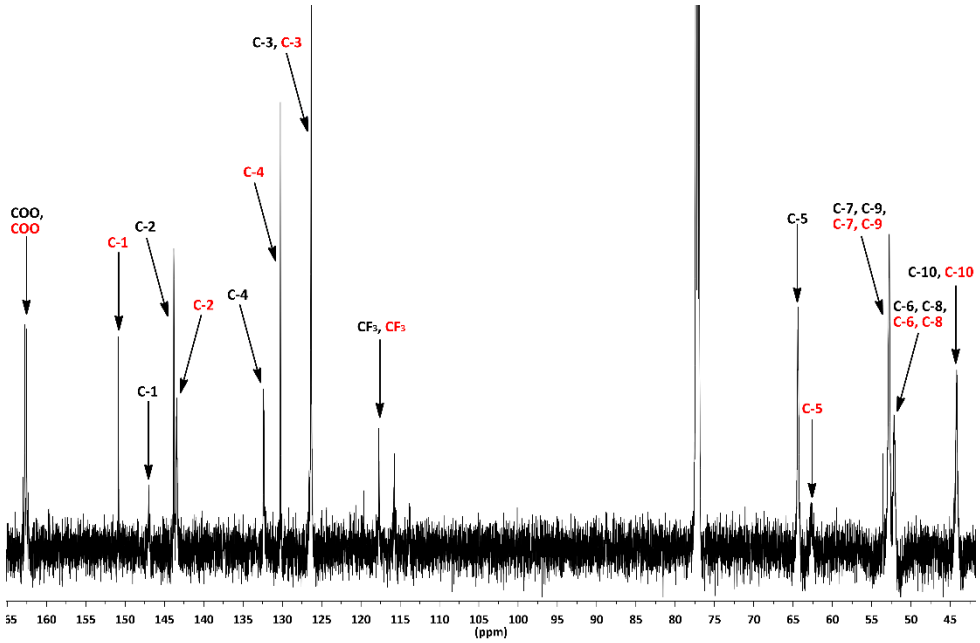


Figure S17. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **5**, at r.t. (isomer **5a** – black; isomer **5b** – red).

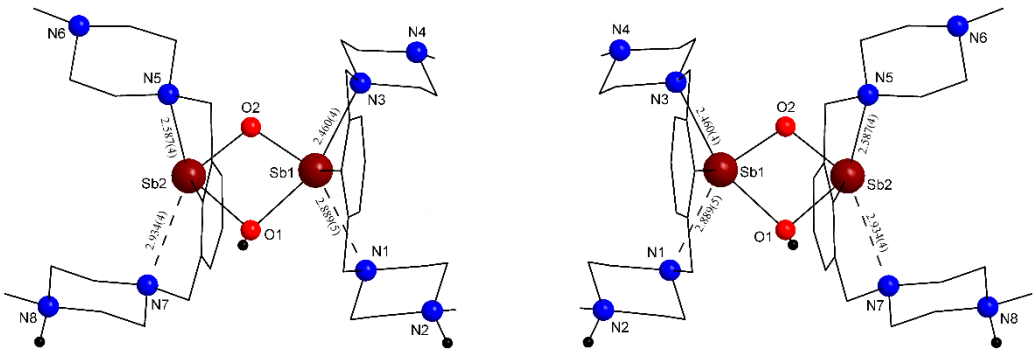


Figure S18. Structure of cations *syn*-(C_{Sb1},pS_{N1},pR_{N3})(A_{Sb2},pR_{N7},pS_{N5})-**5** (*left*) and *syn*-(A_{Sb1},pR_{N1},pS_{N3})(C_{Sb2},pS_{N7},pR_{N5})-**5** (*right*) in the crystal of **5** (only hydrogen atoms attached to oxygen and nitrogen atoms are shown).

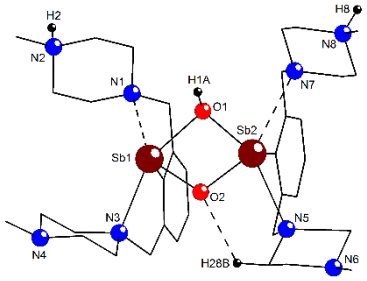


Figure S19. Structure of cation in the crystal of **5**·H_2O·C_6H_5Me, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance O(2)···H(28B)$_{methylene}$ 2.50 Å $\sum r_{vdW}$(O,H) 2.60 Å

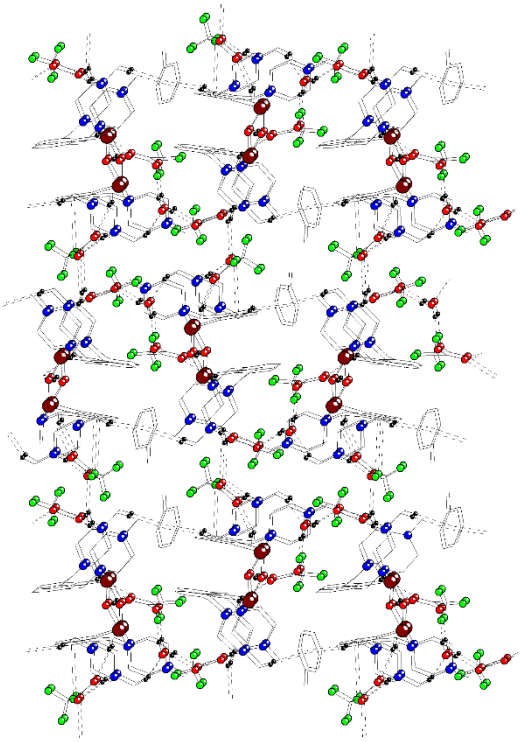


Figure S20. View along *a* axis of the 3D architecture based on O···H hydrogen bonds as well as O···H, C–H···π ($Ar_{centroid}$) and C–F···π ($Ar_{centroid}$) contacts in the crystal of **5**·H_2O·C_6H_5Me (only hydrogen atoms involved in inter cation/anion/water contacts are shown) [symmetry equivalent atoms (*1+x, y, z*), (*1+x, 0.5–y, –0.5+z*), (*–1+x, y, z*), (*1–x, 0.5+y, 0.5–z*) and (*x, 0.5–y, –0.5+z*) are given by "a", "b", "c", "d" and "e", respectively].

- inter cation/anion/water distance

O(3a)$_{anion}$···H(1A)$_{cation}$	1.81 Å	$\sum r_{vdW}$(O,H) 2.60 Å
O(3a)$_{anion}$···H(33A)$_{cation}$	2.44 Å	
O(4a)$_{anion}$···H(9C)$_{water}$	2.15 Å	
O(5b)$_{anion}$···H(8)$_{cation}$	1.75 Å	
O(6b)$_{anion}$···H(8)$_{cation}$	2.57 Å	
O(6a)$_{anion}$···H(9D)$_{water}$	1.93 Å	
O(7)$_{anion}$···H(2c)$_{cation}$	1.88 Å	
O(7)$_{anion}$···H(33Bd)$_{cation}$	2.56 Å	
O(8)$_{anion}$···H(2c)$_{cation}$	2.26 Å	
O(8)$_{anion}$···H(13A)$_{cation}$	2.49 Å	
O(9)$_{water}$···H(12B)$_{cation}$	2.57 Å	
C(7)–H(7B)$_{methylene}$···$Ar_{centroid}${C(43)-C(48)}		2.75 Å γ = 7.1°
C(36e)–H(36Be)$_{methylene}$···$Ar_{centroid}${C(43)-C(48)}		2.71 Å γ = 10.5°
C(41)–F(7)$_{anion}$···$Ar_{centroid}${C(1)-C(6)}		3.81 Å γ = 24.1°

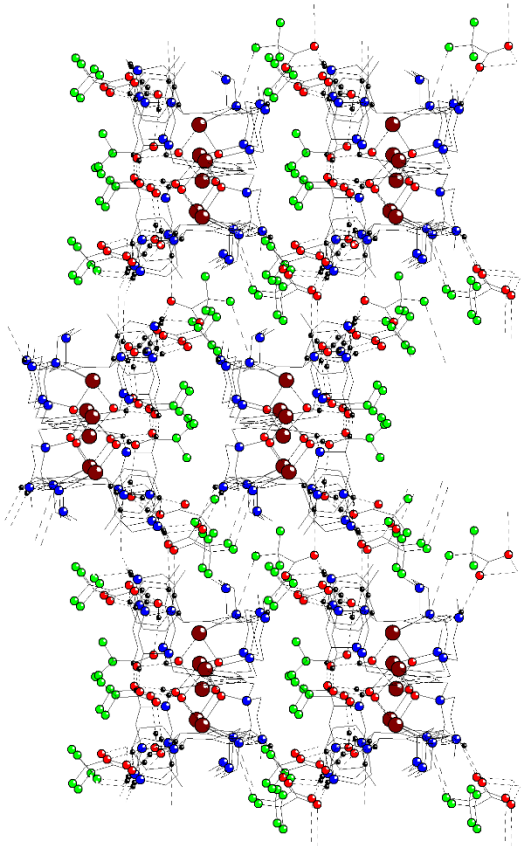


Figure S21. View along *c* axis of the 3D architecture based on O···H hydrogen bonds as well as O···H, C–H···π ($Ar_{centroid}$) and C–F···π ($Ar_{centroid}$) contacts in the crystal of **5**·H_2O·C_6H_5Me (only hydrogen atoms involved in inter cation/anion/water contacts are shown).

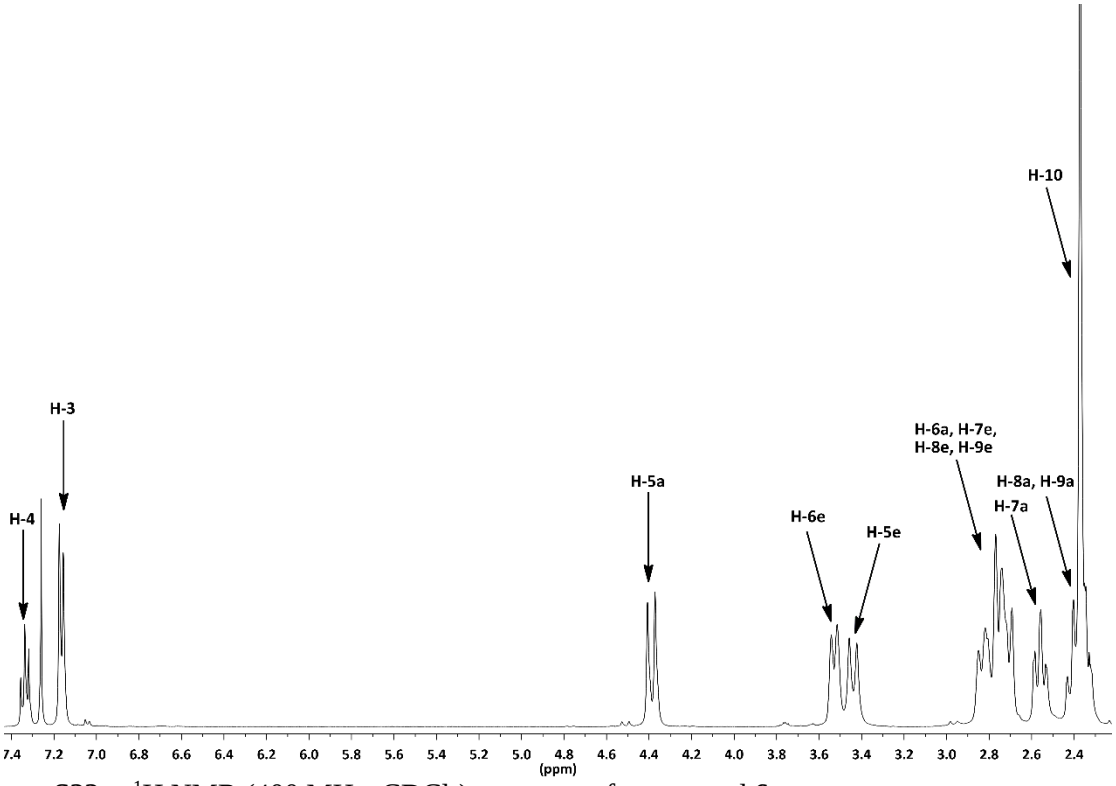


Figure S22. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6**, at r.t.

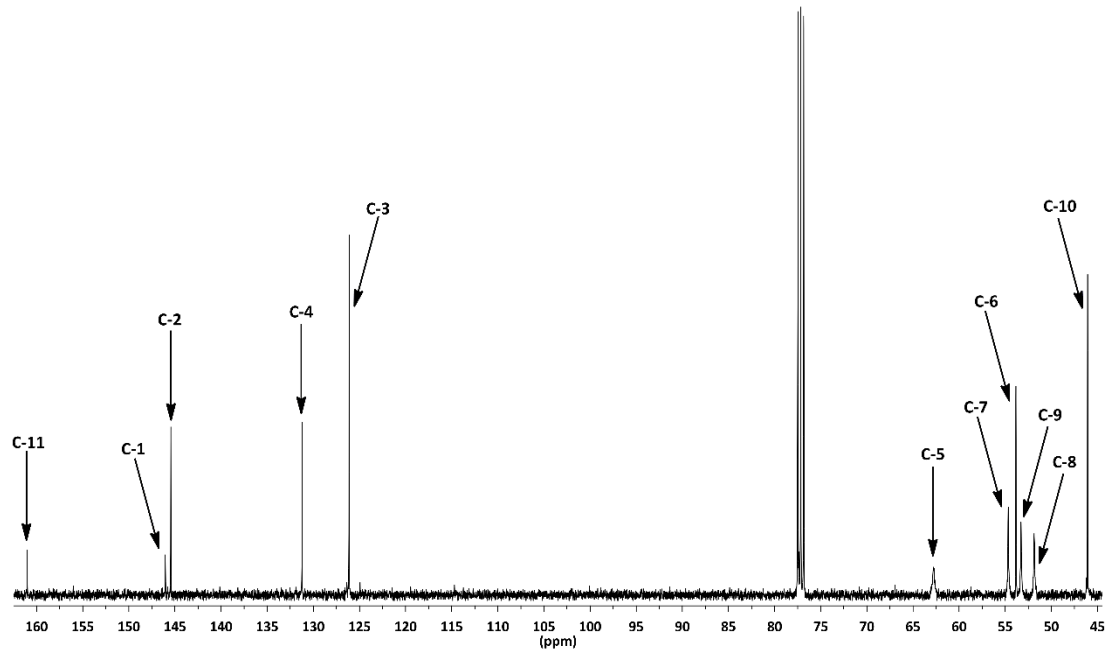


Figure S23. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **6**, at r.t.

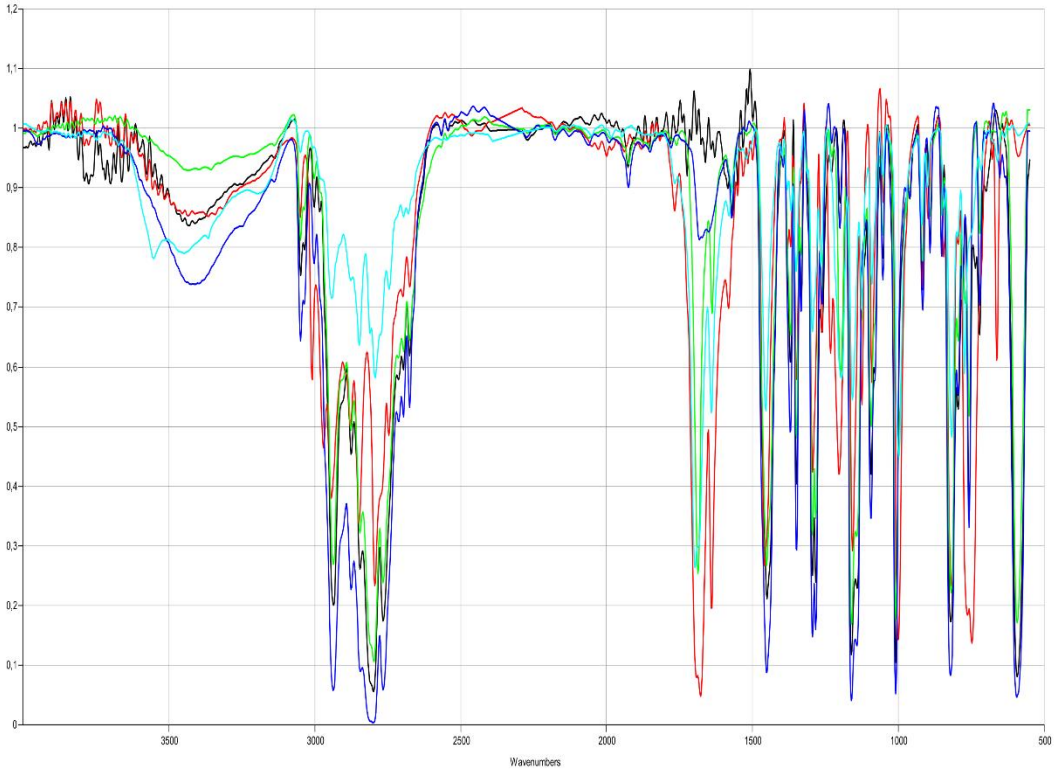


Figure S24. Infrared spectra (KBr pellets) of **3** (black line), **6** (red line) obtained from **3**, **6** heated at 110 °C for 4 h (green line) – partly converted to **3** –, **6** heated at 110 °C for 9 h (blue line) – almost completely converted to **3** –, and **6** (cyan line) obtained from the previously decomposed sample.

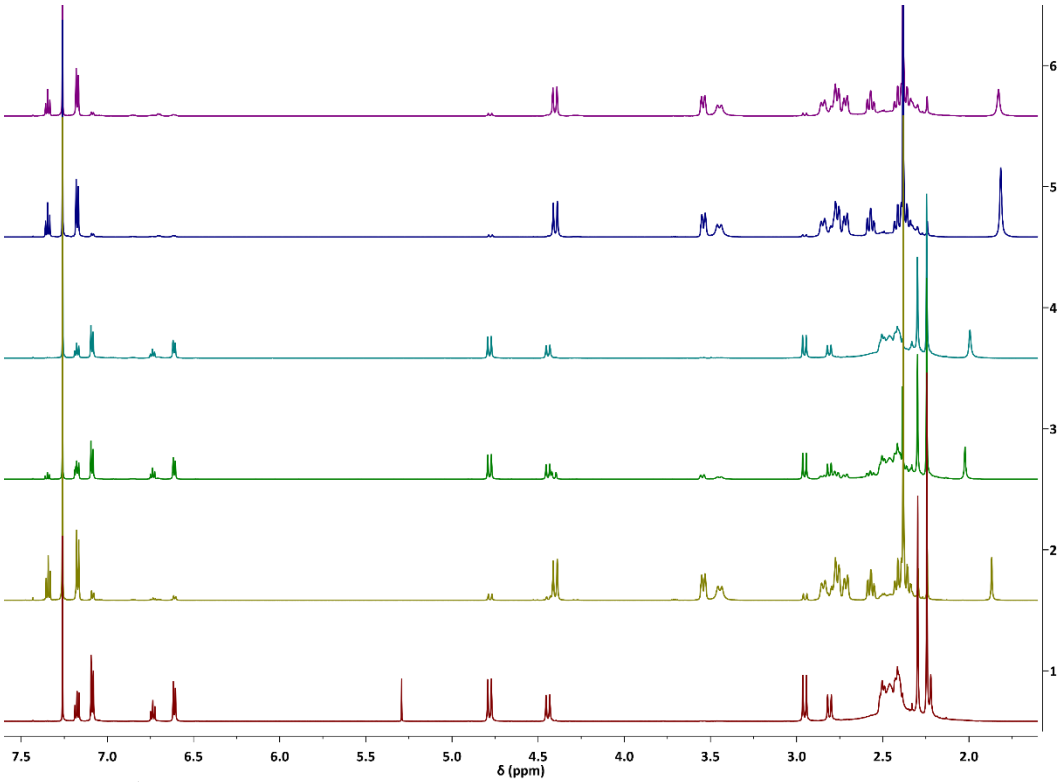


Figure S25. ^{1}H NMR (600 MHz) spectra of **3** (spectrum 1), **6** obtained from **3** (spectrum 2), **6** heated at 110 °C for 4 h (spectrum 3) – partly converted to **3** –, **6** heated at 110 °C for 9 h (spectrum 4) – almost completely converted to **3** –, **6** obtained from the previously decomposed sample (spectrum 5), **6** obtained from the previously decomposed sample dried at reduced pressure (10^{-3} mbar) for 1 h (spectrum 6). All spectra were recorded in $CDCl_3$.

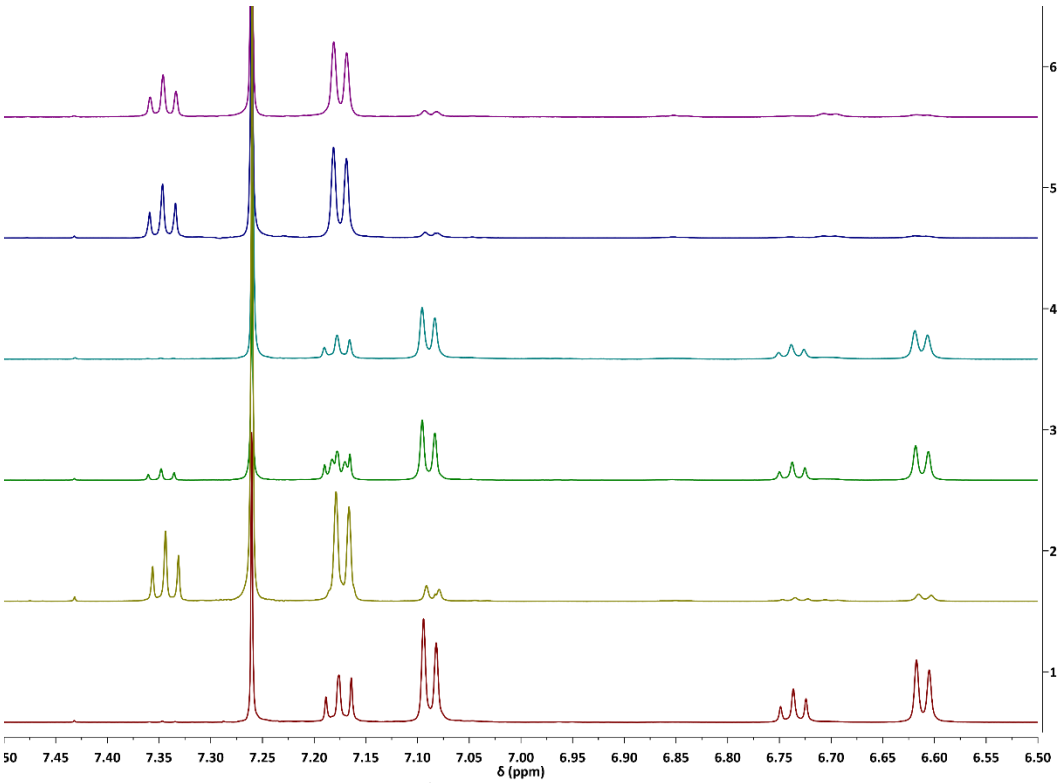


Figure S26. Aromatic region of the ^{1}H NMR (600 MHz) spectra of **3** (spectrum 1), **6** obtained from **3** (spectrum 2), **7** heated at 110 °C for 4 h (spectrum 3) – partly converted to **3** –, **6** heated at 110 °C for 9 h (spectrum 4) – almost completely converted to **3** –, **6** obtained from the previously decomposed sample (spectrum 5), **6** obtained from the previously decomposed sample dried at reduced pressure (10^{-3} mbar) for 1 h (spectrum 6). All spectra were recorded in $CDCl_3$.

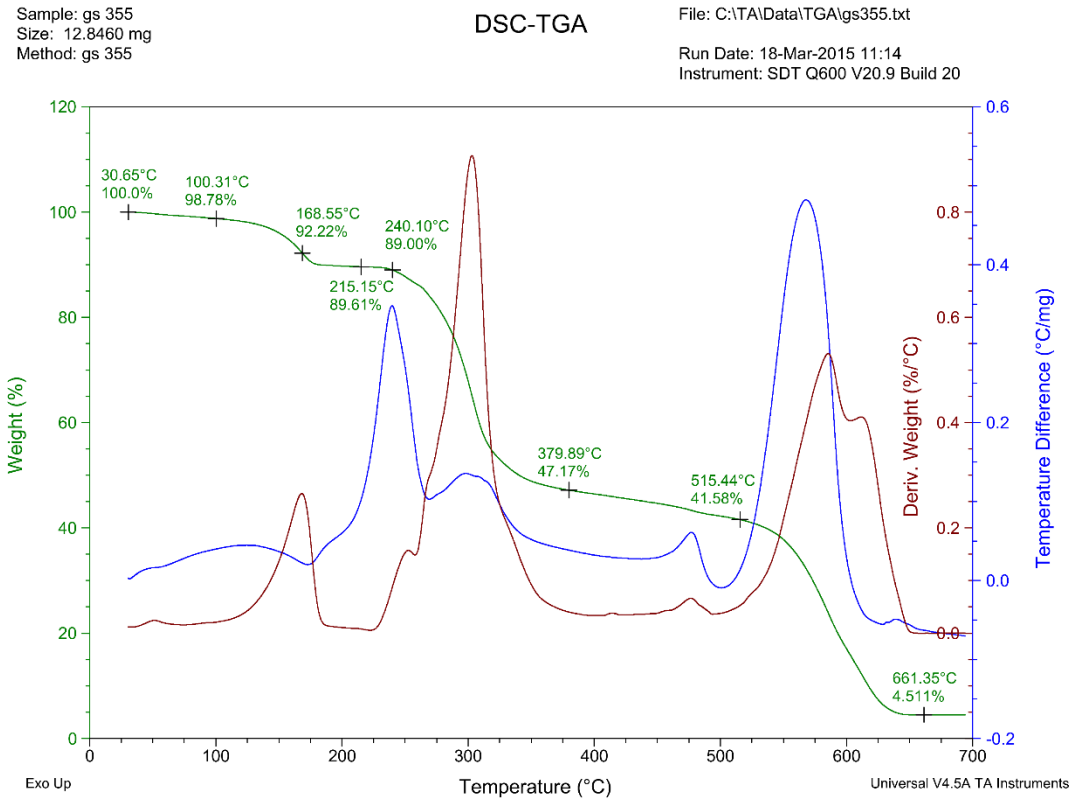


Figure S27. TGA analysis of the sample of **6** dried at reduced pressure (10^{-3} mbar) for 1 h.

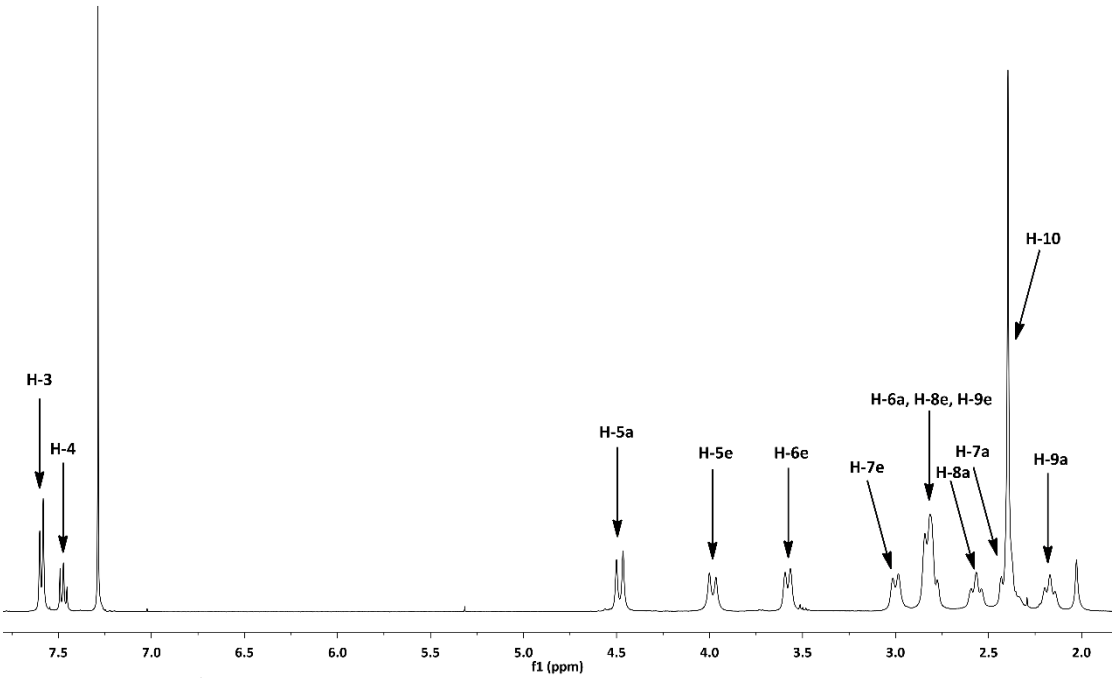


Figure S28. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7**, at r.t.

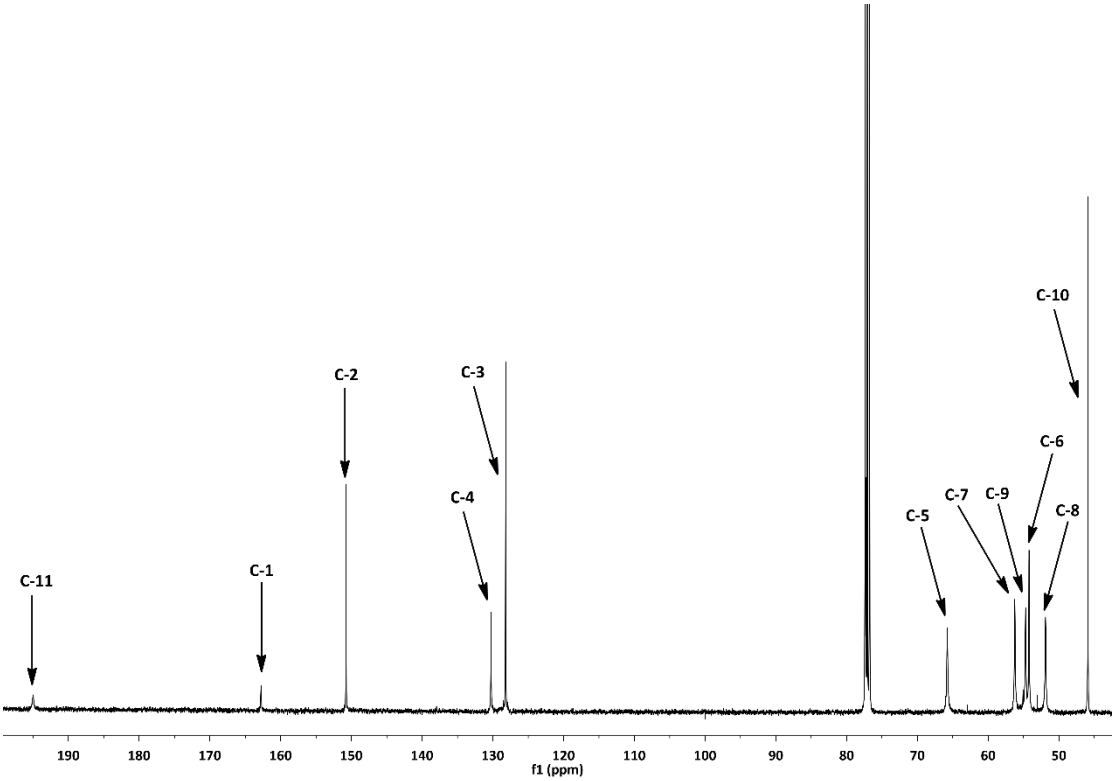


Figure S29. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **7**, at r.t.

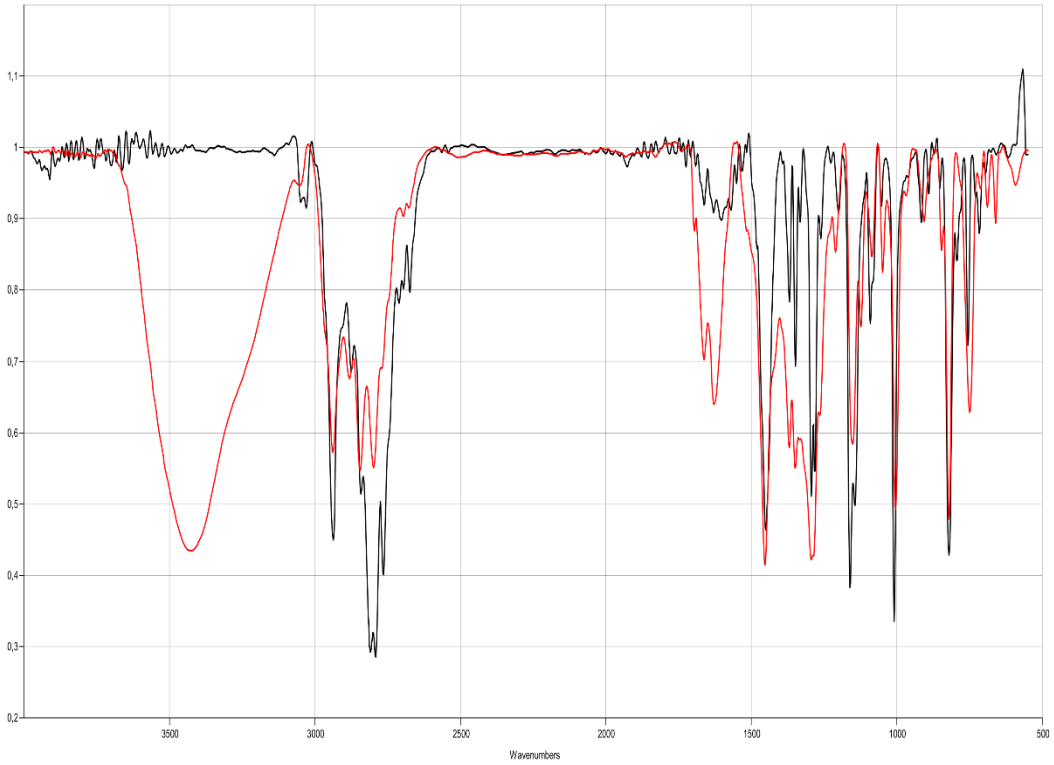


Figure S30. IR spectra (KBr pellets) of compound **4** (black line) and **7** (red line).

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Sb[O(O)CC(O)O] (8)

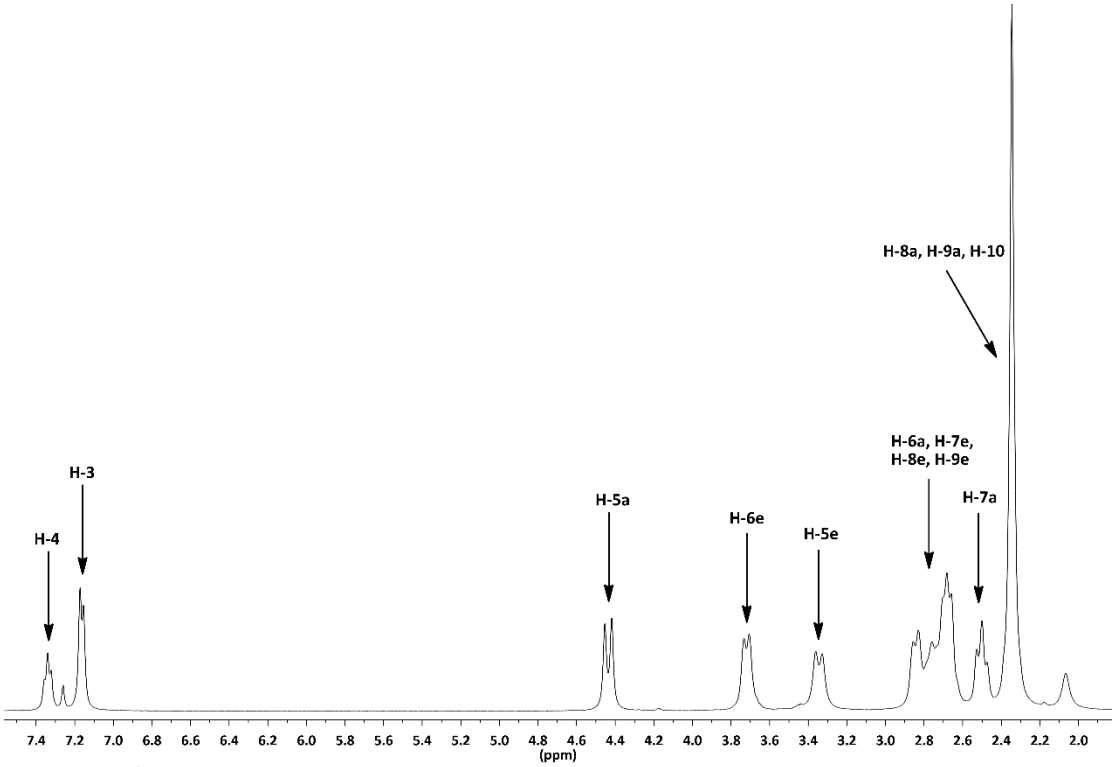


Figure S31. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8**, at r.t.

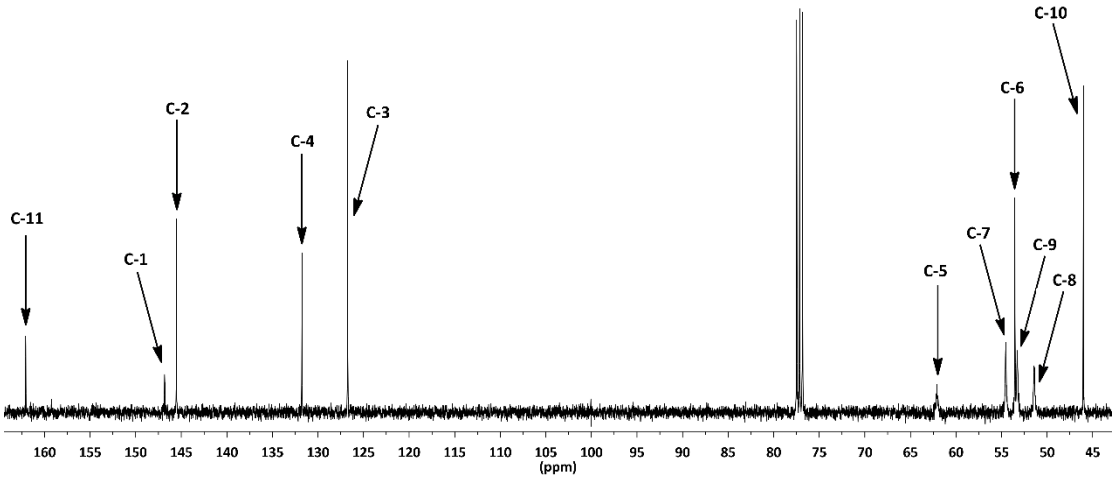


Figure S32. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **8**, at r.t.

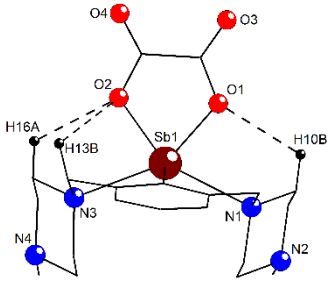


Figure S33. Molecular structure of **8**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

-	intramolecular distance	O(1)···H(10B)$_{methylene}$	2.58 Å	$\sum r_{vdW}$(O,H) 2.60 Å
		O(2)···H(13B)$_{methylene}$	2.54 Å	
		O(2)···H(16A)$_{methylene}$	2.57 Å	

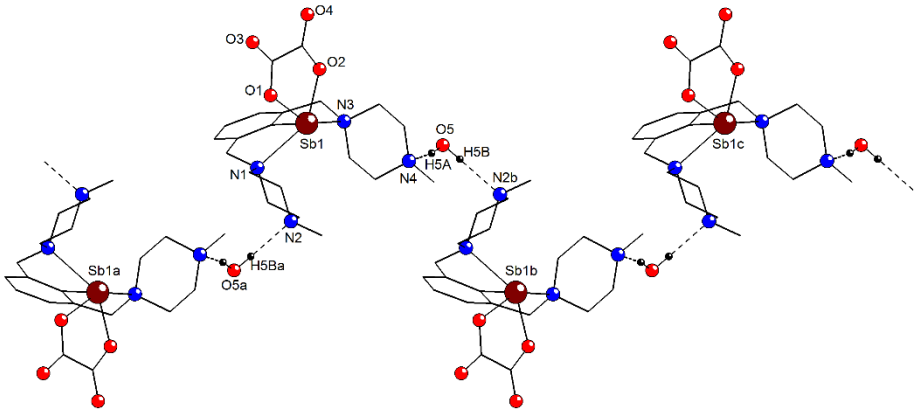


Figure S34. View of the chain polymer based on N···H_{water} hydrogen bonds in the crystal of **8**·H_2O (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*1+x, 0.5–y, 0.5+z*), (*–1+x, 0.5–y, –0.5+z*) and (*–2+x, y, –1+z*) are given by "a", "b" and "c", respectively].

- intermolecular distance N(2)···$H(5Ba)_{water}$ 2.04 Å $\sum r_{vdW}$(N,H) 2.74 Å
  N(4)···$H(5A)_{water}$ 2.02 Å

- no further contacts between parallel chains.

[(2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Sb[O$_2$-1,2-C$_6$H$_3$-3-(CH$_2$)$_2$NH$_3$]Cl (9)

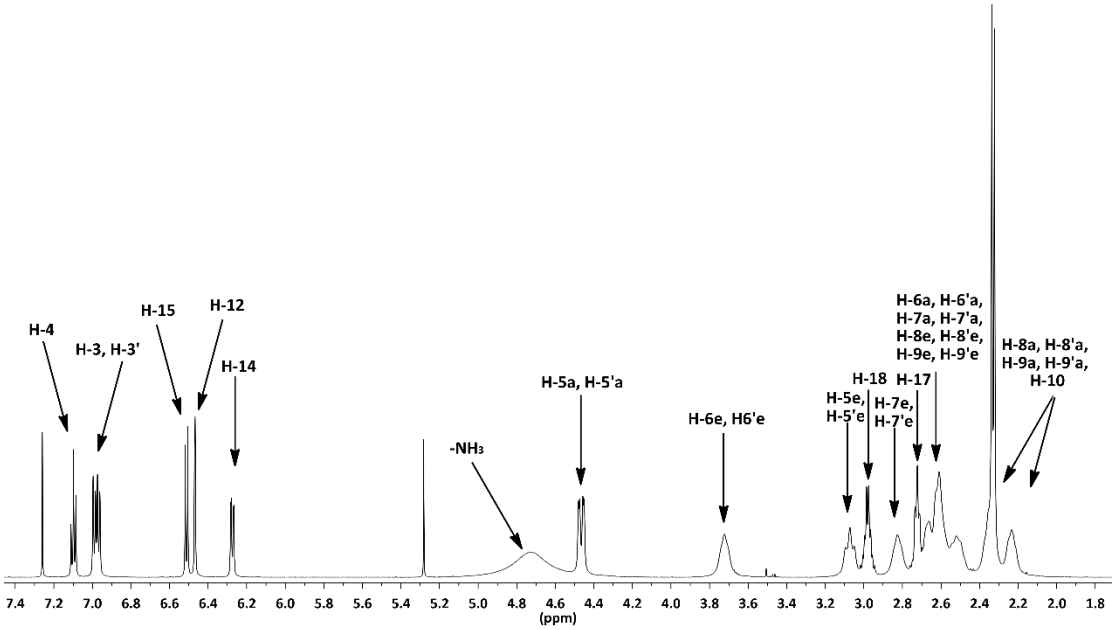


Figure S35. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **9**, at r.t.

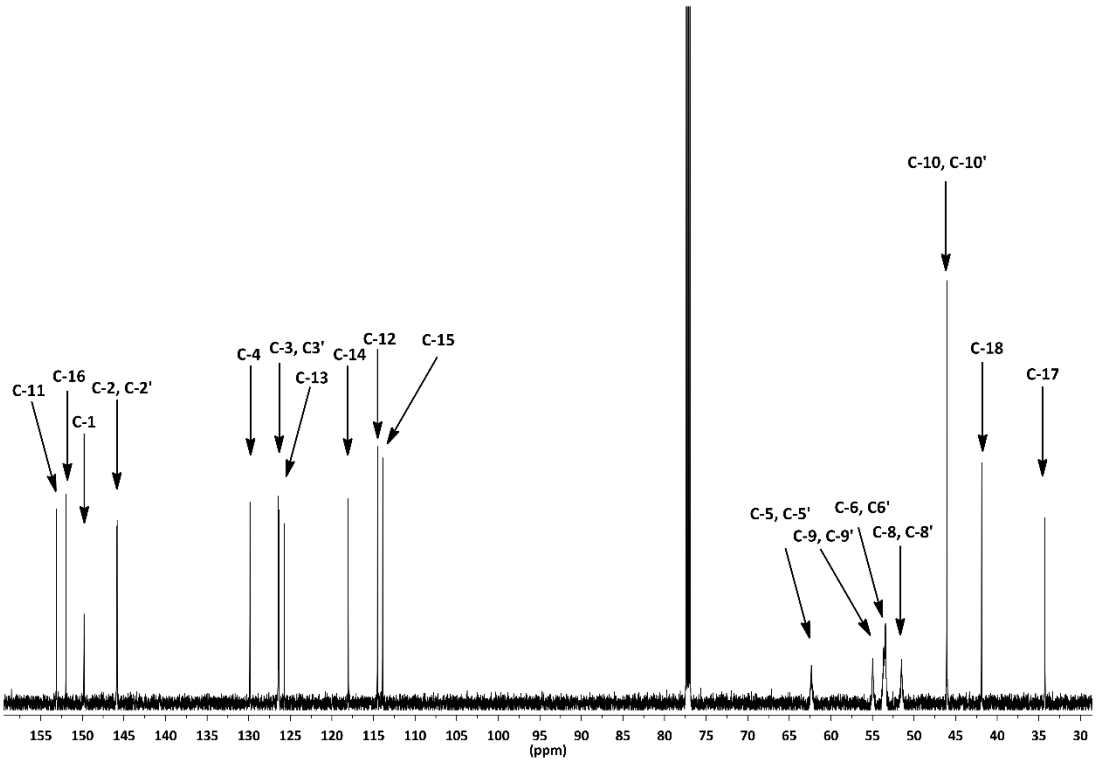


Figure S36. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **9**, at r.t.

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Sb(OCH$_2$)$_2$ (10)

^{1}H NMR (301 MHz, $CDCl_3$, 333 K): δ 2.31 (s, 6H, H-10), 2.35-2.91 (m br, 16H, H-6 – H-9), 2.95 (d, $^2J_{H\text{-}5a,H\text{-}5e}$ = 13.2 Hz, 2H, H-5e), 3.47-3.57 (m, AA′BB′ vicinal spin system, 2H, H-11a), 3.68-3.81 (m, AA′BB′ vicinal spin system, 2H, H-11e), 4.52 (d, $^2J_{H\text{-}5a,H\text{-}5e}$ = 13.2 Hz, 2H, H-5a), AB_2 spin system with B at δ 7.02 ppm (d, $^3J_{H\text{-}3,H\text{-}4}$ = 7.4 Hz, 2H, H-3) and A at δ 7.14 ppm (t, $^3J_{H\text{-}3,H\text{-}4}$ = 7.4 Hz, 1H, H-4).

^{13}C{^{1}H} NMR (76 MHz, $CDCl_3$, 333 K): δ 46.11 (C-10), 52.45 (C-6 and C-8), 54.65 (C-7 and C-9), 62.60 (C-5), 67.08 (C-11), 126.36 (C-3), 128.75 (C-4), 146.23 (C-2), 151.54 (C-1).

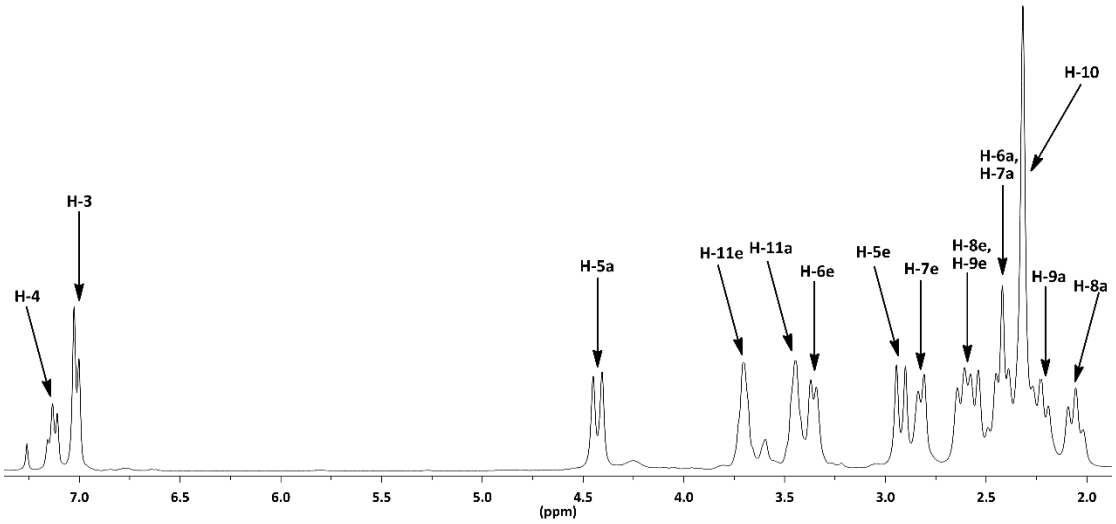


Figure S37. ^{1}H NMR (301 MHz, $CDCl_3$) spectrum of compound **10**, at -60 °C.

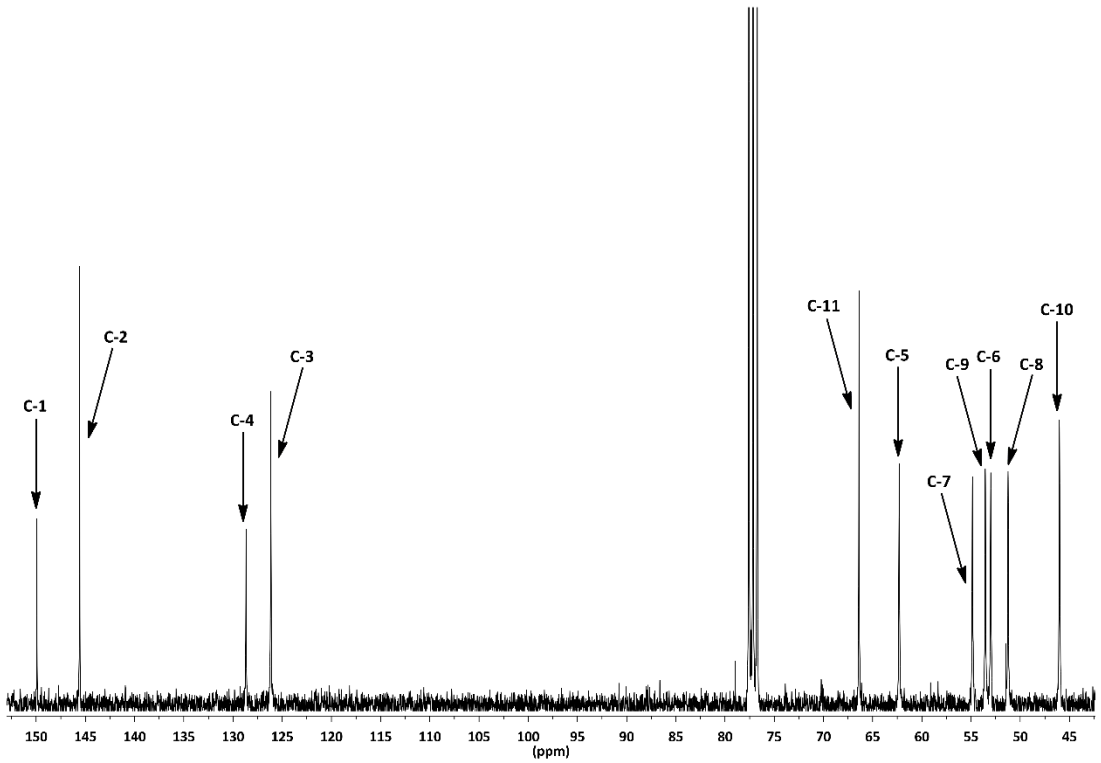


Figure S38. ^{13}C NMR (76 MHz, $CDCl_3$) spectrum of compound **10**, at -60 °C.

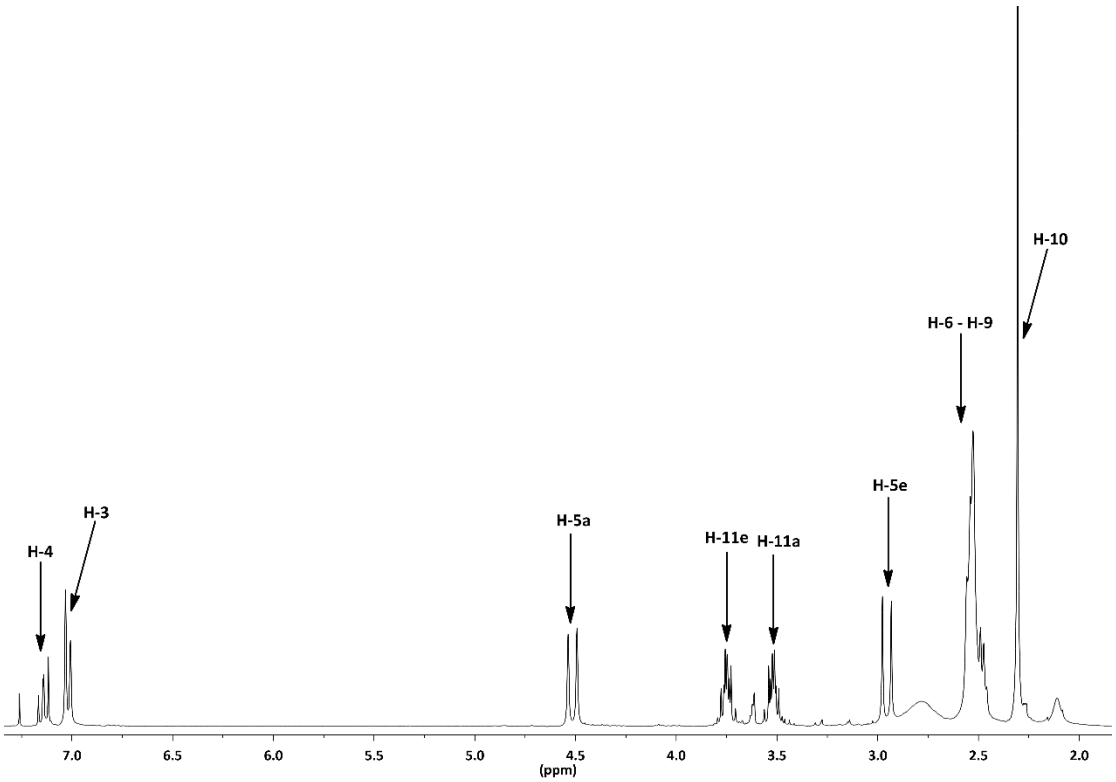


Figure S39. ^{1}H NMR (301 MHz, $CDCl_3$) spectrum of compound **10**, at 60 °C.

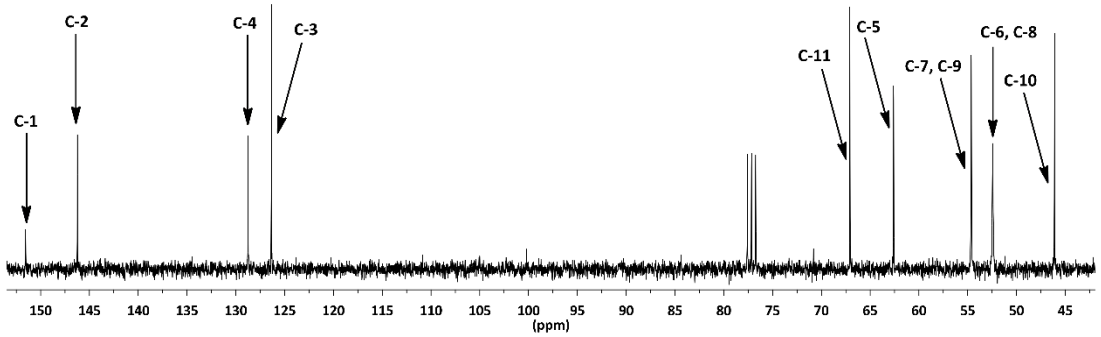


Figure S40. ^{13}C NMR (76 MHz, $CDCl_3$) spectrum of compound **10**, at 60 °C.

- the crystal contains a 1:1 mixture of (δ-pS_{N1},pR_{N3})- and (λ-pR_{N1},pS_{N3})-**10** isomers

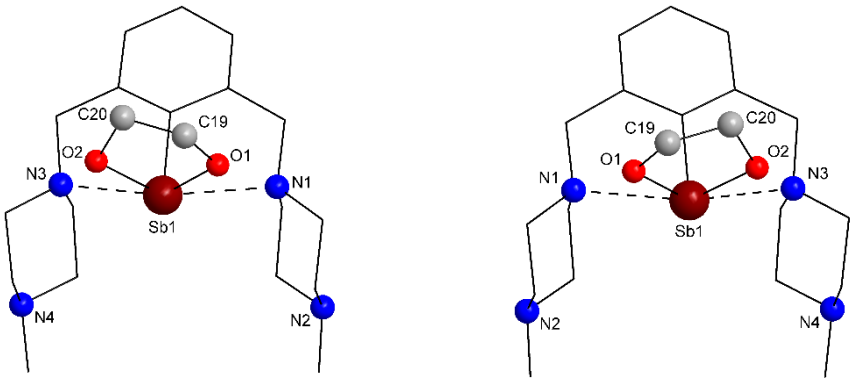


Figure S41. Molecular structure of isomers (δ-pS_{N1},pR_{N3})-**10** (*left*) and (λ-pR_{N1},pS_{N3})-**10** (*right*) in the crystal of **10**.

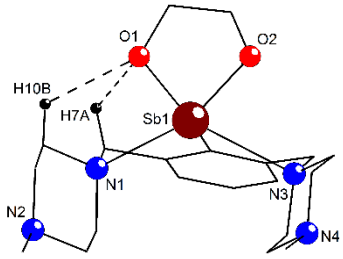


Figure S42. Molecular structure of **10**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

-	intramolecular distance	O(1)···H(7A)$_{methylene}$	2.50 Å	$\sum r_{vdW}$(O,H) 2.60 Å
		O(1)···H(10B)$_{methylene}$	2.47 Å	

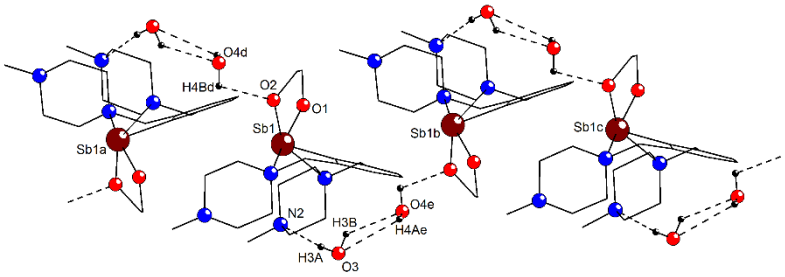


Figure S43. View of the chain polymer of (λ-pR_{N1},pS_{N3})-**10** isomers based on N···H$_{water}$ and O···H$_{water}$ contacts in the crystal of **10**·2H$_2$O (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*0.5–x, 0.5+y, 0.5–z*), (*0.5–x, –0.5+y, 0.5–z*), (*x, –1+y, z*), (*–0.5+x, 0.5–y, –0.5+z*) and (*1–x, –y, 1–z*) are given by "a", "b", "c", "d" and "e", respectively].

-	intermolecular distance	N(2)···H(3A)$_{water}$	2.11 Å	$\sum r_{vdW}$(N,H) 2.74 Å
		O(2)···H(4Bd)$_{water}$	2.57 Å	$\sum r_{vdW}$(O,H) 2.60 Å
		O(3)···H(4Ae)$_{water}$	2.58 Å	
		O(4e)···H(3B)$_{water}$	2.24 Å	

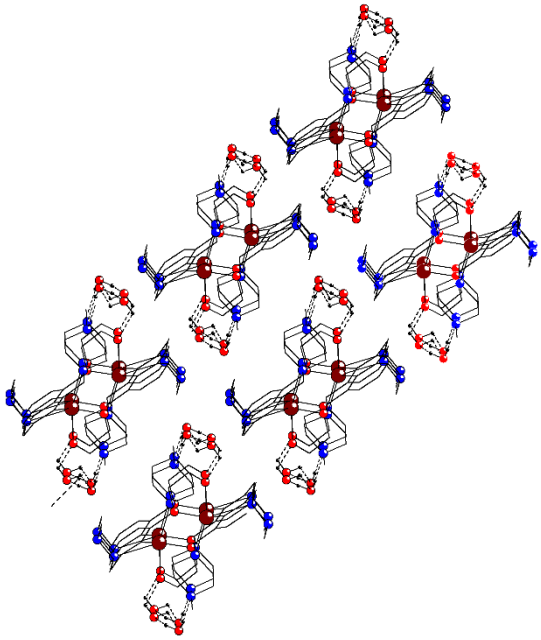


Figure S44. View along *b* axis of chain polymers of (δ-pS_{N1},pR_{N3})-**10** and (λ-pR_{N1},pS_{N3})-**10** isomers, respectively, in the crystal of **10**·2H$_2$O (only hydrogen atoms involved in intermolecular contacts are shown).

- no further contacts between parallel chains

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Bi(OCH$_2$)$_2$ (11)

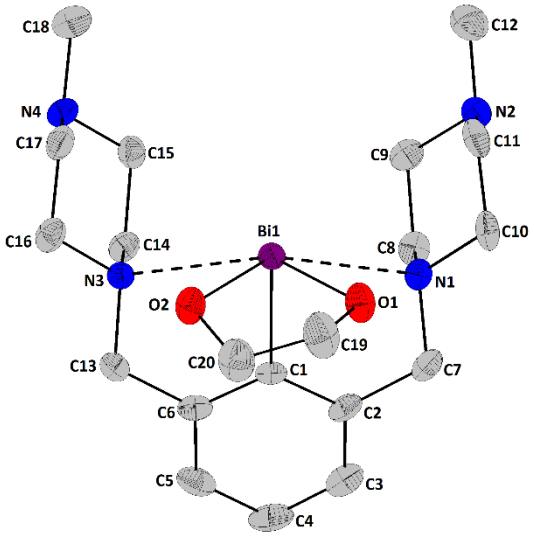


Figure S45. Molecular structure of the isomer (λ-pR_{N1},pS_{N3})-**11**. Thermal ellipsoids are drawn at the 30% probability. Hydrogen atoms are omitted for clarity.

- the crystal contains a 1:1 mixture of (δ-pS_{N1},pR_{N3})- and (λ-pR_{N1},pS_{N3})-**11** isomers

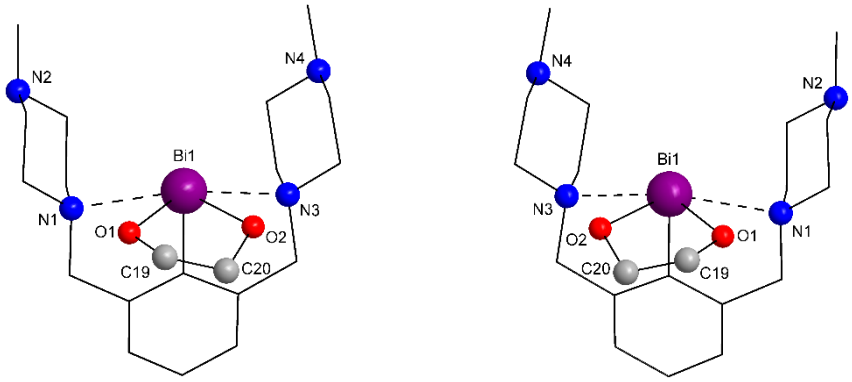


Figure S46. Molecular structure of isomers (δ-pS_{N1},pR_{N3})-**11** (*left*) and (λ-pR_{N1},pS_{N3})-**11** (*right*) in the crystal of **11**·2H$_2$O.

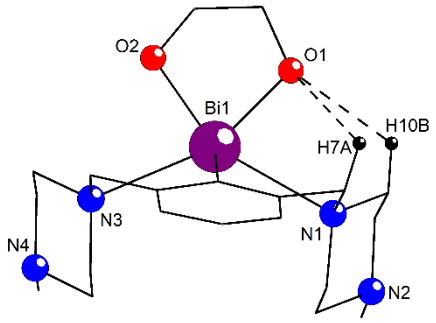


Figure S47. Molecular structure of **11**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance O(1)···H(7A)$_{methylene}$ 2.53 Å $\sum r_{vdW}$(O,H) 2.60 Å
  O(1)···H(10B)$_{methylene}$ 2.53 Å

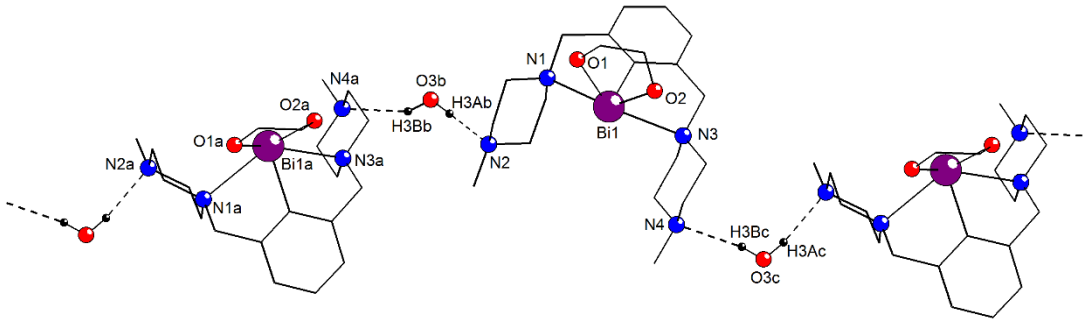


Figure S48. View of the chain polymer of alternating (*δ*-*pS*$_{N1a}$,*pR*$_{N3a}$)-**11** and (*λ*-*pR*$_{N1}$,*pS*$_{N3}$)-**11** isomers based on N···H$_{water}$ hydrogen bonds in the crystal of **11**·2H$_2$O (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*0.5+x, 1.5–y, –0.5+z*), (*1–x, 1–y, –z*) and (*0.5–x, 0.5+y, 0.5–z*) are given by "a", "b" and "c", respectively].

- intermolecular distance N(2)···H(3Ab)$_{water}$ 2.11 Å $\sum r_{vdW}$(N,H) 2.74 Å
  - N(4)···H(3Bc)$_{water}$ 2.26 Å

- no further contacts between parallel chains.

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Sb(OCMe$_2$)$_2$ (12)

A solution of KOH (0.04 g, 0.81 mmol) in ethanol (25 mL) was added over a solution of **1** (0.20 g, 0.40 mmol) and pinacol (0.05 g, 0.4 mmol) in ethanol (25 mL). The reaction mixture was stirred for 24 h at room temperature, then the solvent was removed *in vacuo*. The remaining solid was solved in $CHCl_3$, the colourless solution was dried over anh. Na_2SO_4, then filtered through a glass frit. The solvent was removed from the clear solution and the remaining pale yellow solid was extracted with Et_2O (2x15 mL) and filtered again. Evaporation of the solvent gave **12** as a colourless solid (0.16 g, 73%), m.p. 155-160 °C.

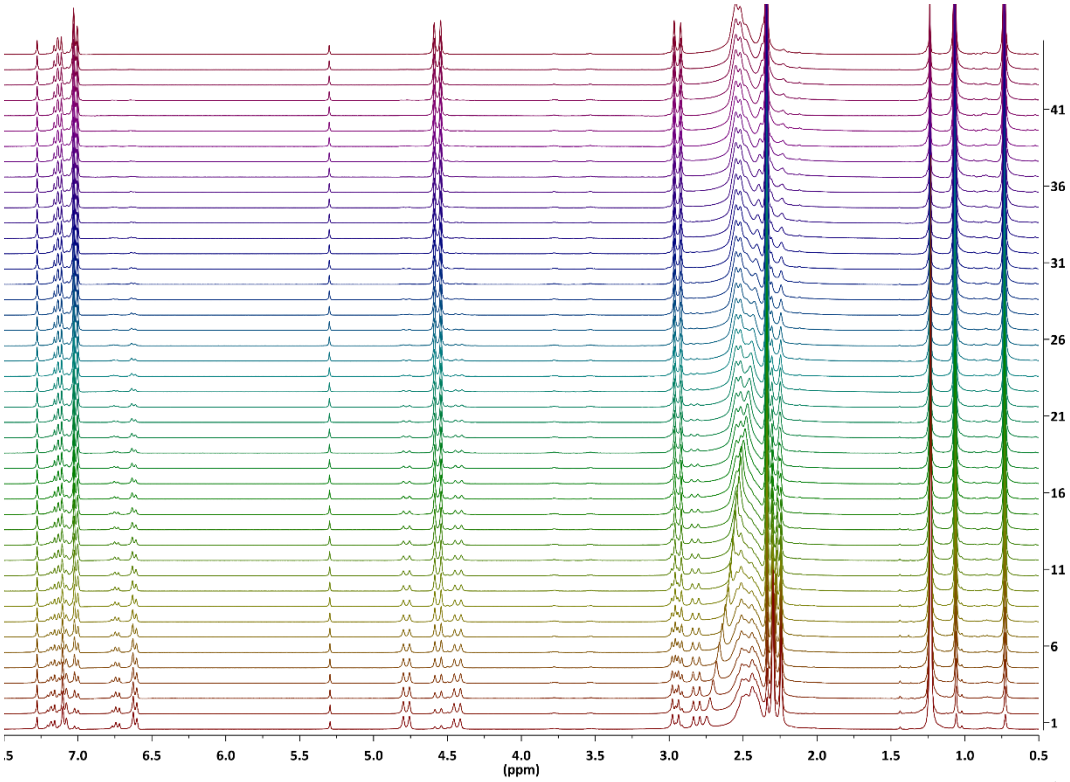


Figure S49. Reaction of the oxide **3** with HO(CH$_3$)$_2$CC(CH$_3$)OH in $CDCl_3$ monitored by ^{1}H NMR spectroscopy (300 MHz). Spectra (1 – 45) were recorded every 5 min. after additon of pinacol to the oxide solution.

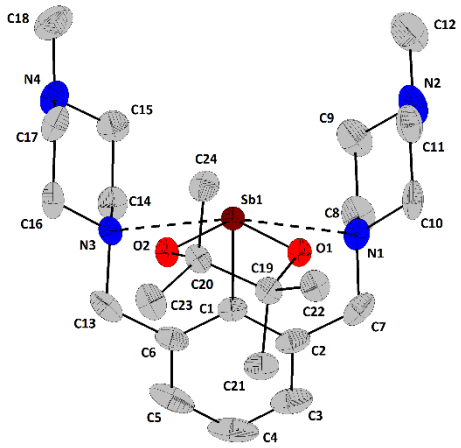


Figure S50. Molecular structure of the isomer (δ-*pR*$_{N1}$,*pS*$_{N3}$)-**12**. Thermal ellipsoids are drawn at the 25% probability. Hydrogen atoms are omitted for clarity.

- the crystal contains a 1:1 mixture of (δ-*pR*$_{N1}$,*pS*$_{N3}$)- and (λ-*pS*$_{N1}$,*pR*$_{N3}$)-**12** isomers

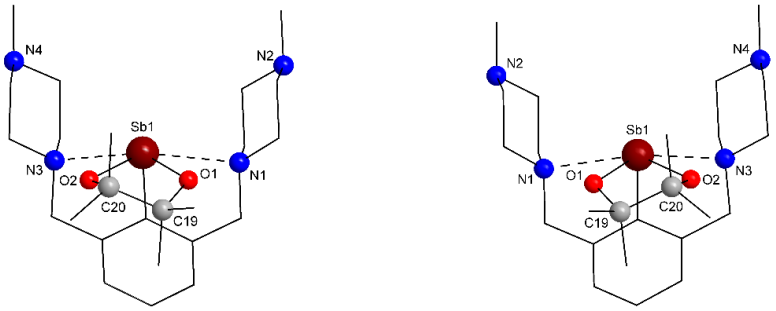


Figure S51. Molecular structure of isomers (δ-pR_{N1},pS_{N3})-**12** (*left*) and (λ-pS_{N1},pR_{N3})-**12** (*right*) in the crystal of **12**.

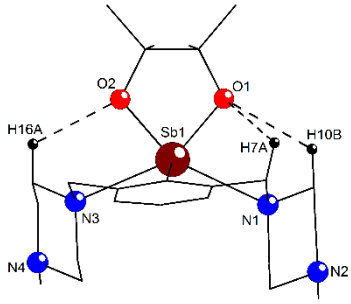


Figure S52. Molecular structure of **12**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance $O(1)\cdots H(7A)_{methylene}$ 2.56 Å $\sum r_{vdW}(O,H)$ 2.60 Å
  $O(1)\cdots H(10B)_{methylene}$ 2.56 Å
  $O(2)\cdots H(16A)_{methylene}$ 2.51 Å

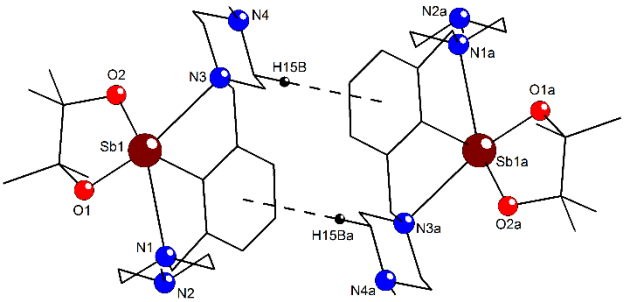


Figure S53. Dimer association between (δ-pR_{N1},pS_{N3})-**12** and (λ-pS_{N1a},pR_{N3a})-**12** isomers based on C–H···π ($Ar_{centroid}$) contacts in the crystal of **12** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*2–x, 1–y, 1–z*) are given by "a"].

- intermolecular distance $C(15)–H(15B)_{methylene}\cdots Ar_{centroid}\{C(1a)\text{-}C(6a)\}$ 3.06 Å
  γ = 16.2°

- no further contacts between dimer associations.

2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Bi(OCMe$_2$)$_2$ (13)

A reaction mixture of **2** (0.20 g, 0.34 mmol), pinacol (0.041 g, 0.34 mmol) and KOH (0.076 g, 1.36 mmol) in ethanol (25 mL) was stirred for 24 h at room temperature, then the solvent was removed *in vacuo* and the solid residue was extracted with Et$_2$O. Evaporation of the solvent from the resulting clear solution yielded **13** as a colourless solid (0.19 g, 89%), m.p. 176 °C.

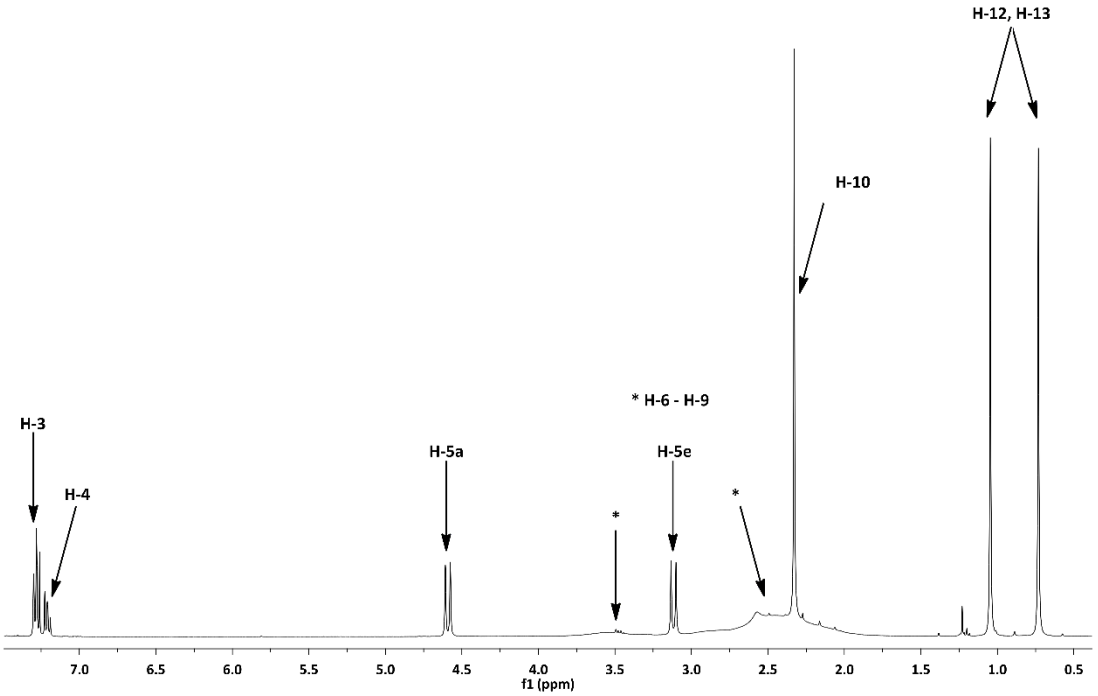


Figure S54. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **13**, at r.t.

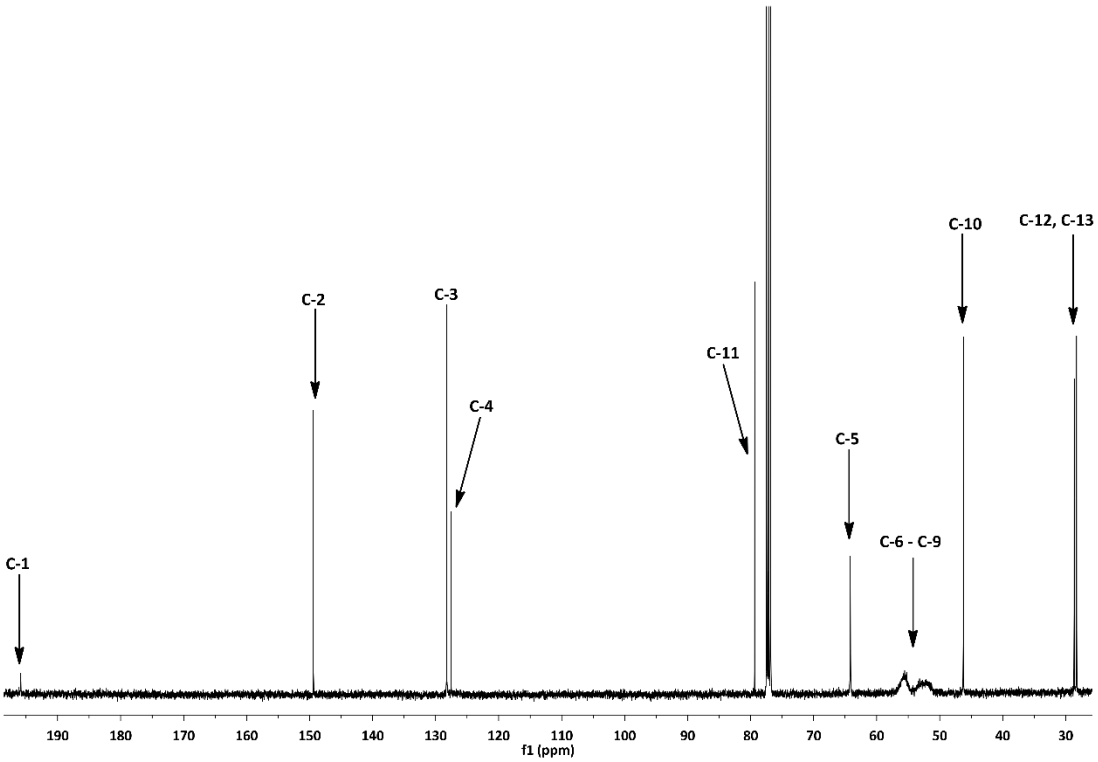


Figure S55. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **13**, at r.t.

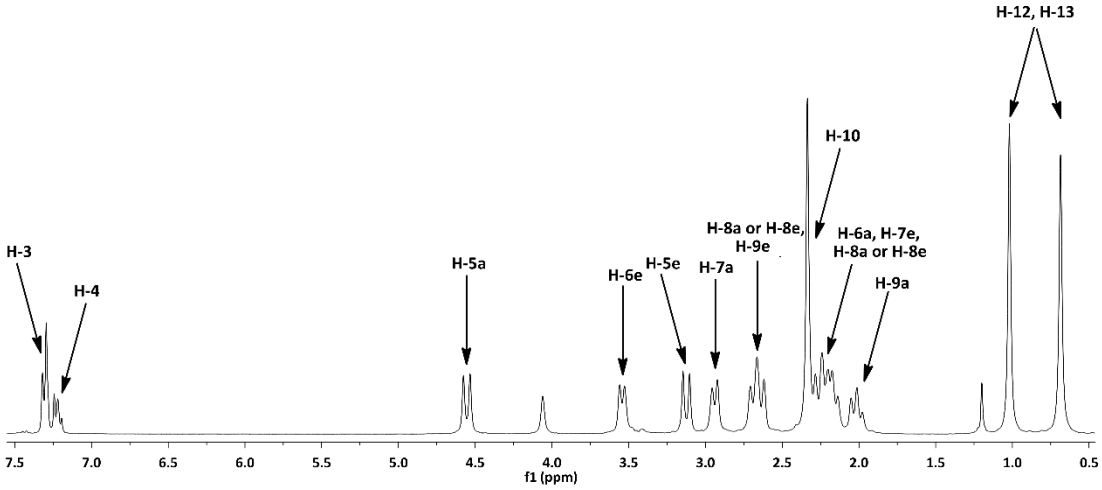


Figure S56. ^{1}H NMR (301 MHz, $CDCl_3$) spectrum of compound **13**, at -40 °C.

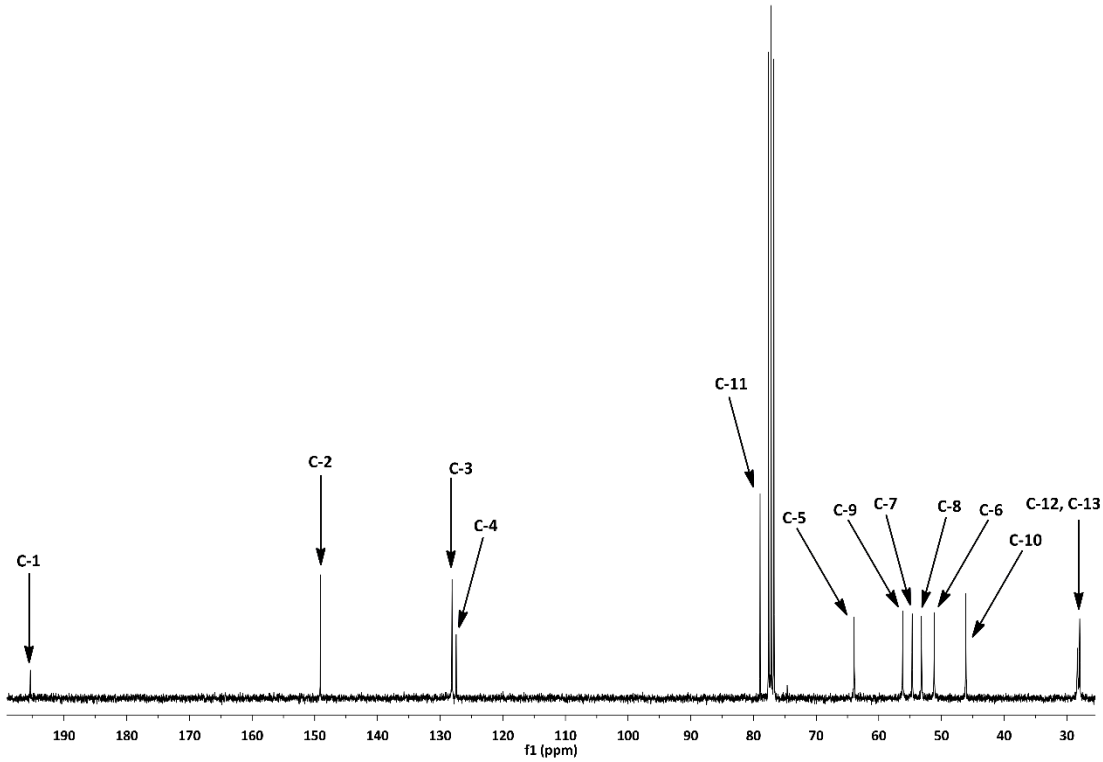


Figure S57. ^{13}C NMR (76 MHz, $CDCl_3$) spectrum of compound **13**, at -40 °C.

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Sb(O$_2$-1,2-C$_6$H$_4$) (14)

KOH (0.03 g, 0.54 mmol) was added over a solution of **1** (0.13 g, 0.27 mmol) and catechol (0.03 g, 0.27 mmol) in ethanol (30 mL). The reaction mixture was stirred for 3 h at room temperature, then the solvent was removed *in vacuo*. The remaining solid was solved in $CHCl_3$, the colourless solution was dried over anh. Na_2SO_4, then filtered through a glass frit. The solvent was removed from the clear solution and the remaining yellow solid was extracted with Et_2O (2x15 mL) and filtered again. Evaporation of the solvent gave **14** as a colourless crystalline solid (0.11 g, 79%), m.p. 225-230 °C.

^{1}H NMR (301 MHz, $CDCl_3$, 333 K): δ 2.30-2.80 [m, 22H, overlapped resonances for H-6 – H-9 with H-10 (δ 2.37 ppm, s)], AB spin system with A at δ 3.10 ppm ($^2J_{H\text{-}5a,H\text{-}5e}$ = 13.5 Hz, 2H, H-5e) and B at δ 4.55 ppm ($^2J_{H\text{-}5a,H\text{-}5e}$ = 13.5 Hz, 2H, H-5a), 6.38-6.48 (m, AA′BB′ spin system, 2H, H-13), 6.56-6.66 (m, AA′BB′ spin system, 2H, H-12), AB_2 spin system with B at δ 7.01 ppm (d, $^3J_{H\text{-}3,H\text{-}4}$ = 7.3 Hz, 2H, H-3) and A at δ 7.12 ppm (t, $^3J_{H\text{-}3,H\text{-}4}$ = 7.3 Hz, 1H, H-4).

^{13}C{^{1}H} NMR (76 MHz, $CDCl_3$, 333 K): δ 46.15 (C-10), 52.63 (C-8 and C-6), 54.57 (C-9 and C-7), 62.49 (C-5), 114.20 (C-12), 117.74 (C-13), 126.35 (C-3), 129.70 (C-4), 146.09 (C-2), 150.57 (C-1), 153.13 (C-11).

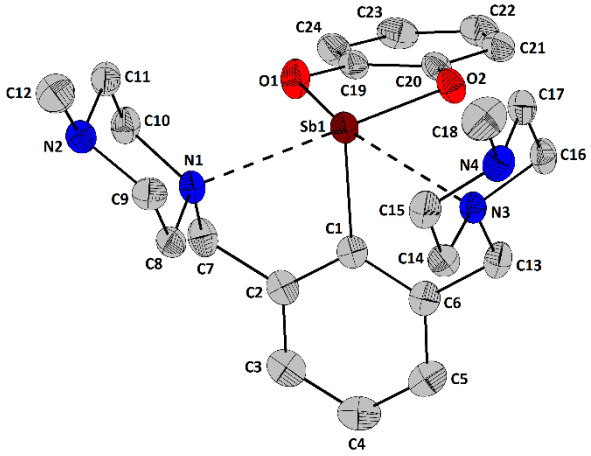


Figure S58. Molecular structure of the isomer (pR_{N1},pS_{N3})-**14**. Thermal ellipsoids are drawn at the 25% probability. Hydrogen atoms are omitted for clarity.

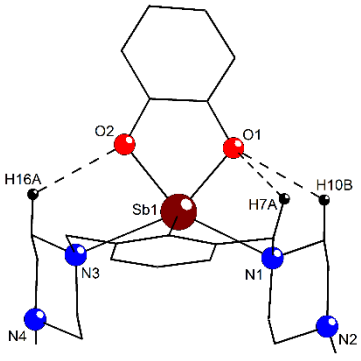


Figure S59. Molecular structure of **14**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

-	intramolecular distance	O(1)···H(7A)$_{methylene}$	2.50 Å	$\sum r_{vdW}$(O,H) 2.60 Å
		O(1)···H(12B)$_{methylene}$	2.53 Å	
		O(2)···H(16A)$_{methylene}$	2.58 Å	

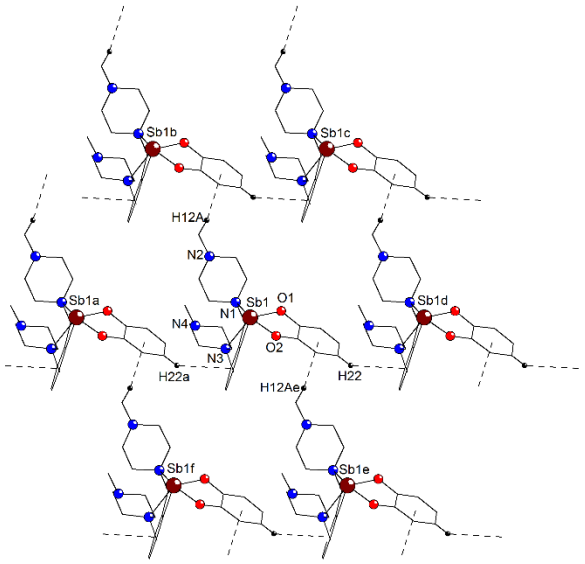


Figure S60. View along *c* axis of the honeycomb arrangement of the molecules in a fragment of the layer based on C–H···π ($Ar_{centroid}$) contacts in the crystal of **14** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*–1+x, y, z*), (*–1+x, 1+y, z*), (*x, 1+y, z*), (*1+x, y, z*), (*1+x, –1+y, z*) and (*x, –1+y, z*) are given by "a", "b", "c", "d", "e" and "f", respectively].

-	intermolecular distance	$C(12)–H(12A)_{methyl}\cdots Ar_{centroid}\{C(19b)\text{-}C(24b)\}$	2.89 Å
	-		γ = 12.6°
		$C(22)\cdots H(22)_{aryl}\cdots Ar_{centroid}\{C(1d)\text{-}C(6d)\}$	3.03 Å
	-		γ = 14.8°

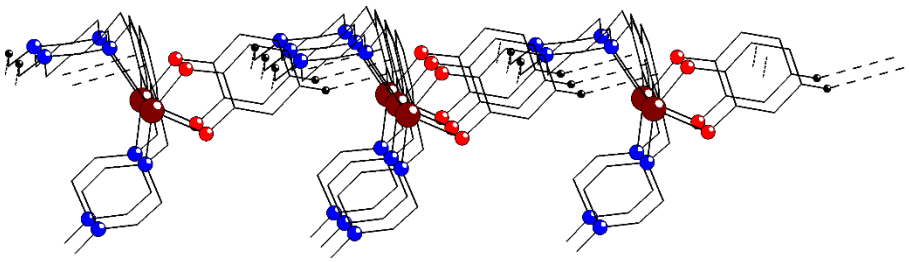


Figure S61. View along *b* axis of a fragment of the layer based on C–H···π ($Ar_{centroid}$) contacts in the crystal of **14** (only hydrogen atoms involved in intermolecular contacts are shown).

- no further contacts between parallel layers.

[2,6-{MeN(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]Bi(O$_2$-1,2-C$_6$H$_4$) (15)

A reaction mixture of **2** (0.20 g, 0.34 mmol), catechol (0.038 g, 0.34 mmol) and KOH (0.076 g, 1.36 mmol) in ethanol (25 mL) was stirred for 24 h at room temperature, then the solvent was removed *in vacuo* and the solid residue was extracted with Et$_2$O. Evaporation of the solvent from the resulting clear solution yielded **15** as a yellow solid (0.07 g, 33%), m.p. 230 °C.

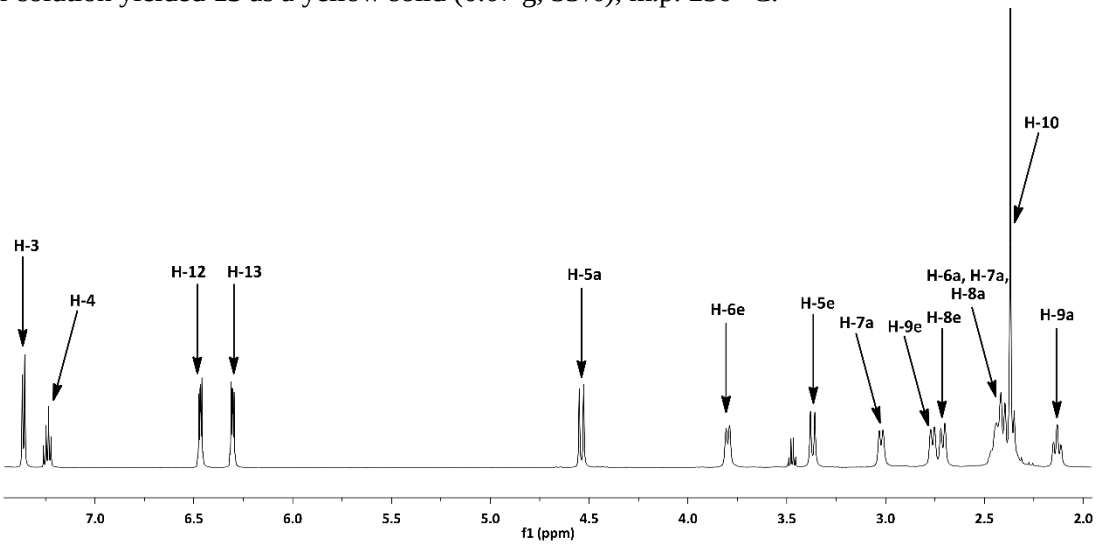


Figure S62. ^{1}H NMR (600 MHz, CDCl$_3$) spectrum of compound **15**, at r.t.

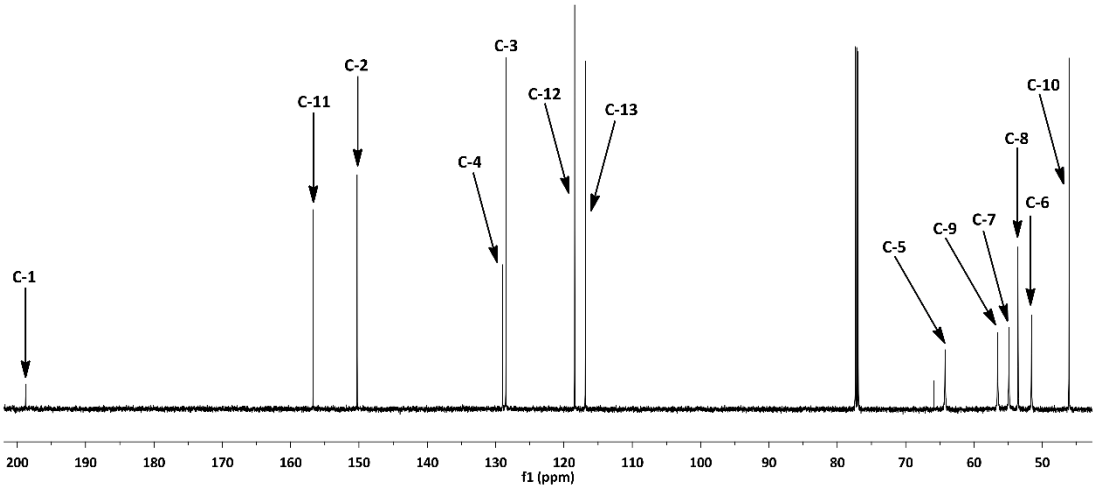


Figure S63. ^{13}C NMR (151 MHz, CDCl$_3$) spectrum of compound **15**, at r.t.

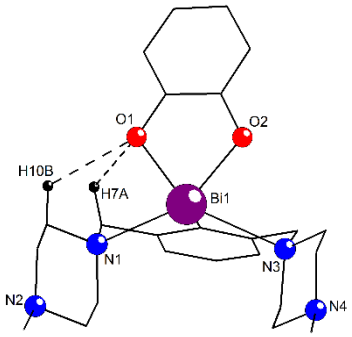


Figure S64. Molecular structure of **15**, showing the intramolecular O···H contacts (only hydrogen atoms involved in intramolecular contacts are shown).

- intramolecular distance O(1)···H(7A)$_{methylene}$ 2.52 Å $\sum r_{vdW}$(O,H) 2.60 Å
  O(1)···H(10B)$_{methylene}$ 2.55 Å

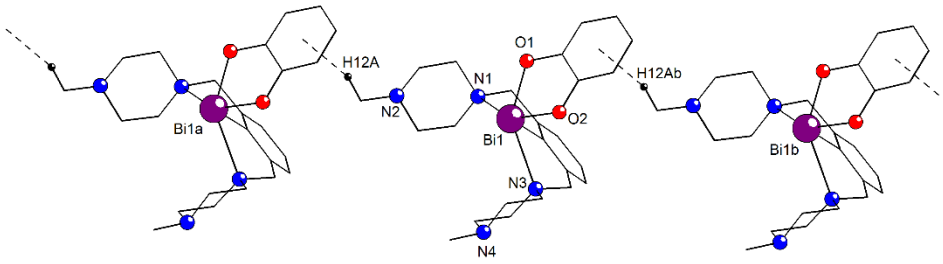


Figure S65. View of the chain polymer based on C–H···π ($Ar_{centroid}$) contacts in the crystal of **15** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (*–1+x, 1+y, z*) and (*1+x, –1+y, z*) are given by "a" and "b", respectively].

- intermolecular distance C(12)–H(12A)$_{methyl}$···$Ar_{centroid}${C(19a)-C(24a)} 2.87 Å
  - γ = 11.1°

- no further contacts between parallel chains.

Table S1. Crystallographic data for compounds **1**, **3**, **4**·4H_2O and **5**·H_2O·C_6H_5Me

	1	**3**	**4**·4H_2O	**5**·H_2O·C_6H_5Me
Empirical formula	$C_{18}H_{29}Cl_2N_4Sb$	$C_{36}H_{58}N_8O_2Sb_2$	$C_{36}H_{66}Bi_2N_8O_6$	$C_{49}H_{71}F_9N_8O_9Sb_2$
M	494.10	878.40	1124.92	1330.63
T/K	293	297	293	203
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	*P-1*	*P -1*	*P-1*	$P2_1/c$
a/Å	10.5551(6)	9.080(2)	11.146(6)	11.0460(11)
b/Å	12.4385(7)	10.126(3)	12.870(6)	28.780(3)
c/Å	16.6000(9)	11.752(3)	16.347(8)	18.4055(18)
α/°	87.275(4)	68.806(4)	107.146(8)	90
β/°	75.794(4)	82.572(4)	99.329(9)	95.829(2)
γ/°	86.572(4)	83.749(4)	92.409(9)	90
V/Å^3	2107.8(2)	996.7(5)	2201.1(19)	5820.9(10)
Z	4	1	2	4
No. of reflections colle	23396	9896	21104	43470
No. of independent refl	7820 (R_{int} = 0.028)	3680 (R_{int} = 0.051)	8093 (R_{int} = 0.075)	10835 (R_{int} = 0.093)
Absorption correction	Multi-Scan[1]	Multi-Scan[2]	Multi-Scan[2]	Multi-Scan[2]
μ(Mo Kα)/mm^{-1}	1.571	1.396	8.033	1.014
*R*1 [*I*>2σ(*I*)]	0.0202	0.0487	0.0442	0.0568
*wR*2	0.0511	0.1214	0.1276	0.1336
GOF on F^2	1.05	1.13	0.93	0.99

[1] R. Blessing, *Acta Crystallogr., Sect. A: Fundam. Crystallogr.*, 1995, **51**, 33.
[2] G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

Table S2. Crystallographic data for compounds **8**·H_2O, **10**·2H_2O and **11**·2H_2O

	8·H_2O	**10**·2H_2O	**11**·2H_2O
Empirical formula	$C_{20}H_{29}N_4O_4Sb$	$C_{20}H_{33}N_4O_2Sb$	$C_{20}H_{37}Bi_2N_4O_4$
M	529.24	519.28	606.51
T/K	297	293	294
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$
a/Å	9.0558(19)	12.626(3)	12.6247(9)
b/Å	17.283(4)	12.291(3)	12.1795(9)
c/Å	16.433(3)	15.792(3)	15.7589(11)
α/°	90.00	90.00	90.00
β/°	105.629(4)	99.53(3)	99.415(1)
γ/°	90.00	90.00	90.00
V/Å^3	2476.9(9)	2416.9(10)	2390.5(3)
Z	4	4	4
No. of reflections collected	23884	23681	23158
No. of independent reflections	4590 (R_{int} = 0.076)	4502 (R_{int} = 0.205)	4445 (R_{int} = 0.059)
Absorption correction	Multi-Scan[2]	Multi-Scan[2]	Multi-Scan[2]
μ(Mo Kα)/mm^{-1}	1.148	1.172	7.406
*R*1 [*I*>2σ(*I*)]	0.0426	0.1086	0.0318
*wR*2	0.0973	0.2261	0.0723
GOF on F^2	1.05	1.19	1.07

[2] G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

Table S3. Crystallographic data for compounds **12**, **14** and **15**

	12	**14**	**15**
Empirical formula	$C_{24}H_{41}N_4O_2Sb_1$	$C_{24}H_{33}N_4O_2Sb$	$C_{24}H_{33}BiN_4O_2$
M	539.36	531.29	618.52
T/*K*	297	295	295
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	*P-1*	*P-1*
a/Å	11.188(9)	9.7365(11)	9.8126(9)
b/Å	11.022(9)	10.1979(11)	10.1505(9)
c/Å	21.870(18)	15.6619(18)	15.7304(14)
α/°	90	81.563(2)	82.242(2)
β/°	93.335(15)	76.977(2)	77.035(2)
γ/°	90	64.391(2)	64.012(1)
V/Å^3	2692(4)	1364.1(3)	1371.3(2)
Z	4	2	2
No. of reflections collected	24813	13491	13523
No. of independent reflections	4980 (R_{int} = 0.096)	5028 (R_{int} = 0.041)	5064 (R_{int} = 0.043)
Absorption correction	Multi-Scan[2]	Multi-Scan[2]	Multi-Scan[2]
μ(Mo Kα)/mm^{-1}	1.050	1.035	6.452
*R*1 [*I*>2σ(*I*)]	0.0522	0.0375	0.0329
*wR*2	0.1041	0.0896	0.0742
GOF on F^2	1.01	1.06	1.01

[2] G. M. Sheldrick, *SADABS, Program for area detector adsorption correction*, Institute for Inorganic Chemistry, University of Göttingen, Germany, 1996.

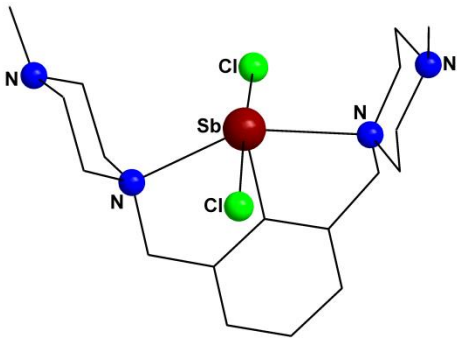


Figure S66. DFT calculated molecular structure of **1**. Hydrogen atoms were omitted for clarity.

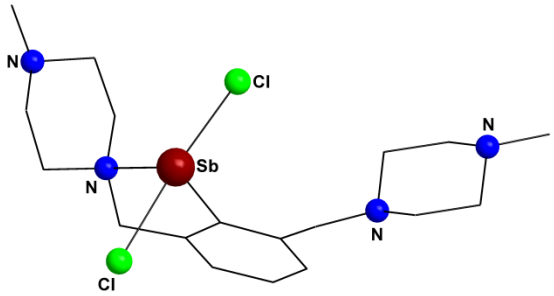


Figure S67. DFT calculated molecular structure of **1**, one arm uncoordinated. Hydrogen atoms were omitted for clarity.

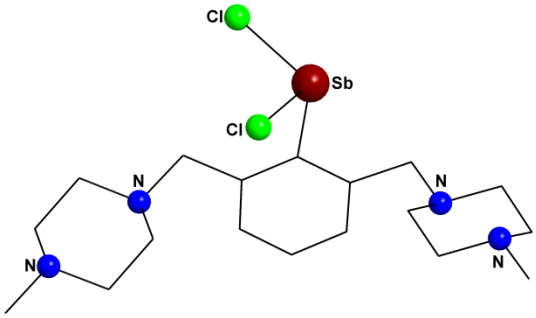


Figure S68. DFT calculated molecular structure of **1**, two arms uncoordinated. Hydrogen atoms were omitted for clarity.

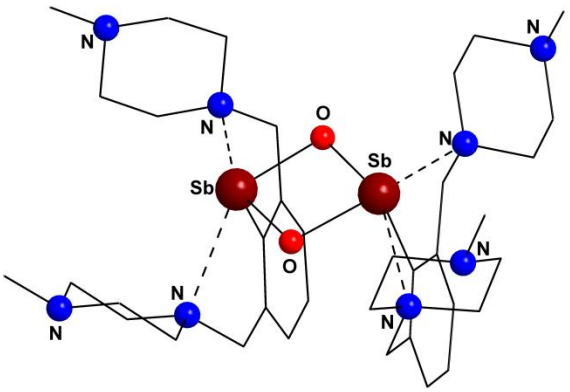


Figure S69. DFT calculated molecular structure of the *syn* isomer of **3**. Hydrogen atoms were omitted for clarity.

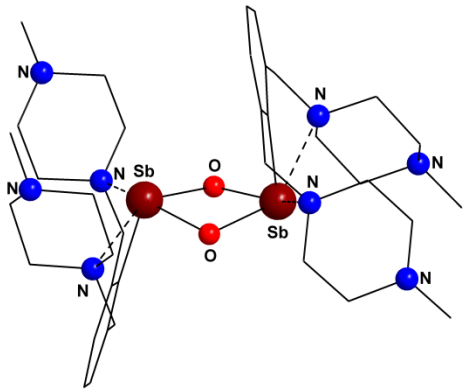


Figure S70. DFT calculated molecular structure of the *anti* isomer of **3**. Hydrogen atoms were omitted for clarity.

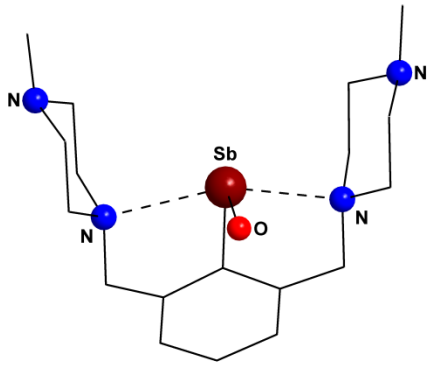


Figure S71. DFT calculated molecular structure of RSbO - the monomer of **3**. Hydrogen atoms were omitted for clarity.

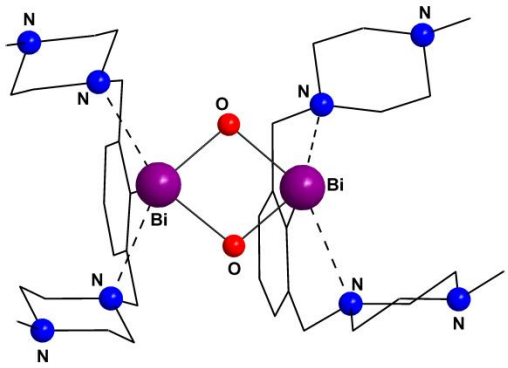


Figure S72. DFT calculated molecular structure of the *syn* isomer of **4**. Hydrogen atoms were omitted for clarity.

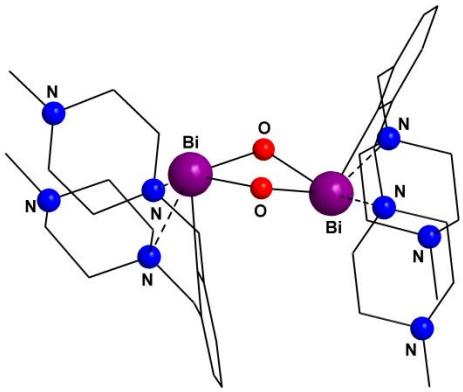


Figure S73. DFT calculated molecular structure of the *syn* isomer of **4**. Hydrogen atoms were omitted for clarity.

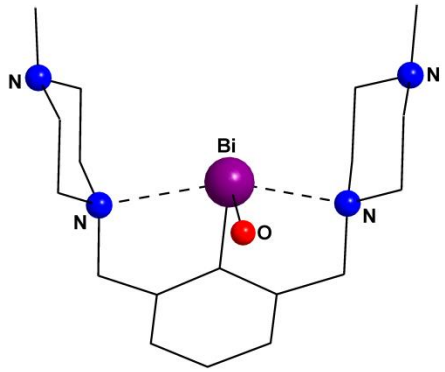


Figure S74. DFT calculated molecular structure of RBiO - the monomer of **4**. Hydrogen atoms were omitted for clarity.

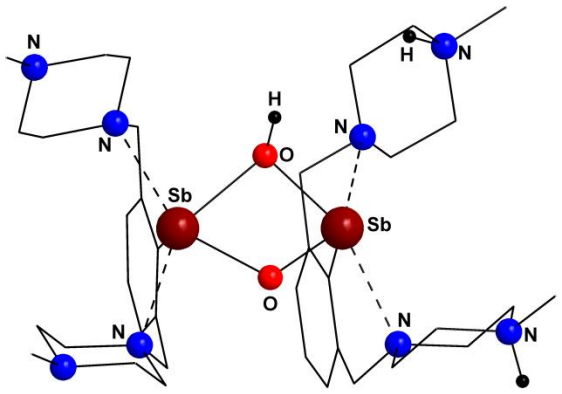


Figure S75. DFT calculated molecular structure of the cation of **5** (protons on the same pincer ligand). Hydrogen atoms were omitted for clarity.

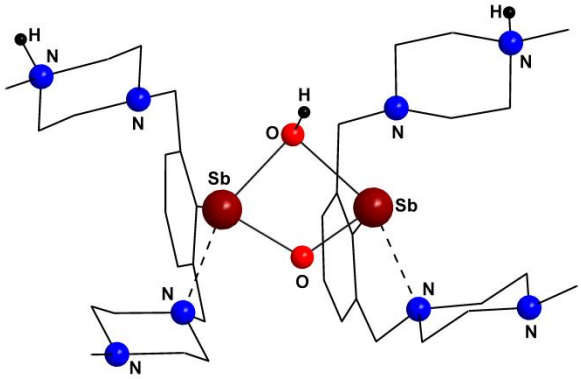


Figure S76. DFT calculated molecular structure of the cation of **5** (protons on different pincer ligands). Hydrogen atoms were omitted for clarity.

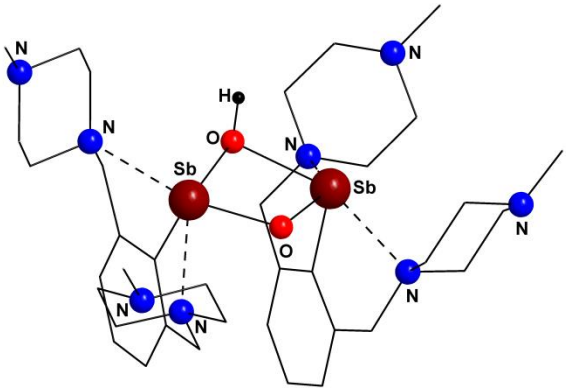


Figure S77. DFT calculated molecular structure of the cation **[(RSb)$_2$(μ-O)(μ-OH)]$^+$**, *syn* isomer. Hydrogen atoms were omitted for clarity.

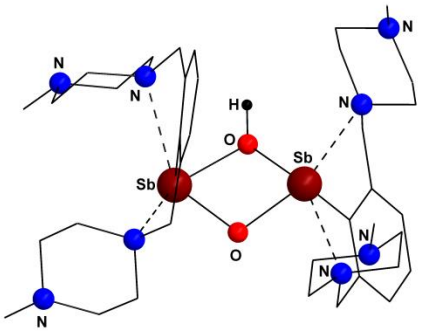


Figure S78. DFT calculated molecular structure of the cation **[(RSb)$_2$(μ-O)(μ-OH)]$^+$**, *anti* isomer. Hydrogen atoms were omitted for clarity.

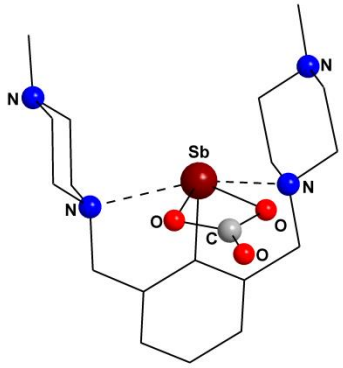


Figure S79. DFT calculated molecular structure of the mononuclear form of **6**. Hydrogen atoms were omitted for clarity.

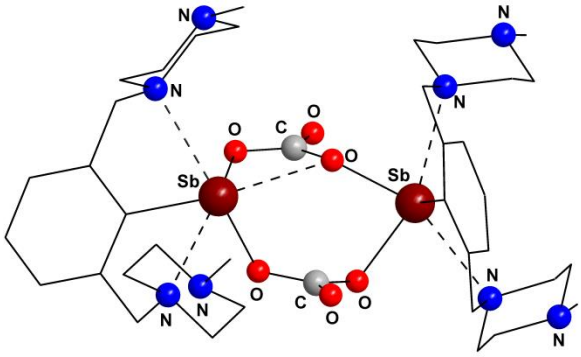


Figure S80. DFT calculated molecular structure of dimers of **6**, *syn* isomer. Hydrogen atoms were omitted for clarity.

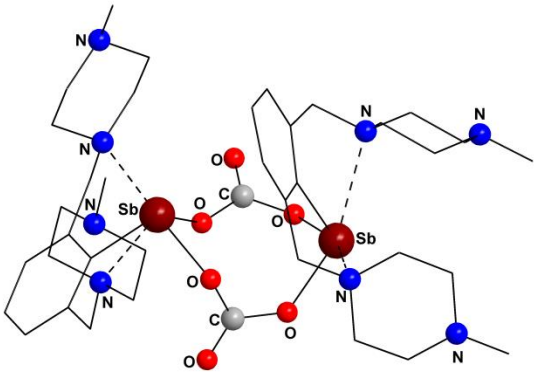


Figure S81. DFT calculated molecular structure of dimers of **6**, *anti* isomer. Hydrogen atoms were omitted for clarity.

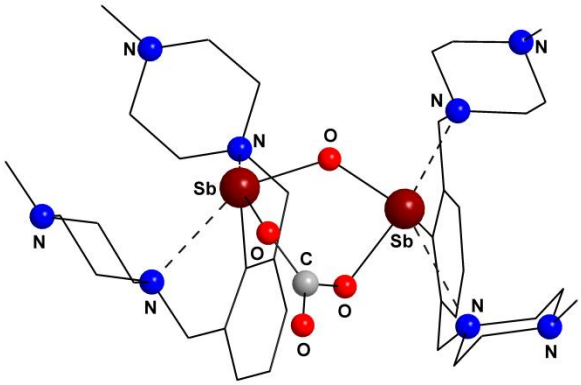


Figure S82. DFT calculated molecular structure of **(RSb)$_2$(μ-O)(μ-CO$_3$)**, *syn* isomer. Hydrogen atoms were omitted for clarity.

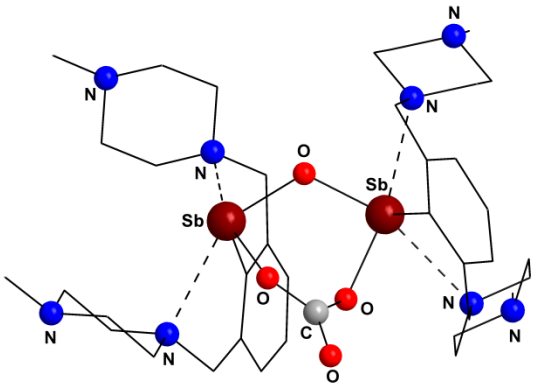


Figure S83. DFT calculated molecular structure of **(RSb)$_2$(μ-O)(μ-CO$_3$)**, *anti* isomer. Hydrogen atoms were omitted for clarity.

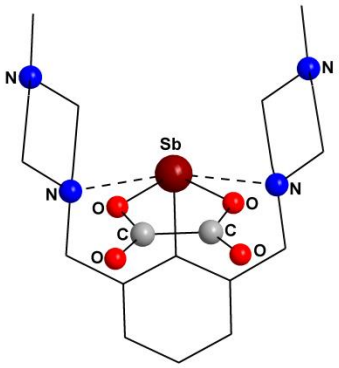


Figure S84. DFT calculated molecular structure of **8**. Hydrogen atoms were omitted for clarity.

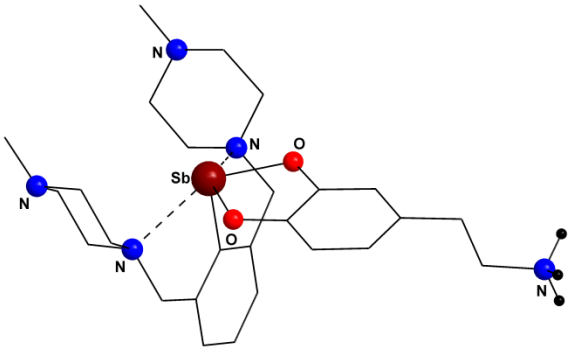


Figure S85. DFT calculated molecular structure of the cation of **9**. Hydrogen atoms were omitted for clarity.

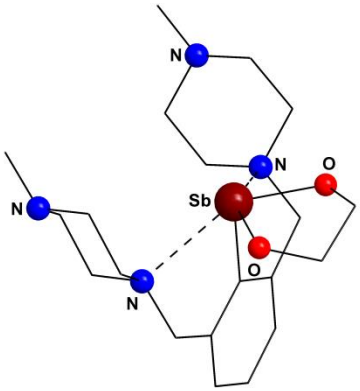


Figure S86. DFT calculated molecular structure of **10**. Hydrogen atoms were omitted for clarity.

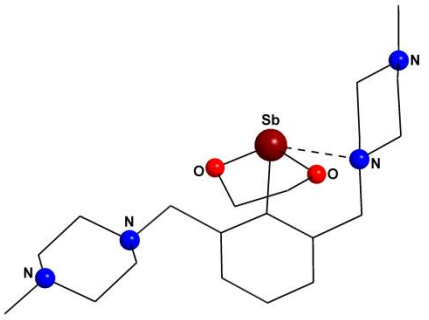


Figure S87. DFT calculated molecular structure of **10**, one arm uncoordinated. Hydrogen atoms were omitted for clarity.

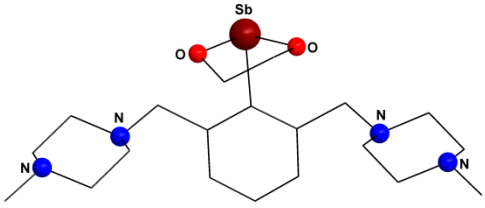


Figure S88. DFT calculated molecular structure of **10**, two arms uncoordinated. Hydrogen atoms were omitted for clarity.

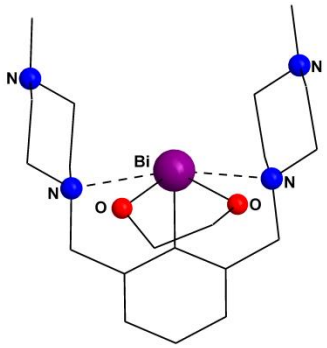


Figure S89. DFT calculated molecular structure of **11**. Hydrogen atoms were omitted for clarity.

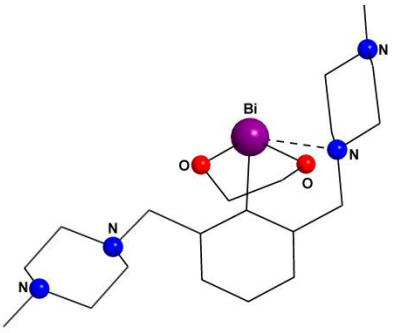


Figure S90. DFT calculated molecular structure of **11**, one arm uncoordinated. Hydrogen atoms were omitted for clarity.

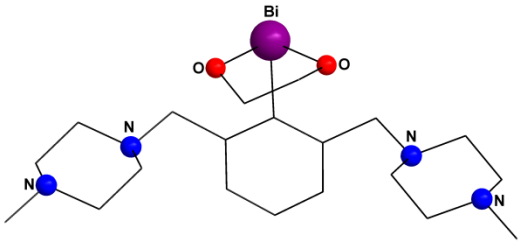


Figure S91. DFT calculated molecular structure of **11**, two arm uncoordinated. Hydrogen atoms were omitted for clarity.

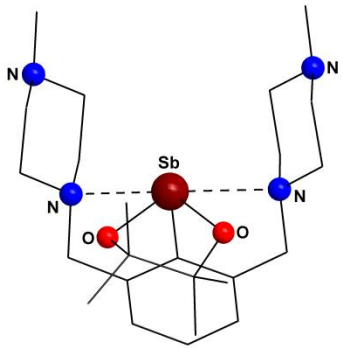


Figure S92. DFT calculated molecular structure of **12**. Hydrogen atoms were omitted for clarity.

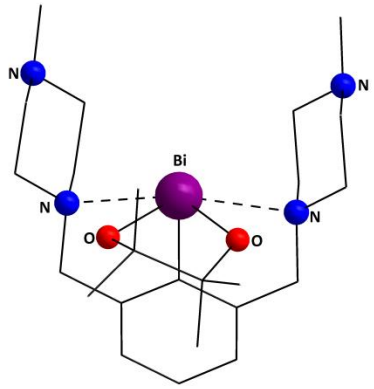


Figure S93. DFT calculated molecular structure of **13**. Hydrogen atoms were omitted for clarity.

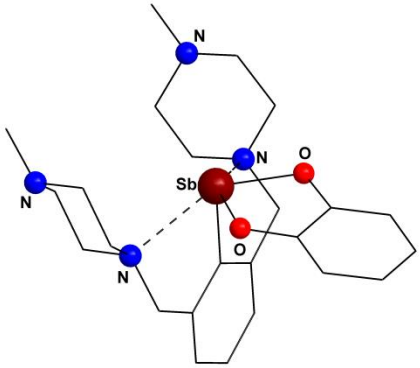


Figure S94. DFT calculated molecular structure of **14**. Hydrogen atoms were omitted for clarity.

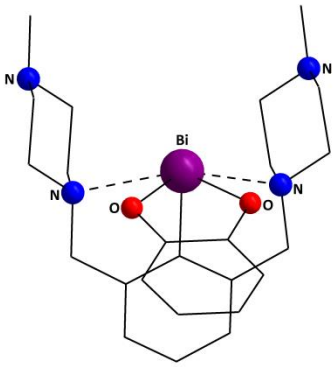


Figure S95. DFT calculated molecular structure of **15**. Hydrogen atoms were omitted for clarity.

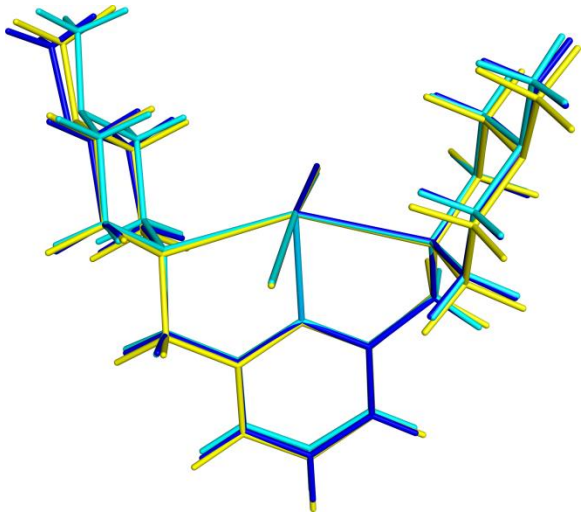


Figure S96. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue and cyan) structures of **1**.

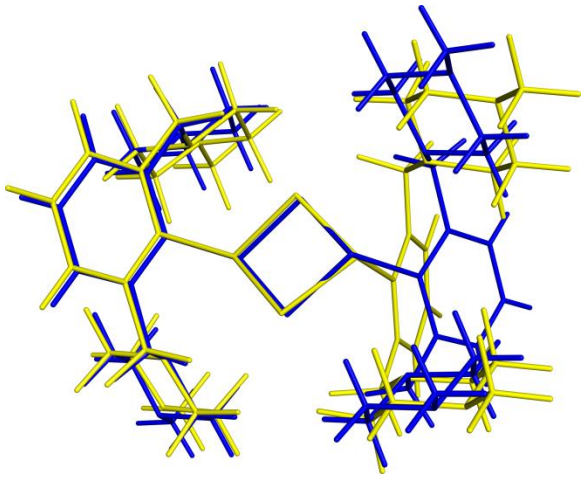


Figure S97. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of the *anti* isomer of **3**.

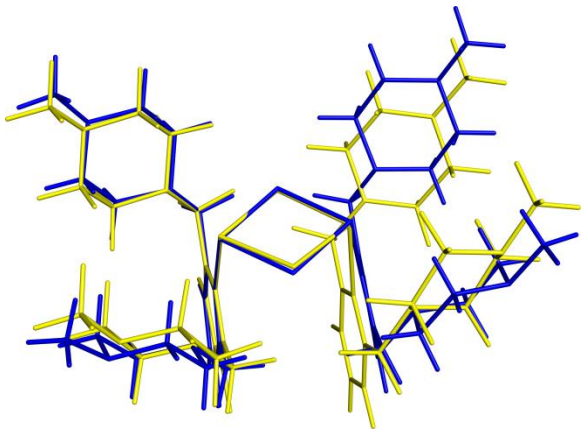


Figure S98. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of the *syn* isomer of **4**.

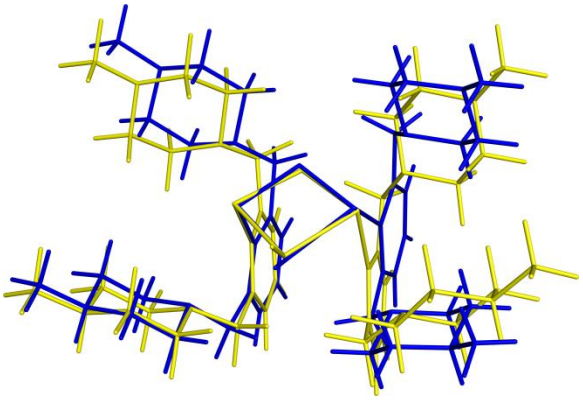


Figure S99. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of the cation of **5**, *syn* isomer.

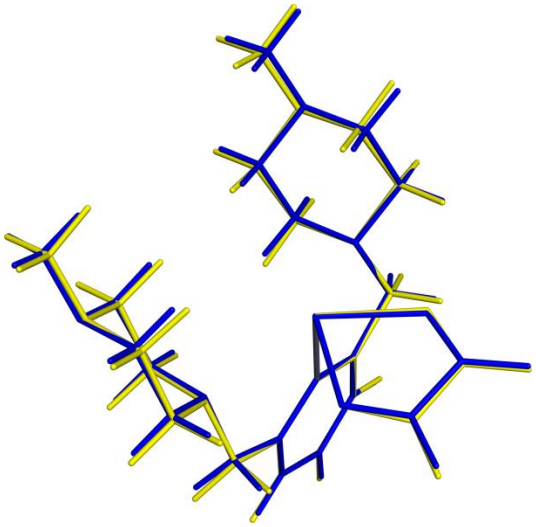


Figure S100. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **8**.

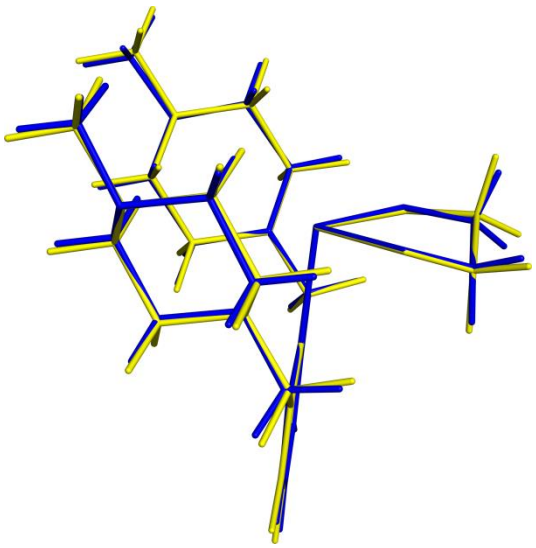


Figure S101. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **10**.

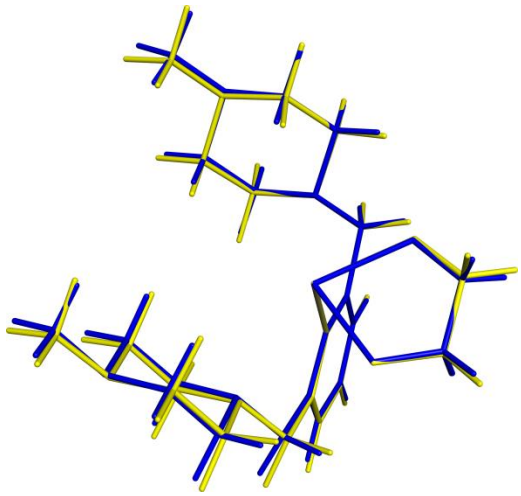


Figure S102. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **11**.

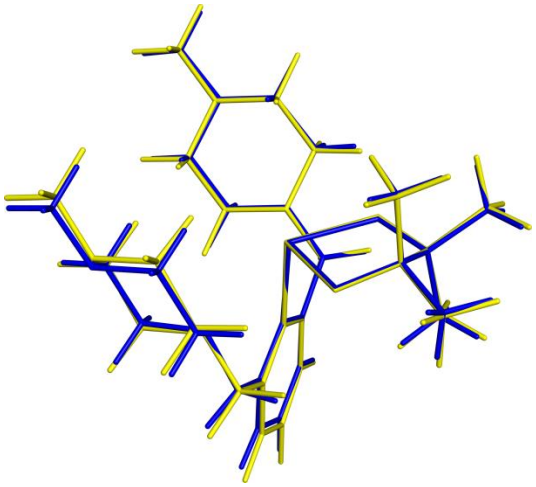


Figure S103. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **12**.

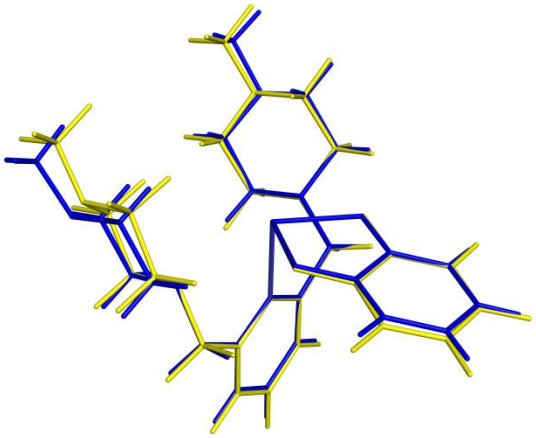


Figure S104. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **14**.

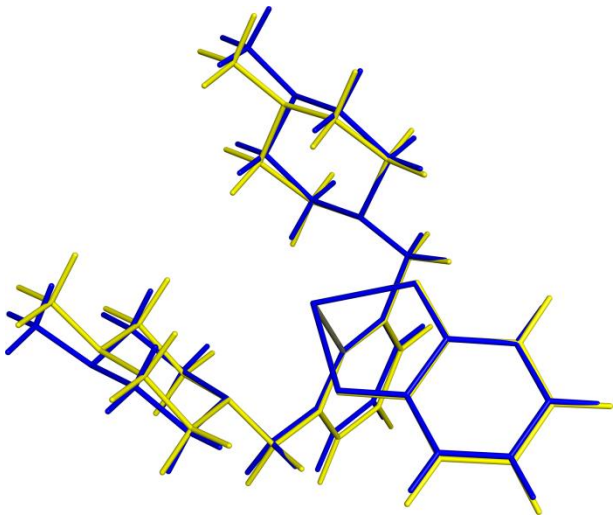


Figure S105. Overlapped capped-sticks representation of the DFT calculated (yellow) and crystallograpically determined (blue) structures of **15**.

Table S4. Cartesian coordinates (Å) of **1**.

54

Coordinates from ORCA-job SbCl2_opt

C	0.00259405110843	-0.00618174206268	-2.08812400433476
C	-0.41977623800874	1.14510250852433	-2.77146527986428
C	-0.37602830626906	1.16598040447099	-4.17746382528657
H	-0.69507324383982	2.06355407898399	-4.72368867675337
C	0.05897609559313	0.02970531027773	-4.88140734752142
H	0.08110205461197	0.04377016030317	-5.97783545501682
C	0.46589069057915	-1.12445171973945	-4.18987685448568
H	0.80729025279827	-2.00783399649564	-4.74564270422287
C	0.45289293899741	-1.13971045939091	-2.78317875873765
C	-0.99537873993124	2.27864383211340	-1.95778745584864
H	-0.92516348721695	3.24835377292308	-2.49267543199963
H	-2.06445275134307	2.05986099071238	-1.77504567315701
C	-1.24069589739906	3.11401569309661	0.31633041211567
H	-2.16780771571498	2.52211141821640	0.41705274660574
H	-1.48844868157531	4.10722667612206	-0.11391348418971
C	-0.57275606771711	3.30179030365807	1.67058413358736
H	-1.25346629207266	3.87345673805435	2.32757017124624
H	-0.41972656275621	2.30002618873158	2.15021743114246
C	0.97106953768750	3.06042794974425	-0.72071420467512
H	0.83085699490278	4.03878743525440	-1.22731854851146
H	1.63558102321792	2.43018075425276	-1.33702034806787
C	1.58928962498672	3.27727415031498	0.65563335131829
H	1.86901957592747	2.29125766327260	1.09594363853965
H	2.52860765130750	3.84588373983012	0.52940120207261
C	1.29794915662685	4.31365645989694	2.81985208350208
H	2.22231648089867	4.89967842974302	2.67289081334130
H	1.56246537720279	3.38994877406404	3.38972547940757
H	0.60608860936519	4.91311937378079	3.43792013791733
C	0.99623884836703	-2.29404969525921	-1.97656131143033
H	0.94825803069035	-3.24948696720817	-2.53891583659901
H	2.05711934426954	-2.08045520856183	-1.74603262216734
C	-1.01697720993751	-3.10706846035141	-0.83776088797920
H	-0.85647285493604	-4.07412252307286	-1.35988017350869
H	-1.65660777254694	-2.46281808390870	-1.46578149899169
C	-1.68891995295215	-3.35347360054801	0.50810066120975
H	-1.98400418280031	-2.37669734152070	0.95885978711962
H	-2.62365063440149	-3.91657698736729	0.33272392542942
C	1.15183044501941	-3.18809930493386	0.28294003603268
H	2.07500887375757	-2.60072156989617	0.43351876894762
H	1.41451446664103	-4.17102656501428	-0.16189324052660
C	0.43246619931228	-3.40724730618236	1.60583879437384
H	1.08640761042397	-3.99735865814330	2.27366472391654
H	0.26466292995055	-2.41702187888685	2.10417629577710
C	-1.48406712229935	-4.43824297611625	2.65843360213400
H	-0.81794588356376	-5.05317736205395	3.28943721237645
H	-2.40315426592055	-5.01822008520353	2.46254712697053
H	-1.76869373220341	-3.52663981303483	3.23800842366836
N	-0.35138461349616	2.38761531200898	-0.62399108562888

N	0.68479976539437	4.03012135056871	1.52802145061236
N	0.29999470776224	-2.43729069234281	-0.67265138929254
N	-0.82051541152795	-4.12778205665199	1.39810048600215
Cl	-2.65134088176202	-0.06066106723819	-0.18858282459544
Cl	2.57464157804079	-0.00131725912605	-0.07650852710714
Sb	-0.04213553524903	-0.03369069360845	0.05194736113300

Table S5. Cartesian coordinates (Å) of **1**, one arm uncoordinated.

54

Coordinates from ORCA-job SbCl2_un1_opt

C	-1.03762448551567	-0.03378757031288	-2.76605019728461
C	-0.10803969582113	0.96501404714038	-2.43488302152003
C	1.15531460525372	0.94897429496624	-3.06014705726073
H	1.87058907881147	1.74268947133389	-2.81103803238580
C	1.47479916401708	-0.04859805272320	-3.99383532492334
H	2.45413368136340	-0.04069994373867	-4.48759875364452
C	0.55052733606547	-1.06503874877946	-4.29380563664554
H	0.80907709504054	-1.85463910462350	-5.01155271294250
C	-0.70653088755406	-1.06669495996336	-3.66592771122890
C	-0.43548953536952	1.99908496274504	-1.37516392063067
H	-1.55421468866959	2.01978455985994	-1.22814274665613
H	-0.01722492765866	1.65696963276849	-0.40729536903053
C	0.12590038308147	4.20472733780838	-0.50767803362127
H	0.64240829151946	3.69647227687038	0.32774937781451
H	-0.90749686385175	4.45906379208453	-0.16753249525650
C	0.86601547188350	5.49357733752981	-0.86177700801206
H	0.83917076381575	6.18462858135274	0.00145650419129
H	1.93982272285783	5.24922744740636	-1.06615223301711
C	-0.53585979592635	3.95963231482812	-2.81209811020352
H	-1.60373259831332	4.18859021930280	-2.59408170665359
H	-0.52301907021354	3.26496674271588	-3.66980766584811
C	0.20536951993413	5.24603280377194	-3.15999127516282
H	1.23895349401958	4.99183261125814	-3.50853749376346
H	-0.31257580384269	5.75452803694876	-3.99406424490469
C	0.87415576064097	7.41848618498296	-2.32566369111883
H	0.33936409193318	7.90631628022956	-3.16018483279883
H	1.94763926217467	7.31007655208641	-2.62126081805238
H	0.82856485165063	8.09071413014099	-1.44998741387139
C	-1.69587100157913	-2.18988570068511	-3.83459785123158
H	-1.53928569187574	-2.75699768682324	-4.77195312271719
H	-1.58721742436913	-2.88439863783099	-2.98059372350610
C	-3.51388895080621	-1.13076339534211	-5.12106753710124
H	-3.28878793191814	-1.89672495654291	-5.88902192088009
H	-2.90119637089635	-0.23277021829257	-5.30697951143742
C	-4.99525166759332	-0.77588635190044	-5.15805987324572
H	-5.18643713379742	0.08695782792565	-4.47795981424573
H	-5.23771730463147	-0.43117071379011	-6.17965833160288
C	-4.02203287001812	-2.83381250455435	-3.43666877219329
H	-3.74366247378690	-3.16532535785174	-2.42100039252854
H	-3.83907488446294	-3.65645286821820	-4.15534847266874
C	-5.48133864855414	-2.41412818652017	-3.49374963224613

H	-6.10877170218934	-3.28811717160636	-3.24146095420130
H	-5.67317828319815	-1.63980935154675	-2.70438706459904
C	-7.24992761535134	-1.62212026974570	-4.94218475328352
H	-7.84745271515484	-2.52324801653167	-4.71818022965812
H	-7.47774137358740	-1.30751059673432	-5.97560512269211
H	-7.57583580714911	-0.80668189625061	-4.25292753646123
N	0.10480676654748	3.30896068607165	-1.66278160526027
N	0.23765256285231	6.14907535938472	-2.00788548107410
N	-3.11437138509991	-1.70253531438867	-3.79754969499290
N	-5.82909295849014	-1.93243998709778	-4.82587489645888
Cl	-3.37390951707331	1.89781871829194	-3.80203301288404
Cl	-2.48172394742789	-2.00122867930225	-0.54819735655937
Sb	-3.08305449171589	-0.03482443010861	-2.10541525383838

Table S6. Cartesian coordinates (Å) of **1**, two arms uncoordinated.

54

Coordinates from ORCA-job SbCl2_un2_opt

C	0.92140266868652	5.04978666241201	-0.34111663109695
C	1.44261030108742	6.24618672542712	-0.90259217760981
C	2.56619212881647	6.18879655545483	-1.74998399923740
H	2.97279900579988	7.12417195134630	-2.15463369995602
C	3.16222637573384	4.95905824300155	-2.05250158600092
H	4.03412997858824	4.91746914885498	-2.71704395581274
C	2.64326637914570	3.77921956712751	-1.50201743578014
H	3.10501480776903	2.80520524375347	-1.70593231512674
C	1.52844266432217	3.80149280356259	-0.64049645955986
C	0.89023409203468	7.62170820951377	-0.58068821214298
H	0.77251274503154	8.20321851110038	-1.51471993714177
H	-0.14490229763952	7.54137185645810	-0.14827140607061
C	1.29827795258311	9.74969646197073	0.49776034441836
H	0.29046294865190	9.77116635540820	0.98189349346278
H	1.20641331870689	10.23007445869714	-0.49417934728317
C	2.28192145609880	10.53337145487968	1.36342788772821
H	3.25454720089847	10.62652273923973	0.81727441299855
H	1.89262434247709	11.55490175071592	1.53006085896933
C	2.93010174242692	8.50745932769484	2.47154680908098
H	3.01564067905221	8.01971492528608	3.45976572856392
H	3.94198430300442	8.48588307628472	1.99388553808331
C	1.96043303787650	7.71408943176037	1.60141248319790
H	2.36054648344903	6.69933019771434	1.43248034148464
H	0.98788045445206	7.61207225133515	2.14974573091562
C	3.31470045375680	10.63962999761301	3.55074834595376
H	3.37441472464188	10.13683331014173	4.53240093898633
H	2.89205339903965	11.64805441254124	3.70792317132389
H	4.35548659779412	10.75840828274701	3.15999496461979
C	1.03657522044233	2.47018927843208	-0.09542002108666
H	0.40373651341754	2.62389311632586	0.80362864807711
H	0.37727097009082	2.00338421843773	-0.85326442609580
C	1.67780715571552	0.17054817650671	0.35363081286761
H	1.09984814985438	-0.12908132318917	-0.54045864634288
H	1.00666559628144	0.07063231095078	1.24136691051518

C	2.87636656290117	-0.76031049054402	0.52595609160118
H	2.52214366503214	-1.79366057723012	0.69963588160196
H	3.47340126671460	-0.76128039930542	-0.42162665404573
C	4.13380584970994	1.03890668210679	1.50508413543341
H	4.81270107432545	1.14869110690577	0.62101520003919
H	4.70592230296285	1.33552760477190	2.40398046401783
C	2.93642985562925	1.96818918509084	1.33124194157935
H	2.32495151423230	1.96763482002837	2.26420687371608
H	3.28613418528759	3.00291895465677	1.16436975588658
C	4.80128800695543	-1.25289474882447	1.90620695594081
H	4.42046560865826	-2.27528646772528	2.08068577567034
H	5.35763067365950	-0.93647246160254	2.80680784292872
H	5.52355793772322	-1.29555957500967	1.05281663267989
N	1.76675608278517	8.37502273809144	0.30945416269454
N	2.45242561771475	9.87710108119547	2.65889101526309
N	2.13727288217615	1.54801028112779	0.17447996463432
N	3.68895983477987	-0.34543226662302	1.66939824311323
Sb	-0.77457789416731	5.31188346848244	1.00125031442506
Cl	-2.15217294480369	3.52788530407979	0.16831208089072
Cl	0.25966511863552	4.28710975582068	2.91328433402662

Table S7. Cartesian coordinates (Å) of the *syn* isomer of **3**.

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Coordinates from ORCA-job Sb2O2_cis_opt

C	2.95631724230962	7.57141243646183	3.55046075973053
C	1.92540411322054	8.05895454896183	2.72229585854589
C	2.23457125461327	8.81630945538786	1.57806342771768
H	1.42569404240713	9.18120475495263	0.93136542159465
C	3.57217163284848	9.10759792873101	1.26828153225287
H	3.81295636337177	9.69938131945731	0.37653779975694
C	4.59928543550852	8.67108316856896	2.12036337270698
H	5.64349284556392	8.93599249223637	1.90378731002852
C	4.29776570686181	7.90465448889264	3.26317507869418
C	0.49570193930913	7.73918851851877	3.09541464318823
H	-0.21485357565755	8.42463422235598	2.57964494138822
H	0.27418308259730	6.70953020933243	2.77035548203226
C	-0.93091450786847	7.11413957718906	4.97313151833736
H	-0.88946015342613	6.07463668438175	4.60291241363990
H	-1.81622652396762	7.63268366794809	4.53711767917970
C	-1.03591640043663	7.10627720057804	6.49388497060246
H	-2.00279141382627	6.66056190350917	6.79245313453552
H	-0.22525827079218	6.45613814119546	6.90659488130809
C	0.29016988361835	9.10481483656823	6.61900132775458
H	1.17987751385035	8.57544330635196	7.04549684522142
H	0.30763213243874	10.14087200846392	7.00562855785674
C	0.40870031590252	9.12930804237411	5.09883280879155
H	-0.39218363043325	9.77652329690646	4.67112519465298
H	1.38407602895071	9.55486782585864	4.80111295875965
C	-1.11518269146044	8.48213869161844	8.48098331313210
H	-0.31076611871944	7.91624971707265	9.01315570168024
H	-2.08647655847987	8.03428422367851	8.75732295037908

H	-1.10053735827344	9.52379126747520	8.84911038838875
C	5.40276782019931	7.41556989875874	4.17798148736759
H	5.65006064405836	6.36870913563166	3.92277222186158
H	6.32513522923011	8.02644374912078	4.04089319684127
C	4.86038908100815	8.75074604189248	6.13999401377466
H	4.15726567008604	9.32815151047518	5.51215929108899
H	5.84841639911207	9.26756426096141	6.11058992141698
C	4.35610270666386	8.69824439843344	7.57833332225568
H	4.34166619025660	9.72136894131341	7.99794605081739
H	3.30265689292122	8.32090748732297	7.58488955545663
C	5.30253098426677	6.50831200033733	7.84603526947319
H	4.30373142900355	6.00615922284424	7.86139386350015
H	5.98719298991981	5.90464884630615	8.46996014481908
C	5.82081104608679	6.53776576267415	6.41185831643589
H	6.87733066547395	6.89465203873462	6.40486970123078
H	5.77824643223378	5.52173517896784	5.97915246684883
C	4.80001251138029	7.84958217828583	9.79484843639395
H	4.80305238330392	8.87868485743703	10.19694104956130
H	5.50103578740233	7.24429830024969	10.39694136900848
H	3.77355161559879	7.42808170108948	9.93305670797350
C	2.26033852877426	4.68755668446574	1.60265847853911
C	0.97003385814107	4.90216720141511	1.07160201683256
C	0.81391119536053	5.67281773880751	-0.09721071587658
H	-0.19064473654897	5.83135784078082	-0.51341570221455
C	1.93517506027880	6.22498949028230	-0.73729453284093
H	1.80742983533797	6.82893923891395	-1.64410685309158
C	3.22192846922844	5.97387382542186	-0.23596193869306
H	4.10393748951438	6.37842862741121	-0.74980955839070
C	3.38594583567019	5.19827979815796	0.92593062482060
C	-0.23589719110477	4.31580221045698	1.77811799291669
H	-0.51403353833792	4.96812905996432	2.62659858889899
H	-1.10904546288756	4.26349549535325	1.08700886715872
C	-0.89447058003802	2.61948240173794	3.39912982281521
H	-1.92475861874980	2.54751952026569	2.97832907609385
H	-0.87364623840634	3.40790370333109	4.17337940429328
C	-0.50097549413133	1.28108176478758	4.01595435676454
H	0.46417226986646	1.40538262612239	4.56642284049167
H	-1.26744932635060	0.97795956318464	4.75287647040782
C	0.58580554235028	0.62932438532342	1.97749103256921
H	0.62315785831653	-0.15275462270962	1.19649438290466
H	1.61179795545500	0.71023467944435	2.41694778465557
C	0.20819315736434	1.96197076469890	1.33925621121121
H	0.99243359846598	2.27779974486048	0.62719641713664
H	-0.74384433109342	1.84513920282319	0.76995085259998
C	-0.08892141483863	-1.05910130591167	3.56591023748936
H	-0.06678346199130	-1.82640750051296	2.77127291552600
H	-0.87081863031279	-1.34136201486793	4.29339997125564
H	0.89690901731823	-1.07992602310347	4.09324924335915
C	4.75640194401448	4.89596135992133	1.48825820522586
H	5.54812227027840	5.06100106150220	0.72240869434070
H	4.94521506002206	5.58298762196050	2.32890785783271

C	5.96553680815093	3.32974968474261	2.91782688698717
H	5.88938583372360	4.07615459957790	3.72822803029484
H	6.91900011262856	3.47762696845266	2.35945114615918
C	5.93226326293192	1.92733968538954	3.51502234259191
H	6.83687198607038	1.76983049780405	4.13109068823650
H	5.04677959763073	1.84446522859184	4.19274020889247
C	4.73561851951767	1.11407019783354	1.59815226046464
H	3.77776910859803	0.97831012179795	2.16191373568806
H	4.75188685866015	0.35802684016384	0.79111835249749
C	4.75624919634510	2.51003532006648	0.98521720191331
H	5.63422360099916	2.60747427504572	0.30488901730675
H	3.84248404648340	2.67484992793358	0.38610520981550
C	5.92444426256427	-0.43891093323000	3.01396069815989
H	6.83548048629703	-0.57578358910938	3.62360608838858
H	5.94583586777179	-1.17960471002391	2.19438440673087
H	5.04004803526600	-0.66435044955879	3.66012257452380
N	4.97287345133541	7.39894176913097	5.57847952088719
N	5.22805446204229	7.86172213635993	8.40302787612548
N	0.31416629760766	7.76906217542835	4.55294765928157
N	-0.95887531130146	8.46682121046490	7.03341142295316
N	0.06860136544721	3.00649036852819	2.36111924670630
N	-0.39818582160674	0.24144746263816	2.98821319715735
N	4.80900502638735	3.53421560006911	2.03670082690452
N	5.89740883035334	0.90822747620937	2.46214927997093
O	1.17381082161480	4.93999918433407	4.37019691705846
O	3.80752479411569	4.86443396508604	4.48968122864232
Sb	2.49331106062325	6.24583477304019	5.23975650335017
Sb	2.49470071053987	3.62942262308015	3.51279476929625

Table S8. Cartesian coordinates (Å) of the *anti* isomer of **3**.

106

Coordinates from ORCA-job Sb2O2_trans_opt

C	6.88824319943843	7.99086468465234	7.88914544530318
C	7.09092855043943	6.60295540916487	7.73862295792403
C	7.76565825988257	6.10946206022783	6.60532811965780
H	7.91168260380783	5.02693862553885	6.48730948623415
C	8.23730678202269	6.99512246367186	5.62260821968998
H	8.75524747213657	6.60699443292329	4.73669671292268
C	8.01895187842239	8.37563964355263	5.76056655837161
H	8.36340567942380	9.06865243056760	4.98069813454785
C	7.34542481524007	8.87693732422309	6.89117242845212
C	7.10690036797257	10.36124205016510	7.07217320564820
H	7.82379605396275	10.74603039543631	7.82205509393070
H	7.26573913313439	10.90975045957139	6.11542158670587
C	4.69267277278274	10.30822375192417	6.66865873164115
H	4.81235961545633	9.26386716039375	6.32773250083734
H	4.76547706576365	10.97080029404191	5.77465596764375
C	3.33072187002811	10.48666616053445	7.33353956860359
H	2.53269749482262	10.31455643802963	6.58736893780853
H	3.21243570805390	9.71153907697218	8.13210579448722
C	4.26435250436888	12.13491105320882	8.81995174128231

H	4.21792662716303	11.47274101062115	9.72013070322047
H	4.15011303096500	13.17741107853117	9.17107075570065
C	5.62579103268159	11.97035167501654	8.15464964471677
H	5.74276408405541	12.72772745195014	7.34482568684446
H	6.42609209125767	12.11002808277798	8.90155595595782
C	1.87294869221036	12.03279235513110	8.47916408112641
H	1.68694072043821	11.35253631293129	9.34666979383513
H	1.08323278159410	11.85258899893796	7.72776198569697
H	1.77595630677154	13.07393175264657	8.83555108752684
C	6.58027817749415	5.67313500834822	8.81906838556484
H	6.56035937181408	4.61847717804104	8.46024794253308
H	7.25885261235104	5.73575352765935	9.69083525236173
C	4.89273233934771	5.47668818186773	10.57058101041313
H	5.69937597368845	5.70550176449314	11.28818457294254
H	4.80465122120175	4.37120239853042	10.45585877407719
C	3.57395564496472	6.04821693940061	11.07789356543859
H	3.28319838849674	5.53035180177857	12.01083279646091
H	3.71918421347465	7.12883611077135	11.32720188165037
C	2.87956668140712	6.48005319265513	8.81388594126486
H	2.96821182711451	7.59158092762237	8.91040203531256
H	2.08148313010067	6.27704396547067	8.07557082050531
C	4.20151668132098	5.91985595720142	8.29678152151302
H	4.08201514443700	4.83862991438792	8.05151642723651
H	4.49878738511041	6.44688747876137	7.37209780502819
C	1.22977534324411	6.35809305780792	10.57238436748523
H	0.95705489120546	5.83851658400094	11.50836500655604
H	0.44145013563752	6.15514699001511	9.82533027155588
H	1.23735872734106	7.45707509825530	10.77754177679028
N	5.76789885313530	10.61100932714494	7.62164481547024
N	3.18377996805117	11.83815296158847	7.87521702588310
N	5.26037958653363	6.10552348561922	9.29708014653188
N	2.50995626180994	5.86137799552360	10.08743143081038
O	7.22262759243782	10.18917202030012	10.10959288725890
Sb	5.82416800773405	8.76145143094276	9.63831034796048
C	6.27020224242582	9.97808741665676	13.02032858393087
C	5.83332869043792	11.31899251529721	12.96643094088440
C	4.68026212350392	11.71371595663724	13.67214519066299
H	4.35057973312837	12.76115152446721	13.63336488651241
C	3.96423150274930	10.77782615079775	14.43615481164094
H	3.06968249466818	11.08963549536213	14.98962550369226
C	4.41597506492469	9.45072903790865	14.52000962754864
H	3.87914311189130	8.72440405777056	15.14577310117370
C	5.56810054302001	9.04848451023787	13.81703278377292
C	6.06837161559690	7.62129851997577	13.88645475268831
H	5.75631886843839	7.09663448311430	12.96519058700431
H	5.63339178484393	7.08960504270126	14.76383164022896
C	8.09617948969648	8.07632930449899	15.16499354030856
H	7.71203099328301	9.09819693654513	15.33663235768547
H	7.76591732869609	7.43823221284180	16.01808049636356
C	9.61971766122593	8.09417696117454	15.10024899762735
H	10.02562269303889	8.41924763761664	16.07627204660313

H	9.94358828913251	8.84699773478388	14.33739357486090
C	9.58567267502324	6.28104299793488	13.52448315367643
H	9.90834390518097	6.92307823227150	12.66749950370671
H	9.96724854731068	5.26063984738992	13.33524535341843
C	8.06153298362525	6.25032497650409	13.57280193263198
H	7.72589056250844	5.49352904751760	14.31994085384451
H	7.66338238671952	5.98148588221893	12.57813368885249
C	11.59732389421366	6.74446670376201	14.78411568930990
H	12.03859110583342	7.41460758419056	14.00531450894538
H	11.98147929890150	7.06626253441374	15.76876969370994
H	11.95799224022620	5.71774459758350	14.59419992563200
C	6.61617673371738	12.30917353766621	12.13064962008044
H	6.36482607624788	13.35662000263781	12.41594246479451
H	6.34927111417623	12.15862064608804	11.06890035500357
C	8.81605697324056	12.70514740229929	11.15409471479743
H	8.40695509162834	12.33288913512019	10.19790363366631
H	8.69707623992276	13.81305476297411	11.19869139625217
C	10.29453596090172	12.34453247344900	11.25555689315360
H	10.85945393176585	12.88997396302290	10.47711742017238
H	10.41576180090051	11.25135598384080	11.05292862611129
C	10.07926426520778	12.03951280136831	13.62887377263914
H	10.18827245391733	10.92674541666608	13.57004769122899
H	10.48222405261752	12.35776275757957	14.60837450238584
C	8.59954881665063	12.39959514324663	13.54840559286882
H	8.46864838267334	13.48834073461505	13.75217621087850
H	8.03126035895707	11.84025126437995	14.31358276400882
C	12.25922140336856	12.42469861342946	12.66354513306987
H	12.80405871006228	12.97895993104395	11.87853376679139
H	12.64242857571641	12.75544912239574	13.64560655522064
H	12.49789215858977	11.33844343070067	12.54767118078481
N	7.53539735772876	7.57974753426140	13.90283858503001
N	10.14127514544979	6.76290531038943	14.79184182478497
N	8.05817405325777	12.05405431778143	12.22875419644618
N	10.83391107373976	12.70732337993413	12.56872681959386
O	6.93917528400257	7.73926275750885	11.02656370263957
Sb	7.97710822056428	9.32109650089481	11.79798174775653

Table S9. Cartesian coordinates (Å) of the monomer of **3**.

53

Coordinates from ORCA-job SbO_opt

C	2.53906518378937	4.19835345872031	1.19490652050362
C	1.33583859746841	4.61073955273073	0.58960500432795
C	1.36589972402652	5.45602965540599	-0.53644172780507
H	0.42796099219015	5.76720295811040	-1.01667851863677
C	2.59724526645865	5.91616863575683	-1.03479129687842
H	2.62222251196804	6.56211547202620	-1.92107311414913
C	3.79412157253472	5.57507601507967	-0.38127363089552
H	4.75063994614358	5.97909352071192	-0.74050791064312
C	3.76329012517832	4.72991702065221	0.74503260908277
C	0.03516438160856	4.25775733168608	1.28427129753911
H	-0.10317726269386	4.97441799653072	2.11620306594984

H	-0.83815991676067	4.37269040602840	0.60493692361106
C	-0.88072112040779	2.79115303426861	3.01022922703163
H	-1.91093989738570	3.05422074822461	2.68307450541912
H	-0.55207792318983	3.50475330716956	3.78814369480814
C	-0.86915318482473	1.37775759008597	3.58109044977891
H	0.12177277319759	1.18379732746783	4.06123993973992
H	-1.63349336629825	1.30780831702606	4.37631804061621
C	-0.18100053694013	0.47761781369738	1.47013542935554
H	-0.43446217199633	-0.25818157979856	0.68472843426112
H	0.84532273330542	0.23239505627694	1.84052911342949
C	-0.17558441020857	1.87375313952204	0.85651336896512
H	0.62386041272288	1.95617075436074	0.09696305693063
H	-1.14969353104337	2.06108623488206	0.35163403879098
C	-1.25841773240096	-0.95807397014740	3.08718355862281
H	-1.53361259918830	-1.66810170283746	2.28692251532157
H	-2.04211658340676	-0.99722090918313	3.86436957856277
H	-0.30040688298001	-1.30667813359356	3.54517712551079
C	4.99353431632457	4.50369995708782	1.60200482052530
H	5.93028641262739	4.70282672150526	1.03608547418992
H	4.95670165129817	5.23080017770942	2.43548746697569
C	5.81687707991473	3.13547684661597	3.45056023143971
H	5.31906330222571	3.81062590979730	4.17081989635817
H	6.84892692718253	3.50265235999283	3.25648656866736
C	5.87434553625713	1.72769146257903	4.03237128150850
H	6.53371862975811	1.73488295265904	4.91930982135691
H	4.85487104176374	1.43350320287669	4.38462633159217
C	5.55694314846336	0.76373030276549	1.86206553053127
H	4.52115156522556	0.41597737520783	2.10088936458072
H	5.98171480575188	0.05758767943900	1.12487519896866
C	5.49103153663782	2.15238126067447	1.23506577818624
H	6.49829997128223	2.43629131159006	0.85617972524791
H	4.79122594509411	2.15426628907861	0.37886559749627
C	6.55786205635415	-0.55596154614106	3.62133150936189
H	7.23720654567004	-0.51565023649567	4.49117143066342
H	7.00168965184388	-1.23423245230751	2.87084833995508
H	5.58968552350720	-0.99989204961602	3.95987153673715
N	0.05901886840253	2.91073079164909	1.87912921260086
N	-1.17242452862400	0.39063966995306	2.54213451882521
N	5.02491367378177	3.16073592277252	2.20582133626113
N	6.40622306063233	0.77723178758458	3.05288709881471
O	2.35785224424331	3.66049117893798	4.33023537557648
Sb	2.51295793351476	2.66663707322306	2.76350125442819

Table S10. Cartesian coordinates (Å) of the *syn* isomer of **4**.

106

Coordinates from ORCA-job Bi2O2_cis_opt

C	2.97004614518348	7.57840874462272	3.59116829911121
C	1.93436205103906	8.04219659286598	2.75773896765590
C	2.24102028265640	8.78433789656407	1.60208495215029
H	1.43190569855443	9.13484425379674	0.94750499029944
C	3.57852594192708	9.07431488022483	1.28737640219836

H	3.81653598982974	9.65352889531312	0.38663446638789
C	4.60997113399426	8.64701659963298	2.13999604385170
H	5.65385182909754	8.90410707223673	1.91171122335184
C	4.31142745411610	7.89789622487267	3.29574735585787
C	0.50565570922851	7.70606552362171	3.12753547771967
H	-0.21264845061274	8.35355824704330	2.57458172179399
H	0.31130249592481	6.65947192596820	2.84164411454795
C	-0.94457193122916	7.12517580056422	5.00320217607154
H	-0.88151230534146	6.07563990105888	4.66394718286431
H	-1.83380617787478	7.61806643603747	4.54536781124390
C	-1.06396964381632	7.15600208792767	6.52275099122129
H	-2.03110789220393	6.71351579101996	6.82479221623164
H	-0.25718328410663	6.51535216072095	6.96122268674920
C	0.24518994191091	9.17130074634562	6.60592862615507
H	1.14291674704644	8.66491218971166	7.04842284233434
H	0.24915226954564	10.21538255177796	6.97052114267399
C	0.36644262605485	9.16095943762653	5.08580289239954
H	-0.44442001647999	9.78492640055292	4.64211235286294
H	1.33506051767490	9.59494855754414	4.77893390367619
C	-1.15760853140503	8.57420403118976	8.47914918112262
H	-0.35059665213458	8.02631703199874	9.02669592592866
H	-2.12609078935777	8.12457144308945	8.76194063671495
H	-1.15218261146261	9.62373702686727	8.82410291193102
C	5.41678653832132	7.40507091820482	4.21003355414175
H	5.61347654489981	6.33888680908078	3.99304628316019
H	6.35855360615464	7.97449720580136	4.03259648039731
C	4.93334988029576	8.82575760326227	6.13300960465349
H	4.24125720319558	9.39529958503184	5.48659337152568
H	5.93083233270257	9.32310501821801	6.08871033165901
C	4.42762538963458	8.82607861502966	7.57174033726420
H	4.42275061731679	9.86099555222166	7.96119897209022
H	3.36742533268766	8.46261987807050	7.58848755906714
C	5.35927262506090	6.63579602363894	7.91067421779700
H	4.35969505171497	6.13276460554721	7.95240936466009
H	6.04507821987916	6.05228057250531	8.55208560874403
C	5.86783183469110	6.61392930283401	6.47252754854501
H	6.92712060247916	6.96209262196011	6.44726101366936
H	5.81420827082096	5.58458866946735	6.07306990597981
C	4.85852026002809	8.04006043091131	9.81488632184884
H	4.86593188702686	9.08127326762899	10.18397700049688
H	5.55581383008052	7.45054744898243	10.43641823384570
H	3.82969622996359	7.62786231356299	9.96524169811917
C	2.23905241380577	4.64050541111715	1.61841278037572
C	0.94639151673530	4.86200410211521	1.10080250055008
C	0.78588795153712	5.64782400630120	-0.05810786236318
H	-0.21997889006127	5.81540462497819	-0.46809988327476
C	1.90637204413975	6.20635379464504	-0.69523669120324
H	1.77581968413805	6.82105121621726	-1.59443338013592
C	3.19552938299553	5.95461716761286	-0.19832113240608
H	4.07447786442967	6.37278515644523	-0.70681088104573
C	3.36412394682811	5.16595445171884	0.95477134493595

C	-0.25546705903040	4.27512844123085	1.81562247018268
H	-0.49403913507219	4.90421298340869	2.69345916635094
H	-1.14557382942805	4.26290106008854	1.14464878150010
C	-0.94062187288341	2.53140459274486	3.37508833616521
H	-1.96969539905441	2.47458365388860	2.94861350650297
H	-0.91991678653563	3.29887859034503	4.17026557767528
C	-0.55620940136209	1.17493242198687	3.95783743067048
H	0.40104061193721	1.28048779583182	4.52925517794620
H	-1.33097859346165	0.85099223365931	4.67688903801398
C	0.54177123070646	0.57910936173199	1.90417117399277
H	0.58255462978826	-0.18493413258884	1.10586241380213
H	1.57028414866019	0.65129291948539	2.34404304646467
C	0.15960715416597	1.92628889742708	1.30032955991318
H	0.93867012670414	2.26047053933124	0.59135254520661
H	-0.79635663656697	1.82259894514526	0.73499208965302
C	-0.12804580171804	-1.15066095726312	3.45125159156368
H	-0.09620042134992	-1.89672151304164	2.63715678875785
H	-0.91347781557974	-1.45523702857829	4.16564403522756
H	0.85430636697847	-1.18031541256416	3.98513287190910
C	4.73656791558045	4.87437225767259	1.52215161497311
H	5.53208530920834	5.08809145004075	0.77216804501524
H	4.89928490463447	5.53336724824796	2.39042982808211
C	5.98499261455269	3.28957681696951	2.89835200977770
H	5.89831562226015	4.01551823429395	3.72685191786689
H	6.93666593407580	3.46144397489979	2.34332222324875
C	5.96875421906369	1.87384482380049	3.46421330478175
H	6.87753332229892	1.70947812512028	4.07200055596347
H	5.08943290204740	1.76900379068074	4.14938074999038
C	4.77130710266225	1.09144339249941	1.53253096939834
H	3.81229124991436	0.93578450809470	2.09287044372452
H	4.79180026461701	0.35039928067861	0.71189680257738
C	4.78282089617751	2.50023567059129	0.94898650997965
H	5.66162244818228	2.61740602875500	0.27245848967449
H	3.86906982611197	2.67046918090989	0.35151065184105
C	5.96932743822604	-0.48230396205118	2.91823410416590
H	6.88331150675150	-0.62605790032482	3.52163368544720
H	5.99057706056576	-1.20691650506035	2.08455180733646
H	5.08863101968494	-0.72453012848808	3.56393528487263
N	5.01784339008879	7.45402690243396	5.62105034414269
N	5.28642372044643	8.00521229379617	8.42367403154224
N	0.29566458240775	7.78584027407024	4.58001826390285
N	-0.99472075143545	8.52693286756847	7.03341115076199
N	0.02961952984425	2.93965949015815	2.35275115638545
N	-0.43823479892433	0.16322152580771	2.90598433306259
N	4.82400137309692	3.49639983833878	2.02502183617585
N	5.93191084954999	0.87502669374412	2.39363291344972
O	1.09547808709917	4.84915875247514	4.50686278217684
O	3.87839937449225	4.78369536921520	4.62500222295236
Bi	2.49316317038254	6.24202281880086	5.39197975866858
Bi	2.48911968017679	3.49223467008437	3.58744190835839

Table S11. Cartesian coordinates (Å) of the *anti* isomer of **4**.

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Coordinates from ORCA-job Bi2O2_trans_pip

C	6.89045321724307	8.36348770092264	8.91795306885698
C	7.36718920819165	7.04218872598267	9.04234051370653
C	8.61225359485579	6.69108054401789	8.48336428148342
H	8.98018655477662	5.65949182203283	8.57421315092037
C	9.37589187614906	7.65284695164562	7.79998420095482
H	10.34322271450269	7.37545327257424	7.36279246756963
C	8.88392617919165	8.96026962707452	7.64494968072153
H	9.46408627040127	9.70316201583040	7.07988531401801
C	7.63955450697217	9.31891781588686	8.20030957152574
C	7.10031355453710	10.72901710269924	8.06855996254282
H	7.29664477920051	11.26357418326171	9.01576756706966
H	7.60776733772232	11.27166080126855	7.23772055591108
C	5.21745732793408	10.20900646150523	6.60253857525262
H	5.64821649227305	9.19921788180286	6.47609392214582
H	5.60041037780329	10.85121390251178	5.77461556527687
C	3.69578023707179	10.13969673041934	6.53185929875391
H	3.38641027090692	9.79256499447575	5.52854110469022
H	3.32950752720770	9.37994722662810	7.27074145957831
C	3.53089966732557	11.96922952986985	8.08210505363439
H	3.15170312127629	11.32674309504473	8.91781754508524
H	3.09948728339691	12.97724424700741	8.22356596007278
C	5.05172677718516	12.04857290316361	8.16991115099227
H	5.42770729908279	12.80983592625900	7.44654512186695
H	5.35197492976105	12.33895671437436	9.19314958953045
C	1.65271272501095	11.42116204796706	6.66072757429523
H	1.16846222947854	10.74400694804343	7.40775876894168
H	1.36691251358487	11.07532157431671	5.65120488414510
H	1.24216870296670	12.43637290338109	6.80499608132136
C	6.54220625695018	6.03005152042508	9.81107271934763
H	6.85607842409223	4.99019980671943	9.56119960353446
H	6.70714688437436	6.20168583532961	10.88993143745102
C	4.29061179738609	5.54751198285726	10.60842291909712
H	4.61624140965721	5.92900523214707	11.59319060173727
H	4.44562566654568	4.44352783874226	10.57213441388234
C	2.81320620645378	5.86240007155161	10.39676724162447
H	2.20683339134493	5.29357325524098	11.12547991904661
H	2.63999151109614	6.95005411339564	10.60110120725988
C	3.20069493682664	6.19108183792307	8.04698765331515
H	3.05864725706518	7.30206318047660	8.10134864126026
H	2.87838854536736	5.87151624222405	7.03860916595943
C	4.67885404886437	5.86804224848691	8.23803509917679
H	4.85120729316521	4.78331089747403	8.04300566615965
H	5.28891002674783	6.44428656209808	7.51901770970991
C	0.96386102189852	5.74702396650126	8.84307491064053
H	0.37582450779549	5.17323414629477	9.58129508070645
H	0.66471057261143	5.41513955498761	7.83276059214347
H	0.68979109033503	6.82635108151737	8.94763257952562
N	5.64188697672872	10.73263745956483	7.90424164992209

N	3.10332676129983	11.45236171693698	6.78085558278252
N	5.10403335089754	6.22640425946384	9.59417346333186
N	2.38471595888509	5.50121405077673	9.04424572901373
O	6.06736902443177	10.69210013291005	10.90605171744660
Bi	5.01332276394952	9.01379268777228	10.07361118171973
C	6.43635681946016	10.36835420604530	14.17221920086485
C	6.29675618745866	11.75924160210633	14.34961287312030
C	5.75684540634605	12.25901406892176	15.55110959485299
H	5.65652949911577	13.34380127428674	15.69540801744475
C	5.35852090554801	11.37401523234545	16.56755966033904
H	4.94568769998758	11.76667750102797	17.50524559920670
C	5.51152844085961	9.98788699915339	16.39413341227695
H	5.21926574183689	9.29731632315834	17.19746230542155
C	6.04996689196981	9.47992696467819	15.19523341637436
C	6.20273624166806	7.98945926426564	14.96396781075025
H	5.40838402469742	7.65615646665061	14.26929123627741
H	6.09715175134866	7.42597211734247	15.91951757965188
C	8.64697656134320	7.91934290304456	15.14980252478603
H	8.60458696094866	8.95934321742603	15.52085194559249
H	8.63420462771781	7.23908807160745	16.03348894930911
C	9.92916041241174	7.70251043806030	14.35080617561538
H	10.80458069589674	7.82865471913002	15.01473815101665
H	10.00213451225448	8.49133981409118	13.55749455620431
C	8.78732429305021	6.11922719038693	12.93874118397623
H	8.77346408569504	6.79133454016525	12.04322998140677
H	8.82566759437053	5.07969663789979	12.56350166961308
C	7.50463342803460	6.32690965306140	13.73581697328848
H	7.43425346277177	5.55937109596232	14.54155355091822
H	6.63080658418378	6.23871358287859	13.06685230366118
C	11.20211718255460	6.13032413997401	13.03317698476827
H	11.32066706017056	6.81784761463323	12.15942090324273
H	12.07106869708280	6.27139378391497	13.70063203801896
H	11.22405738970970	5.09263968311381	12.65518424248447
C	6.71686760202089	12.68289229938988	13.22329092822208
H	6.77829940043006	13.73795703603259	13.57658547086399
H	5.96203121792693	12.62462096096648	12.41599547410565
C	8.24649111832987	12.87575609351304	11.32652617887424
H	7.36948350221306	12.67476187411881	10.68656440992156
H	8.37810629790670	13.97718720133911	11.44027101537865
C	9.49499253645432	12.27050216442722	10.69447376025292
H	9.71703386382721	12.78871209187944	9.74317343559875
H	9.29258851896923	11.19787404327872	10.44508259719799
C	10.38182364771342	11.79273034491223	12.88297730113965
H	10.24716435266554	10.68309967947019	12.79351303863872
H	11.25320170652590	11.96113564661213	13.54283324849989
C	9.13357303542946	12.39479172312105	13.52172037833488
H	9.31185522451249	13.47133953406858	13.75230664559695
H	8.90718199167902	11.87695206853176	14.47119094794053
C	11.86005090731647	11.86051879361395	10.97533866445086
H	12.06518121536310	12.37841195962426	10.02146492104778
H	12.72279440060069	12.02198406572464	11.64622366860499

H	11.78559109587036	10.76511922525504	10.76371628832302
N	7.47688911057295	7.68149804145645	14.29753230112228
N	9.96807807919498	6.36061636117572	13.77139831298139
N	7.98467352461436	12.24192779648282	12.62262689690100
N	10.65255279806505	12.40312279340780	11.58218676771850
O	5.77246813699819	8.10648524104898	11.86760403649967
Bi	7.34075159552709	9.55462452343223	12.24049099464205

Table S12. Cartesian coordinates (Å) of the monomer of **4**.

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Coordinates from ORCA-job BiO_opt

C	2.53593771768331	4.22100907628422	1.24997512102621
C	1.33259804144416	4.61470796127577	0.63370516890843
C	1.36457744424108	5.42933849608994	-0.51536248617497
H	0.42713089178172	5.72740913742209	-1.00523719582061
C	2.59640570959183	5.87313327422340	-1.02696771522812
H	2.62217122921450	6.49547144837482	-1.92996132395528
C	3.79326241584781	5.54185395449875	-0.36875506528426
H	4.75118806958300	5.92765880347394	-0.74453008801981
C	3.76276539438796	4.72795942578604	0.78138435756076
C	0.02343515225658	4.27280384049577	1.32060463459774
H	-0.11451739573077	4.98387575985285	2.15750308523332
H	-0.84153515159361	4.40195992796425	0.63232738098411
C	-0.99797039450522	2.77339917675025	2.95745780055657
H	-2.01027562405296	2.98888861786130	2.54810003806575
H	-0.76944790982545	3.50743037894537	3.75172420992990
C	-0.97057939504076	1.36404330149886	3.53834374351457
H	-0.00830332586644	1.21253284006923	4.09035241681038
H	-1.78552593816278	1.26137647339019	4.27759746115271
C	-0.10533000709000	0.48915775840452	1.47780498414031
H	-0.28293722656720	-0.25547812010013	0.68011060180574
H	0.90739776500453	0.27697453972325	1.90726601673388
C	-0.11397589385463	1.88626276956976	0.86692774965918
H	0.72418744784053	2.00010608446817	0.15541709594902
H	-1.06322622213616	2.03967292256357	0.30534604052945
C	-1.21658254533731	-0.98922655643989	3.03351803144965
H	-1.40527566535537	-1.71250197213863	2.22034564755615
H	-2.04780940183626	-1.06151819751131	3.75690000093358
H	-0.27646456495798	-1.29331610147506	3.55631958668819
C	5.00765883601421	4.51251938336510	1.62216261253304
H	5.93172926993069	4.71014768425478	1.03370718654970
H	4.98623319593883	5.24665768927917	2.45032779815775
C	5.96656534302594	3.13851506935237	3.39851465405939
H	5.58987234157087	3.86209098542673	4.14409423398173
H	6.99575165166857	3.43779066147002	3.09753127504981
C	6.00066784060923	1.74216838546315	4.00946446239439
H	6.73134060011622	1.72756971747309	4.83843993891494
H	4.99922477944296	1.50983966607806	4.45300890678203
C	5.46331856696710	0.76019190802242	1.88692275608937
H	4.43316780901413	0.45659279359796	2.20497580031005
H	5.80067391389140	0.02597933715579	1.13227295083708

C	5.41007383552046	2.14356330880082	1.24695362218372
H	6.39761253550955	2.37888755173063	0.78903866293193
H	4.65022109030515	2.16591508352328	0.44443553397612
C	6.52161462341152	-0.58403427240073	3.59390991346350
H	7.26586827777866	-0.56633605963811	4.40954087992446
H	6.87138215167555	-1.29639682664967	2.82565006061847
H	5.55987115252094	-0.97069133825586	4.01234502949025
N	0.02395667201446	2.92130991187115	1.90642255134521
N	-1.15281536471467	0.36050070163858	2.48884116155438
N	5.05991927297928	3.17617418814345	2.23816371509117
N	6.39506206778627	0.74593530603994	3.01285594362432
O	2.27752367697766	4.00112845525950	4.49617367355055
Bi	2.48526924308085	2.74393868767708	3.00709537728405

Table S13. Cartesian coordinates (Å) of the cation of **5** (protons on the same pincer ligand).

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Coordinates from ORCA-job Sb2O2_2H_cis_1_opt

C	2.92806731772890	7.40628383499402	4.06774880774095
C	1.78727501898139	7.86585217964269	3.36252264984041
C	1.96327363866428	8.75179120218841	2.27844343315953
H	1.08640169573188	9.06320029232851	1.69674641126735
C	3.23171530679851	9.23113770610333	1.92438168254847
H	3.34559297001562	9.92890841122206	1.08698593906133
C	4.35388458163581	8.81015289722121	2.64884017513564
H	5.35000818907155	9.18467108946034	2.37998927114479
C	4.21290897629647	7.88799401272982	3.70440083062430
C	0.37855397695912	7.43619640035150	3.71169788373521
H	-0.24274392419790	7.47549805661103	2.78790711694561
H	0.37934911825982	6.38968261381357	4.05731370215141
C	-1.55099636435349	7.68523547042749	5.13315116314988
H	-1.42511255732220	6.63375148574018	5.44717570529163
H	-2.24485980470222	7.67213320323133	4.25436425126123
C	-2.20577979221741	8.44474197434710	6.28106963549042
H	-3.20867274473510	8.04813689579848	6.51044703909237
H	-1.58737792119182	8.41693260826368	7.19391059043094
C	-1.00643602134456	10.47540065202882	5.52904675293576
H	-0.38635223901221	10.44232760026334	6.44046560426467
H	-1.15657571773823	11.52562659066785	5.22906029782558
C	-0.39622070333241	9.65250224741771	4.40280070020742
H	-1.01964006116234	9.76555368049370	3.47934075600403
H	0.59333627750226	10.07949647435982	4.16400284013128
C	-3.04541886946671	10.70922040309300	6.98857925993584
H	-2.42868606353840	10.68118234581482	7.89932256240932
H	-4.03401923889837	10.26872923733174	7.18879393876270
H	-3.15998420865434	11.74767420312790	6.64225987876292
C	5.46848117106682	7.34988692251238	4.35720906804073
H	5.74600857754460	6.39403294118515	3.87884196921932
H	6.31882427365679	8.04792686086326	4.21475105783072
C	5.29365375960053	8.26485977800416	6.61461782872624
H	4.46566719062440	8.91801542192064	6.28509905299223

H	6.23509226199274	8.83767964044366	6.45244465397272
C	5.11553716983547	7.95553315112529	8.09562541703342
H	5.17773979958308	8.87286899384968	8.70368779324415
H	4.15423131551630	7.45272197298410	8.29799656018040
C	6.16137968350537	5.74588989130558	7.72694557368036
H	5.19355616471014	5.25927615338760	7.93707960458509
H	6.97384830369107	5.08411183210277	8.06893921206259
C	6.31453155184223	6.08349174989675	6.25166384540674
H	7.33689443874053	6.47301579424883	6.04648157690431
H	6.17862841320891	5.15109553964118	5.67322791735064
C	6.10199707680172	6.71300547688064	10.04752504929395
H	6.17090267345012	7.65927402936348	10.60540913429321
H	6.93112729318442	6.04787189579134	10.33316758190612
H	5.13803169728616	6.22222643275995	10.24925862656102
C	2.24244789807571	4.66000953414187	1.95901104856354
C	0.88605795036315	4.82621822936809	1.61575415907559
C	0.55060853225755	5.70800044267288	0.56954435820906
H	-0.49916728495587	5.82427020406147	0.26981562246314
C	1.55593160603299	6.39678902958703	-0.12926366401598
H	1.28533199210741	7.06342202052544	-0.95653322948401
C	2.91057210346014	6.18052544359730	0.17760840538881
H	3.69358511587861	6.67130740859398	-0.41364704445532
C	3.25493202704430	5.29950846283294	1.21561275642996
C	-0.17270673103689	4.03025926247089	2.34680764813431
H	-0.46954988462762	4.55958464726208	3.27085504567270
H	-1.08281966675421	3.92559145682110	1.71866573128320
C	-0.50802817198007	2.08696506915481	3.78977807136425
H	-1.54728163726570	1.97712265822907	3.41291493816041
H	-0.53622076305522	2.76081768417588	4.66590018961660
C	0.03035732207301	0.71547866313999	4.18579254100246
H	1.03351193313076	0.83547197327453	4.67609929418473
H	-0.64468474572125	0.26480378272672	4.93494754808061
C	0.95942436832346	0.42432046057519	2.00320582175426
H	0.97440255398142	-0.23610677343538	1.11799226624140
H	2.02142351937791	0.50527573807906	2.36165762613312
C	0.45632097505357	1.80139167807958	1.58298267161720
H	1.14218525768709	2.26004272002324	0.84762139089639
H	-0.53741151931980	1.69940230180993	1.09811157082961
C	0.45202734482803	-1.53007833246783	3.35237352443921
H	0.41308462718081	-2.15233906961261	2.44262924380428
H	-0.27618469870991	-1.93837075737861	4.07305464032365
H	1.47190656782671	-1.61875389129813	3.79526435823018
C	4.68634914131996	4.96063265965320	1.55448523001203
H	5.36887739410341	5.16326429468712	0.70609398572692
H	5.01630441537477	5.56718764870956	2.41265999464271
C	6.08859972175361	3.27640415419484	2.66166103697527
H	6.11517163885409	3.91621306607199	3.56079122578566
H	6.92101837781634	3.55865360514635	1.98652135871023
C	6.21260229503643	1.80640267450821	3.04846263344532
H	7.20269285916754	1.64061642910070	3.50941255099806
H	5.44447481338781	1.56488761068369	3.83172912649364

C	4.79700163209532	1.16786710625129	1.23322472949099
H	3.94217820377554	0.88281333577944	1.90490748019908
H	4.72181493522146	0.52517044439555	0.33835988500008
C	4.64050045606341	2.62204323755050	0.80803609377987
H	5.41062234910575	2.87791751547267	0.05369420391821
H	3.64825739221070	2.79975457973507	0.35763296586827
C	6.35048451256200	-0.45475591785486	2.16203162471196
H	7.36608361195487	-0.56116242401299	2.57861367435830
H	6.30703499892925	-1.03538210083505	1.22555960817828
H	5.62550063076158	-0.89689344185186	2.88409902243166
N	5.28618178504920	7.03912678032399	5.79573158574478
N	6.19467111843833	7.00415848644742	8.57318932141466
N	-0.24376011038167	8.24798587078576	4.78875053252787
N	-2.35904741554969	9.90817523201206	5.91673353968535
N	0.34371189487178	2.71026971671665	2.75322669362096
N	0.09764147875358	-0.15204826587132	3.02061420963497
N	4.79596004038455	3.53810916628446	1.97637630923553
N	6.08022469181852	0.95409170494824	1.87881430420852
O	1.36315248009512	4.67634626269843	4.89461730682303
O	4.04199560737732	4.62534505223690	4.63108283260154
Sb	2.94461761810498	5.90366964842947	5.65003262608638
Sb	2.86724841555951	3.29010950210183	3.49470761901065
H	0.96806236808505	4.16731156837264	5.62929671315583
H	-2.95289538078842	9.94697088519038	5.07152536893694
H	7.10599826781270	7.46275575458721	8.40607031504811

Table S14. Cartesian coordinates (Å) of the cation of **5** (protons on different pincer ligands).

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Coordinates from ORCA-job Sb2O2_2H_cis_2_opt

C	2.88346128155480	7.54141416094212	3.62338204856173
C	1.79431664075455	7.97817058404623	2.84098892550574
C	2.04058432525819	8.70405920985671	1.66184900406406
H	1.19963976087170	9.05084066648567	1.04833363370302
C	3.35842962097737	9.00584881816030	1.27782305973464
H	3.54204305184989	9.58308416650126	0.36427531922435
C	4.43849672104908	8.61450353857976	2.08496559351817
H	5.46116014556461	8.89909666321898	1.80609308644150
C	4.20540786418197	7.88303496314813	3.26540871441929
C	0.38741522698973	7.69918223682247	3.31926065393792
H	-0.35360236283459	8.25495299491163	2.70529522411035
H	0.16553930852595	6.62175764938582	3.22677395875833
C	-0.97871262768361	7.54049395614275	5.34268852526996
H	-1.04137801911299	6.45128311302666	5.16828838110727
H	-1.87999286360659	8.00125155790837	4.86980013336239
C	-0.99906006339593	7.78454532858813	6.84758139438285
H	-1.94931560114981	7.45958570940647	7.30233240215882
H	-0.15949364622559	7.27121701310619	7.34708481201624
C	0.44536205896342	9.76893247483178	6.49325093583827
H	1.27925497333527	9.25215198320750	7.00074190001607
H	0.51552785604303	10.85128221367093	6.69048505961366

C	0.42395307775390	9.46930311774019	5.00189396616873
H	-0.37898144348582	10.06439820131575	4.50329619985901
H	1.38069846352503	9.80559697648640	4.56436528356972
C	-0.88074614378494	9.56450271949811	8.61983326655456
H	-0.04497528178605	9.04833445340765	9.11570571241799
H	-1.83992740159841	9.20802127521365	9.02508765987960
H	-0.79297930411343	10.65199581696231	8.76509436405787
C	5.34053403097923	7.45028141012486	4.16828992349084
H	5.69031014340378	6.43812765049680	3.89686148643510
H	6.20850377747544	8.13290851987786	4.08368649265401
C	4.76853595434150	8.73908023483592	6.16898053350914
H	4.02595118274702	9.30265802677997	5.57582221512775
H	5.74453897632846	9.25307875981196	6.06811393281341
C	4.37690722172767	8.68368994445835	7.64225319488689
H	4.37065112798483	9.71376921480013	8.04234953336733
H	3.32411422253345	8.28908425794124	7.74170138705580
C	5.39944290856363	6.52877780986370	7.86512118568057
H	4.42474729855721	5.98326051115302	7.97243822841402
H	6.14686767562540	5.95656636960455	8.44209448473946
C	5.82175181995909	6.54179318593623	6.40056351636056
H	6.84484176223465	6.95627763360159	6.30853890758520
H	5.80561553613008	5.52087401039594	5.98172127344398
C	5.09678653058349	7.92876660946495	9.83594296509815
H	5.14086880380872	8.97347452104321	10.18714539038270
H	5.89080942366795	7.36582162109998	10.35388093548661
H	4.11215093227012	7.49543249114352	10.13276832804351
C	2.15655556680455	4.60972778065754	1.83530714444565
C	0.84669276368917	4.76834036086099	1.32933709079899
C	0.65180099653431	5.52514634185053	0.15723711991293
H	-0.36022468802423	5.64679730387975	-0.25066049144814
C	1.74722396936383	6.09066119407811	-0.51742460579873
H	1.58431045511087	6.66831833775143	-1.43464165946649
C	3.05306867305289	5.86364595406646	-0.05585646187521
H	3.91037509094287	6.25330823138646	-0.61838596415721
C	3.25930013762500	5.11542329567033	1.11683292388423
C	-0.31490241315967	4.05843595261855	1.99295205223870
H	-0.51190129226566	4.49639306770789	2.98888071071133
H	-1.23507355624201	4.16449137747030	1.37797252620346
C	-0.95599938833128	1.95733005101508	3.07464017364005
H	-1.97321010069044	1.93050172044189	2.61252889448886
H	-1.05525003711539	2.51047014041690	4.02570911957613
C	-0.49685805339844	0.54005109255254	3.40097835850833
H	0.47362743789274	0.54481573360409	3.92607566544260
H	-1.23971184488201	-0.00031286379796	4.01054324032413
C	0.69099889833229	0.48692414858144	1.22591158922773
H	0.78604761240909	-0.08832064672325	0.29029933100694
H	1.65964994282304	0.48387081811753	1.75628431341228
C	0.20179181945113	1.90415379777516	0.96775888250471
H	0.95614151631054	2.42693314432962	0.35336836348234
H	-0.73795777894603	1.88207596590725	0.36401554707041
C	0.13499190791941	-1.67197632892776	2.38775175004167

H	0.22959220912324	-2.20074287487145	1.42707959700400
H	-0.62756820931840	-2.16178382305666	3.01223095071383
H	1.10300798377520	-1.66201371139610	2.91088850341392
C	4.64222307236512	4.79740017518728	1.63341702282665
H	5.40068716383961	4.84262250663308	0.82801994992813
H	4.92380879456265	5.52738177455392	2.40768494735934
C	5.88728625553068	3.27208536296648	3.10519370487502
H	5.86596863492251	4.04172765576668	3.89451027002292
H	6.77821267226220	3.42436891545547	2.46456429145979
C	5.92230893179617	1.87891362757883	3.72157394402332
H	6.86701694895521	1.76082366065740	4.28058040204548
H	5.09039954088336	1.77957687821192	4.46777807412886
C	4.63790315833372	0.99633197624195	1.90501741006714
H	3.71404066567938	0.83312927015898	2.53455349190906
H	4.62554899294749	0.22948062516288	1.10931938505253
C	4.56908198721646	2.37543085381436	1.25732775526758
H	5.40708461177887	2.49031085548476	0.54192943457680
H	3.62535658411981	2.50840922694809	0.69903575228864
C	6.04205750039842	-0.49882643441869	3.20406562083839
H	7.01036725205558	-0.56109726435401	3.72763154772880
H	6.06594571256037	-1.21631897647355	2.36650773085339
H	5.24092364587889	-0.80958325726266	3.91629826201475
N	4.88926293754214	7.37129362768374	5.58343352715587
N	5.32201980777651	7.88378497359071	8.39370806584973
N	0.26567533316455	8.03288253317297	4.75669103296786
N	-0.82593645626055	9.26117360399961	7.14747906107518
N	0.02108901398335	2.63520484305560	2.22508262905017
N	-0.28276714704920	-0.25080644092124	2.12535147815940
N	4.66011224253450	3.45543160601289	2.28058666877209
N	5.84617962013852	0.85357343313306	2.68931208898818
O	1.06454452133626	4.85628602479179	4.62911048840402
O	3.76037267010153	4.85405786218050	4.62990083413117
Sb	2.69721261216539	6.36718380142244	5.42185111039392
Sb	2.63468396110954	3.50819830322289	3.63407708218664
H	0.74939274512683	4.41362753939604	5.44121635953869
H	-1.61452543275383	9.75661860933586	6.69871832661267
H	-1.18972827813115	-0.28022325536239	1.63015947831323

Table S15. Cartesian coordinates (Å) of the cation **[(RSb)$_2$(μ-O)(μ-OH)]$^+$**, *syn* isomer.

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Coordinates from ORCA-job Sb2O2_H_cis_opt

C	2.94351887297241	7.60407454735913	3.51413658462189
C	1.89976899543372	8.08043061725269	2.69823714527384
C	2.20834564457602	8.81905545171249	1.54195186950740
H	1.39859024620199	9.19175066472726	0.90211153036645
C	3.54595738669049	9.09489950802152	1.21623853423509
H	3.77995264727827	9.67876806935267	0.31824838163612
C	4.58318857440285	8.66381685482509	2.05951500479921
H	5.62429284239817	8.92433353814864	1.82772639944590
C	4.28555498807081	7.91876136915858	3.21573484734544

C	0.47202167503428	7.79903493740322	3.10740638375257
H	-0.22602102623970	8.50787683143406	2.61008401407627
H	0.19578671851248	6.78001972607758	2.78443054310876
C	-0.94889542636859	7.27942470784098	5.02149120755130
H	-1.01931896872511	6.24801825194725	4.63486074291310
H	-1.79841797715787	7.86769340871330	4.60837321082504
C	-1.02362597393892	7.28402893656627	6.54483452111075
H	-2.00408562456994	6.88840894016397	6.86648153286018
H	-0.23625589744840	6.59732732022614	6.95335310557951
C	0.39543838920203	9.21762569978011	6.62068323688636
H	1.27049606184669	8.66297563448131	7.05072672265643
H	0.46281803011092	10.25828058760669	6.98655596252092
C	0.49661532883633	9.21245581879463	5.09897573600766
H	-0.28228143139973	9.88088832501420	4.66941266367213
H	1.48234406511130	9.59607928165809	4.78044525662057
C	-1.02803320043241	8.70366414309220	8.50932793998749
H	-0.25029279753018	8.11840328505233	9.05775634701608
H	-2.01901081190678	8.30989407391279	8.79426770646452
H	-0.96860522485168	9.75334033874886	8.84558701727492
C	5.37590462292476	7.43584283690384	4.14790444080733
H	5.67789124903461	6.40798123450996	3.87648057544297
H	6.27858689969759	8.07782281223986	4.07654423369875
C	4.80268910276723	8.72350366961903	6.14386338329622
H	4.09453079773015	9.32062022346031	5.54148082576957
H	5.79733963645883	9.21368165087116	6.08864908073505
C	4.34949066350370	8.65456283923755	7.59797181726984
H	4.35914747703705	9.67513634477516	8.02150036412811
H	3.28903409764573	8.29448996487566	7.64703832707341
C	5.27624716701298	6.45696279269862	7.81513058741464
H	4.27264953511648	5.96219155650922	7.86794524204227
H	5.97267536978305	5.83678692575113	8.40750509768412
C	5.75245725740524	6.48521357682512	6.36735190098512
H	6.80274549089296	6.84293298243970	6.32700914117984
H	5.69615896373274	5.47422562018607	5.92611904270430
C	4.90256223964290	7.80416866893286	9.79546640193197
H	4.94781177315775	8.83407810019241	10.18970492718062
H	5.63298651676079	7.19311355869370	10.35317615235177
H	3.88221919673844	7.39825946257018	9.99776753899428
C	2.20067330259872	4.69870014248419	1.65238857575827
C	0.90698647536658	4.89101990938171	1.12457646843720
C	0.74752210265115	5.66981336485021	-0.03845194553882
H	-0.25591381579537	5.81744137588868	-0.45901679661161
C	1.86469878334284	6.22802897577135	-0.67960598776273
H	1.73042012045191	6.82706679485720	-1.58800754057414
C	3.15671165441225	5.97700801854256	-0.19080113315714
H	4.03359596184320	6.37214000681633	-0.71875505052313
C	3.32578959499039	5.20565941020286	0.97113679762283
C	-0.28575129028708	4.24064408768886	1.79336238562375
H	-0.62129264929957	4.86170156702498	2.64480089017072
H	-1.13644097733008	4.16633332500707	1.07996037964969
C	-0.93919933006202	2.43528308841010	3.29559847418340

H	-1.92778640063221	2.32267651224087	2.79632858939604
H	-1.05140453861313	3.18680332114886	4.09846662013996
C	-0.51337405373981	1.09272476035759	3.88144264262519
H	0.42015183622984	1.23398983273347	4.48569239848137
H	-1.29825767404402	0.72653875775482	4.56772779672578
C	0.68632166550278	0.58042411993309	1.87064239648452
H	0.78548729778745	-0.15892915446222	1.05524835773507
H	1.69272719132404	0.66900206210539	2.35607234691291
C	0.29055054353594	1.92909584255105	1.27813472555755
H	1.08788273513919	2.30286768441231	0.61067576643509
H	-0.63313978691303	1.81073226857736	0.66850425462461
C	-0.01246991346290	-1.21479917354526	3.33561624467184
H	0.06255594990689	-1.93297139687352	2.50071482611543
H	-0.82353068735874	-1.55228789256615	4.00385936439520
H	0.94609279015771	-1.24620713116097	3.90844630939059
C	4.69275864560599	4.88255381832190	1.52427002039522
H	5.47943951664945	4.98255979989731	0.74823907000785
H	4.92339081173262	5.58667173237109	2.33848526964323
C	5.89079221608074	3.33362183579356	2.98885250675718
H	5.81600710223697	4.07877324059315	3.79979547404448
H	6.81902996122169	3.51140356180626	2.40605682979239
C	5.90957111200433	1.92591431023667	3.57264794381958
H	6.82729879763444	1.79906647276591	4.17466908627522
H	5.04092732771528	1.80430953007376	4.26968109668636
C	4.70576647568307	1.08603624519596	1.68173748776621
H	3.76592204797432	0.91018624289303	2.26759942395300
H	4.72249142973493	0.33532093007065	0.87114513787004
C	4.66485260609180	2.47939454393923	1.06565461468017
H	5.52879979894578	2.61076694860642	0.38071753080099
H	3.73996547592053	2.61914869069566	0.47816535600616
C	6.01554864512056	-0.43490137060943	3.03402696009777
H	6.95250659620578	-0.52934627276462	3.60957980841153
H	6.05550458675777	-1.15365524664661	2.19734706386804
H	5.16715311544306	-0.72286701918699	3.70048723591472
N	4.89402833476748	7.36945212894237	5.54426204837590
N	5.24229359669026	7.80450232650745	8.37654890331162
N	0.33423162774431	7.84300532231892	4.57201605320239
N	-0.86898860060176	8.64008624116951	7.06157157235265
N	0.07050608186410	2.92561814594071	2.34430282562458
N	-0.32018670485774	0.11276356791862	2.81712027784363
N	4.71071659462546	3.52491686850159	2.11584498593288
N	5.89250014702905	0.92200008792795	2.51233486717849
O	1.04719962137264	4.91670159015159	4.40465447588701
O	3.69451177028079	4.89473657652450	4.47926261552428
Sb	2.58399372011949	6.39293642895869	5.26958897972278
Sb	2.55622455857188	3.55422736551416	3.45740554709181
H	0.61857067577956	4.48771072907462	5.16965643438626

Table S16. Cartesian coordinates (Å) of the cation **[(RSb)$_2$(μ-O)(μ-OH)]$^+$**, *anti* isomer.
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Coordinates from ORCA-job Sb2O2_H_trans_opt

C	6.83201184511707	7.86372890285205	7.75195528552886
C	6.89374654737959	6.46534756558114	7.58405492679143
C	7.46741302504105	5.93635914865136	6.41116006548984
H	7.50940748245027	4.84843567259303	6.26992526585954
C	7.96941847381771	6.79087966123400	5.41698781264963
H	8.40863217658368	6.36941358550406	4.50510304087195
C	7.87519176306360	8.18414076317555	5.57044204071200
H	8.23339464857483	8.85159741414541	4.77599365007119
C	7.30151982131179	8.72218770910802	6.73562355174499
C	7.14546221153852	10.21235165523622	6.93969253427212
H	7.94003052389720	10.58243795299893	7.61367105990340
H	7.21449861375866	10.76347739973283	5.97906199662409
C	4.70035206994251	10.23496455368343	6.72027246047207
H	4.74303776271868	9.18074421427090	6.39475068759311
H	4.78300900497018	10.87605287405414	5.81745199637279
C	3.38648498451349	10.51944025675219	7.43963516139842
H	2.55025835223722	10.37027040183857	6.73295391825407
H	3.24817726362794	9.77753994045226	8.26870676001198
C	4.47661523753784	12.13868647405328	8.83295216491174
H	4.41887587587765	11.49943654556745	9.75255530178410
H	4.44398832075402	13.19191025787949	9.16691015341338
C	5.79904828237974	11.88226384210166	8.11932595290196
H	5.91406324903130	12.59608213321922	7.27651120521690
H	6.64890494328569	12.01021800244272	8.81112358470967
C	2.07189651576543	12.21070201433862	8.56504506960605
H	1.86087555979923	11.58349945876478	9.46481435851746
H	1.25306688383498	12.06047380511567	7.84046744428408
H	2.06363339720837	13.27047365410311	8.87356698522225
C	6.35595050370706	5.54851441522739	8.66180257724858
H	6.14897955973351	4.53803818049217	8.24502740186585
H	7.12571720141596	5.43166077894101	9.44817247730461
C	4.81876048885653	5.41445026658575	10.55364765436072
H	5.70990223018334	5.39708049502906	11.21006559264380
H	4.55162884044640	4.35333479239692	10.34863300877185
C	3.65157649527814	6.10786513797007	11.24816354662347
H	3.39233282802953	5.55823031511451	12.17188560832393
H	3.95965859251965	7.14238588347966	11.55116245772369
C	2.79512395749852	6.78457590464852	9.10450921897380
H	3.01330765127250	7.87275014859624	9.25597320150746
H	1.91178427686477	6.72079467127808	8.44350680089904
C	3.98655712730444	6.12512853824463	8.41411911559735
H	3.72324071349852	5.08569791358506	8.11660461402826
H	4.25021320689751	6.68068680816969	7.49612136452431
C	1.31934012374547	6.71170754289474	11.02039275683113
H	1.07878971663632	6.14580308582890	11.93725217758766
H	0.44747949744467	6.65379685773303	10.34605791027177
H	1.47290201605441	7.78191026173389	11.30118312170067
N	5.85523991152500	10.49585960843410	7.61290318583717
N	3.34959423619415	11.88981939368462	7.93908755744234
N	5.16143783898483	6.11625078893461	9.30829026042794

N	2.48552051380088	6.12543463692476	10.37024023969150
O	7.47149004948341	9.99560065906985	9.98482611746185
Sb	5.91535132032785	8.78320652150478	9.47967759827038
C	6.27413923337489	9.79820212877377	12.79780506295226
C	5.73554509828954	11.09263679867107	12.62679289660749
C	4.45523242342018	11.39297722585531	13.12507952376488
H	4.03923598577751	12.40095230903589	12.99770676750926
C	3.72046001321976	10.40975516836890	13.80855503665935
H	2.72350919544834	10.64434714288180	14.19980604316283
C	4.28456528528324	9.14580333122870	14.04231594453240
H	3.73373071537503	8.40185806216285	14.63288160076853
C	5.56753864146440	8.83616061067288	13.54892078679549
C	6.19105039401764	7.48482908746844	13.84402289139312
H	5.88938544429019	6.74419108659998	13.07387724009707
H	5.78629971964393	7.08134076304294	14.79955194788624
C	8.13728393018581	8.21640907272347	15.09609077082468
H	7.69710979684669	9.22915159627001	15.13643376682997
H	7.78792560078875	7.65799752828943	15.99306054487557
C	9.65987759224076	8.30005897183895	15.10977570751700
H	9.98756889464388	8.74853746741647	16.06519383884334
H	10.00199936232283	8.98678736250274	14.29232883883446
C	9.79905617719599	6.33748992917514	13.74304603624181
H	10.12843546972506	6.90355615750942	12.83493593178288
H	10.24144547150402	5.32715403518387	13.67810901923562
C	8.27871116458437	6.21967548590350	13.73513771711338
H	7.95331547182664	5.54975234353227	14.56216970832806
H	7.94919075681464	5.77070694484938	12.77983555262968
C	11.70769365118743	7.01204652150690	15.07702584543888
H	12.18408947301683	7.61611272254633	14.26753823488318
H	12.00248977159654	7.44496434589612	16.04866200539482
H	12.11157375502396	5.98632666967603	15.02388990703504
C	6.56537569665033	12.13052079938885	11.90392363067836
H	6.27499576872755	13.15807994444843	12.20714927445286
H	6.40355150671625	12.03490912492605	10.81763150029789
C	8.82794451290171	12.62096686285260	11.12493181205206
H	8.54898955248519	12.22018126655098	10.13456791499356
H	8.59827783571354	13.70698752350788	11.15779599979499
C	10.31446138319618	12.40214317340488	11.38184720405392
H	10.89552141805444	12.99142670588651	10.65000154262079
H	10.56627416255118	11.32429629802576	11.20762296415159
C	9.90257136688763	12.08250804313826	13.71802262839774
H	10.13525227261724	10.98637697093043	13.68175384458372
H	10.17199089248391	12.43329245151088	14.73058880108343
C	8.40822003674982	12.29362889241594	13.50339452594967
H	8.15586827419664	13.36196251252132	13.67147355012268
H	7.82255420351457	11.68805673972555	14.21797686525611
C	12.11158906247100	12.73588390281853	12.97400294757251
H	12.65334781243032	13.35496633972444	12.23837669667178
H	12.34426351446486	13.12172551429565	13.98157851504700
H	12.49967077205270	11.69137958218744	12.90250614853015
N	7.65738470987397	7.54989538161429	13.86793662097916

N	10.25302051768262	6.97545233893852	14.97582510591502
N	8.00911320996515	11.90575930010878	12.13020705221060
N	10.67569755903193	12.82663405924355	12.73130634887297
O	7.24281592898736	7.59562615849619	10.85001410246640
Sb	8.16144269951332	9.38669305921836	11.78587423356984
H	6.74080530325006	7.03793062758508	11.47215956662952

Table S17. Cartesian coordinates (Å) of mononuclear form of **6**.

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Coordinates from ORCA-job SbO2CO_opt

C	2.64375172266579	4.42124600656431	1.23290728760688
C	1.42936762976542	4.74617718983395	0.59708364517401
C	1.45015837933832	5.44755315894644	-0.62297796939319
H	0.50649516813605	5.69519378477644	-1.12700325834639
C	2.67550867201708	5.82864936602720	-1.19475067549401
H	2.68828910486118	6.36902388289073	-2.14914581545572
C	3.88489817616385	5.51182148549105	-0.55393866947504
H	4.84124568768263	5.81003788595558	-1.00375285979440
C	3.87345240808234	4.81016715782791	0.66605915766322
C	0.13310520058644	4.37393388884203	1.28442618144634
H	-0.07484957970919	5.11869429995978	2.07529982503947
H	-0.71869390545887	4.38329483518627	0.56930118839501
C	-0.81875021892139	2.85174805938017	2.94609878715464
H	-1.81419968826409	2.89680746409172	2.45075412637461
H	-0.75004529723973	3.66358580076403	3.69059569737210
C	-0.65170393995084	1.49861209310787	3.62914485532661
H	0.28222347633821	1.50659227484800	4.24474300235974
H	-1.49621019484982	1.33894253616675	4.32386094468790
C	0.43835393205763	0.61584196211289	1.67919767089658
H	0.40258192109923	-0.19379182535709	0.92702152563887
H	1.44618347788587	0.56534983776019	2.16719001398909
C	0.28425056683122	1.95955876514541	0.97430982633784
H	1.13101885166512	2.13087079737489	0.28497770535878
H	-0.65171811850376	1.95940792637574	0.37198150378364
C	-0.55721430330674	-0.89555657934386	3.28088238969096
H	-0.60437713506600	-1.68779941632114	2.51265864249294
H	-1.41269672903267	-1.03120060916937	3.96577677919806
H	0.38222116677044	-1.03869163460116	3.86932783416481
C	5.14672871887439	4.50359445622417	1.42516076741139
H	6.03536108903696	4.55773961750619	0.75857900012107
H	5.27188698451040	5.25615445209260	2.22601050463779
C	6.07610437739224	3.02993612832567	3.14311150653751
H	5.92179691229936	3.83783159660048	3.87891374663575
H	7.09615574411459	3.12341147562791	2.70841468743062
C	5.93335265904051	1.67042156076581	3.81858140570675
H	6.73923428873954	1.55189923642771	4.56541404883526
H	4.96303723374056	1.63345656017676	4.37399266408516
C	5.01264935329512	0.73344409728851	1.80600545803495
H	3.97954743526710	0.62801206763363	2.22792164613277
H	5.13960758900497	-0.07157197379551	1.05874072968302
C	5.14005007212125	2.08481833923666	1.11010193927979

H	6.10902185356418	2.13339947668799	0.56462045702750
H	4.32808713273812	2.21391654974290	0.37152175975717
C	5.97923631671738	-0.72528571946667	3.47295632072035
H	6.79655998048240	-0.81822430100450	4.20962998416181
H	6.11251183618401	-1.51453376523683	2.71182225603621
H	5.01353235697161	-0.91425747010842	4.00303186379934
N	0.25000475635308	3.06453680911967	1.95098737911328
N	-0.63709144378511	0.41332329606984	2.64606922696601
N	5.05952718451046	3.18864817665025	2.08521451559630
N	6.03338160064627	0.58569286430313	2.83987000598364
O	3.66717662294440	4.80719839144983	4.14163382746368
Sb	2.62079901151064	3.31098866483823	3.08807864371395
C	2.52491927606851	5.42974283622439	4.56093490451748
O	1.44157032772465	4.75024437402506	4.07997357736511
O	2.48056241528871	6.42826174495775	5.25159065505301

Table S18. Cartesian coordinates (Å) of dimers of **6**, *syn* isomer.

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Coordinates from ORCA-job SbOCO2_cis_dim2_opt

C	-6.93290593504869	-8.89577021850498	-8.38704442622281
C	-7.66057855674868	-7.71086311170698	-8.62659258838534
C	-8.91868274072254	-7.52976232568406	-8.02238767684205
H	-9.48057586654475	-6.60364812892071	-8.20389495905734
C	-9.44099320906106	-8.51644634662002	-7.17043063985127
H	-10.42016663330092	-8.37026044999692	-6.69785870663908
C	-8.68881472407859	-9.66686261113558	-6.88489029832906
H	-9.07505237276200	-10.41829290886818	-6.18347960303164
C	-7.43080134936121	-9.85851862469749	-7.48525290298871
C	-6.59396130522592	-11.08056394079862	-7.19273023770865
H	-6.72305023110356	-11.78456631329606	-8.03638953801107
H	-6.92852834184814	-11.58113717630083	-6.25727690684930
C	-4.85525116516603	-9.95068823360240	-5.90322169060464
H	-5.48478292507782	-9.04210235203936	-5.89929933171670
H	-5.11048300011258	-10.54552638646859	-4.99706637813572
C	-3.37923876569947	-9.56875468604632	-5.86592690342384
H	-3.16378175395834	-9.03530656568224	-4.92147448410129
H	-3.16407817181355	-8.85369972095170	-6.70132586426494
C	-2.83016180300200	-11.50840966871353	-7.16694376493303
H	-2.58592438457428	-10.91705911449904	-8.08427440165785
H	-2.20096330898906	-12.41687702076070	-7.18764493933653
C	-4.29872398601623	-11.91401521893163	-7.20871286787145
H	-4.51689635682735	-12.61111005952867	-6.36858650649848
H	-4.52561457525728	-12.41534228121878	-8.16462415303174
C	-1.11698079556808	-10.41183310530532	-5.85464498582730
H	-0.77196809141258	-9.75282174308063	-6.68882745106600
H	-0.91962837540839	-9.88965324235449	-4.90133911477768
H	-0.50785757299015	-11.33284145837732	-5.87355700167374
C	-7.04559304691333	-6.63864943985522	-9.49806067634269
H	-7.54479943815040	-5.65818370237230	-9.33049218159104
H	-7.16722478149979	-6.90982832215026	-10.56213787875780
C	-4.90499750345840	-5.75786914037478	-10.28244284220105

H	-5.08752493315101	-6.23983978826514	-11.25636236442848
H	-5.31282281832069	-4.72179052194188	-10.30728340789971
C	-3.40617788731868	-5.71857140654062	-10.01356071721630
H	-2.91926285390603	-5.08469423070915	-10.77653627880854
H	-2.99411990156397	-6.74796582570839	-10.13389607576648
C	-3.80736004512636	-5.94228122568893	-7.65813228738999
H	-3.41320878459297	-6.99094216473672	-7.61570012024676
H	-3.61621798833153	-5.48533389837649	-6.66921514872067
C	-5.31043171005444	-5.98679779567522	-7.90995340819829
H	-5.73374087997948	-4.95998077897325	-7.82810550380087
H	-5.80800816555390	-6.61959622518081	-7.15317130175570
C	-1.69877522713197	-5.06038036582910	-8.42946470000972
H	-1.22430474527338	-4.42835139329683	-9.20077124120753
H	-1.52525362130758	-4.58968836430211	-7.44499612598039
H	-1.18571634882131	-6.05323035743742	-8.43524845868159
N	-5.16462721310229	-10.72504440539394	-7.11798632745563
N	-2.53013293216441	-10.75374465413490	-5.94742007687864
N	-5.59600580012831	-6.54428172629120	-9.24479725947691
N	-3.12960674677852	-5.15880573438771	-8.68543997250193
O	-6.18770459664379	-11.49062399484422	-12.04821931895492
Sb	-4.97782529920288	-9.16919258450607	-9.29685172989979
C	-6.94483784754867	-11.05750771505778	-15.07479066180227
C	-7.13606965292366	-12.44603970475216	-15.24270185871550
C	-6.88498999295208	-13.04328375213325	-16.49148129260491
H	-7.03933645428563	-14.12315172173400	-16.61792938193757
C	-6.47065551106191	-12.25738077151092	-17.57889661497586
H	-6.28272272115076	-12.72405640322807	-18.55367305034421
C	-6.34832418437757	-10.86719050991580	-17.43108599050176
H	-6.07789120206246	-10.24402088505354	-18.29408733879546
C	-6.58678981281787	-10.25949210082187	-16.18278675687466
C	-6.47617217975318	-8.75863598293822	-16.02267015053993
H	-5.49511639038744	-8.51507816219734	-15.57794540411471
H	-6.54308917155027	-8.25338972915549	-17.01205952237873
C	-8.84918980514999	-8.24823123320807	-15.69394521575623
H	-9.08617149210616	-9.27804098710478	-16.01806231165207
H	-8.87273804921165	-7.59405938989779	-16.59543984855966
C	-9.88333148709607	-7.76672930744331	-14.67977478116666
H	-10.87639024124554	-7.72046763136593	-15.16402877216771
H	-9.95903422651880	-8.51558828833360	-13.85138543596354
C	-8.20421965347434	-6.44461431793379	-13.57907993844871
H	-8.14833442647988	-7.11268246285169	-12.68279703323049
H	-7.96069128031921	-5.42054231184452	-13.24094120153124
C	-7.16961213967239	-6.90086259731613	-14.60000365452895
H	-7.13190623996200	-6.17390646134851	-15.44280251898082
H	-6.17114634155999	-6.95338090855960	-14.13484711913745
C	-10.54573197846633	-5.95935130052496	-13.22289427782795
H	-10.63275878581801	-6.60407746470715	-12.31398594588168
H	-11.53539574373790	-5.92247342191676	-13.71211699934472
H	-10.28773306129316	-4.93690712057947	-12.89410117007766
C	-7.69334536102237	-13.24073680601990	-14.08274907688652
H	-8.06205508790267	-14.23312513627513	-14.42626184190686

H	-6.91044276229989	-13.40823079328822	-13.32008984267646
C	-9.20307983038911	-13.09703239250295	-12.16803072175389
H	-8.33175451506145	-13.16580805534976	-11.49784306353849
H	-9.60212928310166	-14.11703637620048	-12.37130985045005
C	-10.27190419597475	-12.24694884492424	-11.49472556638823
H	-10.60865909786817	-12.75367412372630	-10.57224549056734
H	-9.81343912159002	-11.27834987474452	-11.18559964173291
C	-10.99842822758104	-11.44104289475260	-13.63199456270909
H	-10.59358641186817	-10.40981553706085	-13.46178758942708
H	-11.87157702228863	-11.33943120819906	-14.30366817726535
C	-9.92867371611972	-12.28230605842611	-14.31903033348484
H	-10.35555669823138	-13.27117869677241	-14.60325608068338
H	-9.58929259153809	-11.78317245940895	-15.24390357854166
C	-12.47524738764804	-11.27785209462249	-11.73436277398824
H	-12.80409162728910	-11.78855588920580	-10.81194178438238
H	-13.34703392601122	-11.18852264309684	-12.40761265319388
H	-12.14392551009936	-10.24659755863493	-11.45600646095037
N	-7.50354325115441	-8.24542174003073	-15.09789183930795
N	-9.54507430403613	-6.44041532815989	-14.16624678679747
N	-8.76830209618503	-12.47069771321830	-13.42925753341045
N	-11.42682809268135	-12.05485844551952	-12.38007801176273
O	-5.87314561382475	-8.73864041544012	-11.16968401197941
Sb	-7.37340966341018	-10.13553400101691	-13.14977442165500
O	-5.49517517652944	-9.13005672801117	-13.33811388250497
O	-5.24109852232180	-11.13945956520000	-10.03400618160049
C	-4.97652086898055	-8.71727596101730	-12.19248858420360
C	-6.36838649651702	-11.39566715137930	-10.71970943337508
O	-7.46817258093981	-11.54605528685885	-10.16881543588664
O	-3.81434387439693	-8.32461569743807	-12.06226033913956

Table S19. Cartesian coordinates (Å) of dimers of **6**, *anti* isomer.

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Coordinates from ORCA-job SbOCO2_trans_dim2_opt

C	6.59693435428798	7.59430095297455	7.16686409928288
C	6.57406609068901	6.19706508384934	6.98509657192809
C	6.82321303767602	5.65412076629482	5.71128680983028
H	6.80664239337974	4.56502522386257	5.57308896441082
C	7.07560234145476	6.50149911870140	4.62121516244946
H	7.26673888039468	6.07569351164460	3.62852962500607
C	7.03776325336882	7.89464536825342	4.79090061715578
H	7.18371215428175	8.55863116301398	3.92852307172664
C	6.79421442380277	8.45074108255615	6.06103948782865
C	6.69769117836371	9.94715974699631	6.24962853626233
H	7.64122269352808	10.34276858331621	6.66960593859388
H	6.51542419387313	10.45279616341033	5.27539072853195
C	4.28762598510183	9.96998141110071	6.70374682850229
H	4.24652340491598	8.90001752164753	6.43028292679530
H	4.08789684049298	10.56358345982754	5.78303192672041
C	3.22817329244681	10.28171884508284	7.75769665583849
H	2.22448668029630	10.08897521629916	7.33471193481635
H	3.35552464983039	9.58209147088768	8.62301952452983

C	4.64644355196547	11.97887629786470	8.69110604458613
H	4.88253535692179	11.38772581358025	9.60949299388110
H	4.68812130716897	13.04847888381087	8.96841879729663
C	5.69744547488234	11.69289578531784	7.62978607000831
H	5.52071768554430	12.34826470780158	6.74681264431590
H	6.71330206343585	11.88884975721411	8.01675652070339
C	2.27999020673270	11.97111296789062	9.19007651321007
H	2.39031838081913	11.36028864809886	10.12020324835516
H	1.27651946103644	11.77723734249752	8.77044444533416
H	2.33311311297575	13.03769642130588	9.47252620884314
C	6.26007952574337	5.32251601619469	8.17273187237167
H	5.97293396926035	4.29811484593517	7.84856728906210
H	7.16838435041632	5.25076404476875	8.80485781326429
C	5.06750819933991	5.27532552175314	10.29494987335847
H	6.04975149778817	5.33914159279555	10.79093954315657
H	4.79933394060755	4.20306795495778	10.16201140383213
C	4.00857555709572	5.97426228750687	11.13436750151320
H	3.90523508698473	5.45791015945875	12.10691317819921
H	4.34920390772545	7.01708534536491	11.34135157009480
C	2.82756493278642	6.60989286763407	9.14839909755703
H	3.08708128173902	7.69402078213614	9.25490901111974
H	1.85069424754107	6.55850396233281	8.63270485100897
C	3.89086495000729	5.92984894054860	8.29323802341681
H	3.58090846308008	4.88436605136306	8.06776204945708
H	4.00517655923168	6.46293756739281	7.33227533412168
C	1.67872883394717	6.59826997303366	11.26889534651271
H	1.58408538765923	6.06552276934711	12.23194382670722
H	0.70504563884832	6.54334931687047	10.75012682744734
H	1.89504962504439	7.67319826072681	11.48663229422718
N	5.63413751561566	10.27702526360585	7.21841137452653
N	3.30074835511956	11.67323915998742	8.19528388072520
N	5.19067116758593	5.93554268717242	8.98653933546088
N	2.71009499028556	5.96791613903799	10.45582763622615
O	9.43019055009972	10.37497956637493	10.41604256301379
Sb	6.21460687133186	8.46346763308922	9.11762156541234
C	7.00767614631704	9.65860853585457	12.38779725028194
C	6.43565429049517	10.92704650368170	12.12832582588628
C	5.04730542489988	11.11128231048120	12.28695458777067
H	4.61020933839014	12.09836232341660	12.08812503998751
C	4.23572522057170	10.06437226036208	12.74695139379515
H	3.15780255716966	10.21949931373147	12.87742031238611
C	4.82204417819438	8.84355214860897	13.11451782203899
H	4.20852090214484	8.05154153008572	13.56277068082726
C	6.20324381216426	8.63602120041991	12.94123501408101
C	6.83798609248818	7.33062427497076	13.35694141844843
H	6.97057665659239	6.71032844423643	12.45266717565897
H	6.17701392269937	6.78084113476643	14.06403034570997
C	8.07297667121794	8.16518649535654	15.28231093253291
H	7.53360152774883	9.12551173029249	15.18787272080562
H	7.48060415922056	7.50724983386857	15.95785735203686
C	9.45776013567271	8.39623429289558	15.87803012253639

H	9.34911284192244	8.80248297167655	16.90075860683129
H	9.99335356920562	9.17182557747049	15.27347374681331
C	10.33202879312353	6.56893279286233	14.59719302055700
H	10.90813693784026	7.23394614934908	13.90780606121574
H	10.88415886104941	5.61433280166325	14.66751096590713
C	8.95524505894780	6.30650891532782	14.00028247087006
H	8.42136373722971	5.54620735848456	14.61373154010480
H	9.06482612841157	5.92831485571643	12.97044265682312
C	11.51852012894394	7.34126240414446	16.56130732485186
H	12.17104077622578	8.05308093855697	15.99878633877289
H	11.38894213644332	7.73222898003375	17.58631324237493
H	12.04655088089932	6.37367893166413	16.62737851405685
C	7.32069136167991	12.10505926026447	11.78037738805542
H	6.76733391267036	13.05489762144529	11.96017883692754
H	7.60608147588454	12.10357768155905	10.71272431239393
C	9.58762654217673	12.96377393346227	12.01987683389341
H	9.76124960303771	12.67422843717834	10.96985658385924
H	9.22712769993483	14.01732547741065	12.05013618702517
C	10.87579475400495	12.84537095901050	12.82371650748663
H	11.62086269779055	13.55891936825887	12.42728358694293
H	11.29696861072758	11.81781780984859	12.69070032167759
C	9.62053359085281	12.25529301374144	14.78337856174752
H	9.96830513272815	11.19042041944001	14.77806261422698
H	9.42901437279150	12.52880269115571	15.83783025717654
C	8.32145166785981	12.35734753103928	13.99038053185047
H	7.89284663816037	13.37977532670914	14.10566003028082
H	7.58082364509926	11.63581283831370	14.38187614316342
C	11.86861003715306	13.09892098340620	15.01762801109892
H	12.60156296825581	13.81448757389987	14.60486920579492
H	11.66162216145421	13.38520371054025	16.06447599395002
H	12.34152292474900	12.08565734292422	15.02297116080103
N	8.16924025698383	7.55311461009141	13.94396537615990
N	10.21567667860797	7.14972332616644	15.93733084597361
N	8.56125435814697	12.06064321644981	12.56997422210898
N	10.63923865783546	13.14797844520815	14.23854467406331
O	7.34026700203080	7.25595875811010	10.39874056075703
Sb	9.17876425124679	9.36517000036235	12.22030101189530
O	9.43375850357738	7.56137800914584	11.19662386810132
O	8.06856473616198	9.39111093216834	8.88939427336084
C	8.65329165039631	6.95399198903790	10.29021629975722
C	8.67690890933704	10.49047429812352	9.31954292900491
O	8.62886951345946	11.57505073302519	8.71743164028515
O	9.09680822442300	6.11569466103385	9.51248267868004

Table S20. Cartesian coordinates (Å) of **(RSb)$_2$(μ-O)(μ-CO$_3$)**, *syn* isomer.

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Coordinates from ORCA-job RSbOCO2_bridging_cis

C	2.03541084859367	7.81058437120796	3.59476124507381
C	0.67079482103800	7.92470429936971	3.25046435338205
C	0.28579012805519	8.72320829007194	2.15563021261721
H	-0.77736481585793	8.81188458105271	1.89395704421092

C	1.25489753861909	9.41504699045507	1.41281507006522
H	0.95339478042095	10.03430788551510	0.55894999893844
C	2.60301337823350	9.36173373248652	1.80224945100239
H	3.35580577267306	9.95187813470901	1.26296750957286
C	2.99768641371212	8.57750176321980	2.90164822100069
C	-0.37095556176826	7.16689059069639	4.04723881904946
H	-1.37183572159388	7.64109967436191	3.93580646225602
H	-0.45442869384085	6.13648450685692	3.65859539454412
C	-0.70986484315570	5.94148816767357	6.12347767504301
H	-0.43175408300397	5.01433307355934	5.59061644454361
H	-1.81057871869227	6.09448112408422	6.05353433433134
C	-0.30022643750735	5.83422333750189	7.58753539195115
H	-0.89399206222413	5.03744189688864	8.07169921847603
H	0.77386598776760	5.52933021973536	7.64647002881212
C	0.21393333883754	8.17381795853762	7.65092097709560
H	1.31665949454176	7.99839833295766	7.72109290705742
H	0.00262745291031	9.12308019837621	8.17686723177086
C	-0.18230358259993	8.31685285739649	6.18533881427603
H	-1.24607659063978	8.63939264661196	6.11688212912833
H	0.43879645115201	9.08865285349642	5.69499789188223
C	-0.22560990637206	6.99213651122875	9.71001334424010
H	0.84875710976275	6.75283952050609	9.90218038417924
H	-0.84043246201443	6.19901773030584	10.17118755341619
H	-0.45985613543881	7.94562062895015	10.21603137899406
C	4.42588460947890	8.59253298105712	3.40232247643468
H	4.94399941043302	7.66783533023471	3.09070617061870
H	4.97660227281474	9.45947267102322	2.97067299300940
C	3.91699869118689	9.88054102993815	5.41704994257282
H	2.90659136118374	10.05416407297847	5.00453873329448
H	4.56092997812789	10.73885700229184	5.11252388615840
C	3.85000578074791	9.80475636867989	6.93907442446954
H	3.48794421808465	10.76879441600488	7.34348129954930
H	3.10078816895091	9.02175994016958	7.22622712420900
C	5.69782861638170	8.26911091163038	6.94745844665001
H	5.07410014777382	7.38736361490425	7.23776640633675
H	6.71020024004945	8.09879716269243	7.35600771124288
C	5.77207388175542	8.33927278835945	5.42792892304686
H	6.49261955674671	9.13405771803295	5.12512821444791
H	6.11487074318248	7.36677552427947	5.03650537234241
C	5.11950434077260	9.47758166692831	8.96323849988042
H	4.76356617318080	10.44805861531173	9.35414529640408
H	6.13320136274934	9.29699160232376	9.36281784910041
H	4.44650847707577	8.67675987293940	9.35991377579423
C	3.57194497745890	4.46100995088921	1.91676408710612
C	2.67801182140595	5.27278941072683	1.18544090719693
C	3.16815737364411	6.16174946307020	0.21247110332213
H	2.46795917808364	6.80765153543141	-0.33295449332907
C	4.54339743839692	6.21069291930003	-0.06394106792966
H	4.92774397042615	6.90633458559256	-0.82009899297875
C	5.41708254307590	5.32151769441806	0.58197490570660
H	6.48208620146979	5.30451657108461	0.31358953294402

C	4.93764713204999	4.43655758609323	1.56757632832810
C	1.19549233829845	5.14427072815933	1.44608572254531
H	0.94478035699651	5.72338773452034	2.34517449982416
H	0.60452553020283	5.55081579929537	0.59557958011878
C	-0.48833911092607	3.62149644875743	2.34556405670719
H	-1.27429868313907	4.04436417430388	1.67852165333747
H	-0.46762236712506	4.19984945038977	3.28607822074650
C	-0.80566129209342	2.16266849561985	2.65641686775886
H	-0.09960753225744	1.79874672314416	3.44484618775775
H	-1.82873174942128	2.09133749493368	3.06944141100430
C	0.61393390764844	1.44625841939823	0.86671202631856
H	0.65256909646857	0.84046136827231	-0.05739917450129
H	1.39057099224841	1.04045515161235	1.56192355047891
C	0.94813234801048	2.89538959965923	0.53503332123563
H	1.98122104908918	2.97211952384566	0.15145694703836
H	0.26000786299325	3.26417793348217	-0.25991322038366
C	-1.08804837831309	-0.04498616875328	1.71269806314223
H	-1.05973471384675	-0.62503936934131	0.77309194304795
H	-2.11614321113897	-0.09186784933021	2.11371982927659
H	-0.40739866047324	-0.54221141469993	2.44684106128383
C	5.88000464564285	3.45770241072414	2.23732029173759
H	6.73473916416679	3.23590214095497	1.55716358920216
H	6.31776968290456	3.90550907456801	3.14785612459173
C	5.95541179486197	1.47876796396399	3.64867041263484
H	6.09824498359393	2.14636567939546	4.51525991434120
H	6.95343559864393	1.18807846293802	3.24693058363103
C	5.19728893064171	0.22765873511388	4.07127019983111
H	5.80316770676794	-0.33874736851930	4.80197334126961
H	4.25128904546162	0.53092454848837	4.58530238926347
C	4.16170398923558	0.10134920651785	1.91178328132744
H	3.15124537673253	0.38590630191435	2.30312897025185
H	3.99792880071563	-0.55161214777689	1.03402203471982
C	4.89999168118158	1.36297301664298	1.47473691764139
H	5.84418519142468	1.07874040600716	0.95386399352151
H	4.28131878658611	1.93683865743035	0.76023012823758
C	4.25546106005533	-1.86615313196285	3.30324939737583
H	4.87671374276085	-2.41715776320744	4.03157630223240
H	4.11215469202856	-2.51054442668489	2.41715149699139
H	3.25339924826693	-1.69054066410371	3.76837615585757
N	4.43913892046862	8.62076896604328	4.87278931405285
N	5.16192852882326	9.51371933643090	7.50893742025640
N	0.00489057865211	7.04710611236460	5.46188534544472
N	-0.53982636037699	7.09669191316643	8.29046322996657
N	0.83943193458993	3.74466771876627	1.73099240147571
N	-0.72392499859327	1.34077364376661	1.44845193918914
N	5.19081601069828	2.22016303693269	2.63187549292450
N	4.92571206950608	-0.63337160865546	2.91596666375498
O	1.71778423321366	4.85583227486888	4.39457664235064
O	4.44128777325686	5.88080073590199	4.38554459642562
Sb	2.59966715436073	6.48174666044785	5.23618513183100
Sb	2.77039561658258	3.31262130474051	3.59937082550839

O	4.31796850303450	3.69732755278861	4.99998232859981
C	5.05576200078108	4.81346920829807	4.92154453527218
O	6.23313056181139	4.84900191426579	5.28944771871116

Table S21. Cartesian coordinates (Å) of **$(RSb)_2(\mu\text{-}O)(\mu\text{-}CO_3)$**, *anti* isomer.

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Coordinates from ORCA-job RSbOCO2_bridging_trans

C	6.50453793828048	7.47159655849106	7.77015980200522
C	6.07786043962436	6.14566167384757	7.53593696515498
C	6.55582075128920	5.45753747984487	6.40194158114241
H	6.22275032373563	4.42740947539146	6.21817900711885
C	7.43911164665990	6.07924953627113	5.50748344687090
H	7.80520990012884	5.53301413337212	4.62941914715945
C	7.81828154789167	7.41624123795526	5.71265694066556
H	8.46820664881055	7.92521299244813	4.98817198555817
C	7.34391842603729	8.11525156034907	6.83609417143627
C	7.64989891304562	9.57995515155270	7.04811572754196
H	8.37229049706786	9.70094948765773	7.87717249341908
H	8.08322696576774	10.03359113814416	6.12894199917746
C	5.39342107095103	10.30307464618956	6.41316734630331
H	5.17893691249521	9.26206389900224	6.11373987022075
H	5.76797915166868	10.84695105199219	5.51598266890570
C	4.12498897188828	10.97245164571238	6.92999486853852
H	3.37687754124062	11.02177880466204	6.11736829954056
H	3.68757642247779	10.34146465183369	7.74514479218054
C	5.43200398569820	12.30627920370654	8.43893466961278
H	5.07997750440413	11.75430789369942	9.34710978785008
H	5.65026885265013	13.34468589552178	8.75023817047382
C	6.70691627124506	11.64555803438894	7.92893835182774
H	7.14363913038902	12.25834696200568	7.10742318970048
H	7.44621829046821	11.55553015922457	8.74298733481231
C	3.19206196968624	13.00038406051501	7.85448731621711
H	2.70970398152553	12.48831719480856	8.72362913273851
H	2.45605964832693	13.04312342638203	7.03197158441947
H	3.42911619936084	14.03605278130302	8.15661976562191
C	5.12637594247606	5.46653989967280	8.49637339568738
H	4.61722487917575	4.61190398134995	7.99622118001095
H	5.71700275060063	5.06064754687393	9.34140176103748
C	3.53560333261631	5.91777302465296	10.28891690314487
H	4.35468205052208	5.70349421396287	10.99489017371280
H	2.96618216616079	4.98024296068025	10.09301056957575
C	2.60362954018689	6.96895568360598	10.87767603331559
H	2.11750845299856	6.56161371458930	11.78322707622712
H	3.20444872929358	7.85420459815760	11.20177471967447
C	2.16347238331972	7.82647744727729	8.67180924732951
H	2.72442439519605	8.78154789247839	8.83795841724458
H	1.35675675896612	8.04611148461256	7.94738978558171
C	3.11166666722264	6.78960392569403	8.07356546905644
H	2.53265948858192	5.89175619632944	7.75456458974873
H	3.60754775062874	7.20598058721887	7.17682060056656
C	0.63658653826509	8.31543307620606	10.47280593867826

H	0.16543097886341	7.90295080916943	11.38281993899958
H	-0.16247278426727	8.53812964474760	9.74284541796922
H	1.13152447825549	9.28015461573672	10.74869485505238
N	6.42228685788600	10.28384947745000	7.46470909689289
N	4.40217121381892	12.32922290268368	7.40059346337335
N	4.14637562136766	6.41558591213838	9.04632621922821
N	1.56345384141524	7.34262227604369	9.91363295768722
O	7.45534806717259	9.55990813246586	10.09426483201294
Sb	5.76694388347783	8.57628585912579	9.50041930025865
C	6.59577537653292	8.78297062637880	12.98056550639668
C	5.59918736188432	9.78385656550269	12.93668491845552
C	4.35286579048437	9.56438702913886	13.55435661751282
H	3.58145077170049	10.34515609488220	13.51296384226493
C	4.10861905347219	8.36687989757317	14.24440586400067
H	3.13737957088482	8.19727786160613	14.72513333502192
C	5.13195089078954	7.41444615951866	14.36915653684894
H	4.96729442931835	6.50478641046572	14.96232410366686
C	6.37790111276417	7.61881468810407	13.74632781005797
C	7.48059799777608	6.59201033723822	13.89506759347517
H	7.43764508891251	5.86405628993686	13.06433529277766
H	7.32801470097391	6.00565239047633	14.83054470875936
C	9.08754025639772	7.94742632564620	15.12246864845700
H	8.30219347852547	8.71306839968793	15.26175558543621
H	9.04760587309610	7.25614287307917	15.99652185987457
C	10.45992531988456	8.61122805363357	15.06145956734232
H	10.66840453112680	9.11163659724941	16.02563042234555
H	10.44631667972826	9.40748860888639	14.27358389184328
C	11.22751632139469	6.91425785579178	13.55004001149822
H	11.24810826538719	7.60614057452872	12.67151876590592
H	12.01425170360964	6.15455876397569	13.39018971512222
C	9.86903367055861	6.22841681817776	13.60960342826399
H	9.88199199567718	5.44963634128074	14.40649554723786
H	9.64617189805205	5.74953692283766	12.64117229553563
C	12.82833928416690	8.23953213410837	14.79143724908650
H	12.94735531261259	9.01014954407581	13.98966799450083
H	13.02348031254533	8.72565280609950	15.76429828709984
H	13.59873821721830	7.46371129157532	14.63478919893281
C	5.90112963571381	11.10367554977368	12.25876899639479
H	5.20419478210802	11.89478341460094	12.61788089173095
H	5.76330687983257	11.01187841142150	11.16567234835611
C	7.73511549050683	12.55137747783647	11.56627779140080
H	7.57985258451184	12.18619543634948	10.53782140632561
H	7.12437532145299	13.47171268657309	11.71616788710948
C	9.20971377969093	12.87359261529260	11.78215980698659
H	9.50344718650185	13.70963437968164	11.12101546650231
H	9.82126078225088	11.98329573443755	11.48958070911640
C	9.04182044008090	12.18476181564036	14.07158796990846
H	9.64940260643323	11.25971224043118	13.90774920174310
H	9.20921083279552	12.50607908095620	15.11621718932554
C	7.56704642441085	11.85303953392362	13.87481025425918
H	6.94491815282738	12.73059745775331	14.16666711086922

H	7.27822107756095	11.00309627118280	14.51840313322836
C	10.84984818533287	13.63436156504549	13.38896678021670
H	11.11913997670627	14.47484535587560	12.72486427230020
H	10.98952992211080	13.96473155657025	14.43372064546398
H	11.56331363850619	12.79654383815530	13.19305502110532
N	8.81028542913753	7.21641452273615	13.87808221948004
N	11.50722114702726	7.62793333458431	14.79974285187918
N	7.30312755209190	11.48435761336052	12.47558683458831
N	9.45878518536421	13.25966305788309	13.17187160012778
O	6.30803050667669	6.96080957939685	10.74108288119250
Sb	8.42204358067552	9.04866132453682	11.78351653540193
O	8.57264476588759	7.10547972115438	10.98713212654803
C	7.50210357285449	6.34305279131487	10.74723713406073
O	7.59720444545927	5.12054450987994	10.60437767337657

Table S22. Cartesian coordinates (Å) of **8**.

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Coordinates from ORCA-job Sboxa_opt

C	4.91729671117113	0.14693343849685	3.07698456012117
C	6.07457205741447	-0.02234840667544	2.29021448174252
C	6.68987416036375	-1.28648209609716	2.22659786722270
H	7.59496663235489	-1.42219196390801	1.62003613700426
C	6.15472361057100	-2.36800191437590	2.94520436436819
H	6.63975456622903	-3.35037819302647	2.89548521776024
C	5.01867444298958	-2.18872027485361	3.75135649267825
H	4.61934351478741	-3.02844572262804	4.33523030068246
C	4.39530856337271	-0.92912435606545	3.82324460891954
C	6.61964132053632	1.16631408844400	1.52816958942239
H	7.68745870320511	1.01052209416438	1.26076239364303
H	6.04833538756263	1.29562642775388	0.59075688626879
C	7.36421649387210	2.45069597675059	3.46631868776265
H	8.41843505146472	2.40036983805597	3.11417731902957
H	7.17495004494036	1.56243160320901	4.09610214811591
C	7.15674045615333	3.72712180994092	4.27498228629389
H	6.13936914151627	3.70751309469645	4.74602610663597
H	7.89187052332865	3.75641292527070	5.10032055853644
C	6.61699050956462	3.61063945069446	1.47124592055001
H	5.87056278338801	3.56064901193635	0.66057124374057
H	7.63626349700774	3.62181694608519	1.02587190396093
C	6.41071745397795	4.87203093514134	2.30180948851023
H	6.59114947519106	5.75735629644547	1.66562721612266
H	5.34522689829240	4.92179788641908	2.63997719777851
C	7.21095487663920	6.14117884523562	4.20354126006956
H	7.96162196123072	6.15512418096088	5.01359115917417
H	6.20087428104240	6.26826595854870	4.66479497263324
H	7.39857199938642	7.00930438530320	3.54760783024409
C	3.17144666166919	-0.69488102906834	4.68242342813199
H	2.26444292467378	-0.73818262442734	4.05217234205826
H	3.08190246103744	-1.47708138793613	5.46734645737578
C	4.24694545116540	0.74288479398578	6.33425439801993
H	5.22293994616256	0.47971649164034	5.88753894083924

H	4.03063953711060	0.00554236344997	7.13893923394396
C	4.29700424108164	2.14657404873293	6.92797329454456
H	5.03944298687497	2.16732655043239	7.74703528030381
H	4.65412840336215	2.86737005019284	6.14689412776367
C	1.89836394493026	1.06009197900077	5.81599018100149
H	1.56821095866911	0.34373707234904	6.60037060714306
H	1.17785323274688	1.03610060890466	4.98101020493875
C	1.97499325521680	2.46282818917649	6.40788556064984
H	2.17894698711574	3.19922320249081	5.59036069341256
H	0.99411384407889	2.72533204850035	6.84385078350214
C	3.03248905192499	3.84348867960659	8.09386863124242
H	3.77246088118838	3.83906951380698	8.91378648187139
H	2.04391328135886	4.07865498439349	8.52577147710763
H	3.30441802029480	4.66447663124232	7.38588736422717
C	2.82050905396581	1.71722215107012	0.47076273345577
C	1.74791028480367	1.13947432581424	1.45475933364718
N	6.44799876487524	2.40667778459464	2.30982834818738
N	7.33473692119736	4.90837808334713	3.43692491016912
N	3.21404127629241	0.65257288347653	5.28355029529519
N	2.99333462054632	2.53349508713369	7.45740543247626
Sb	3.96600956969716	2.08706255395354	3.18272135860083
O	3.88004078339821	2.26829362273962	1.07859839828368
O	2.05833122697992	1.28663552383474	2.75019698189499
O	2.68644930537548	1.67189284514660	-0.73769358019063
O	0.72214130965201	0.61441740049224	1.06433055011059

Table S23. Cartesian coordinates (Å) of the cation of **9**.

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Coordinates from ORCA-job Sbdop_opt

C	4.92425018868465	0.20677543681850	2.90266698617866
C	6.10981560968330	0.06066635671552	2.15536884894030
C	6.71890123792221	-1.20468091960966	2.06045942149350
H	7.65038677597389	-1.32173797977313	1.49104535820645
C	6.14995198469104	-2.31061439733758	2.71384773516957
H	6.63542747935291	-3.29190636604183	2.64898693526195
C	4.98637195397238	-2.15496547422681	3.48597955206935
H	4.56878675413910	-3.01240695235926	4.03042534478938
C	4.36938152078093	-0.89394701785947	3.58533277329937
C	6.69783536301878	1.28413885934440	1.48541698792393
H	7.77518005337579	1.13425095952096	1.25779730074595
H	6.17038774802192	1.47298868968012	0.53282909852380
C	7.36756795139427	2.44564436914558	3.52534621572918
H	8.43288466730344	2.39153168202007	3.21172372999825
H	7.13568974820790	1.52914331760726	4.09742515056069
C	7.15337408618412	3.68148062732583	4.39267700737449
H	6.12032417674613	3.65788708784711	4.82860658472627
H	7.85914890694778	3.65097832319720	5.24283196105634
C	6.71614981616031	3.72913892432493	1.56884859386793
H	5.99925455167361	3.73729993064086	0.73050318090563
H	7.75061318614589	3.74967287250011	1.16199659783937
C	6.49700957979166	4.94397096999570	2.46335213342639

H	6.70947109595773	5.86115705947543	1.88505845921010
H	5.42060267372568	4.98912618792204	2.76838864664782
C	7.26591339562104	6.09565910412168	4.45258005269512
H	7.99248000906155	6.04812527576832	5.28253838809090
H	6.24619901327409	6.22428540613097	4.89054711219073
H	7.49510760634571	6.99082578056480	3.84878206163742
C	3.12571709830701	-0.67528880282004	4.42074386340816
H	2.23612686938341	-0.67474674584705	3.76483042991283
H	3.00209652435330	-1.48703522819854	5.17032992502784
C	4.17873338310797	0.67922608701041	6.15578146761792
H	5.16311014540852	0.42915348495984	5.72064019470013
H	3.93734030805962	-0.09336560927443	6.91849187917411
C	4.22408794164620	2.05209588035451	6.81744860906609
H	4.94660156316988	2.02584670294403	7.65348973391808
H	4.60557743321660	2.80747420193723	6.08200859489288
C	1.84619040745539	1.04928618197028	5.59178090265373
H	1.48237912523941	0.30133529946842	6.33027871312848
H	1.15031791414611	1.07863645134110	4.73588141852412
C	1.92356681826092	2.42053948552645	6.25445919803868
H	2.15940772746655	3.19328984043180	5.47940753159143
H	0.93371549738772	2.67456023992704	6.67494184793411
C	2.94241662607243	3.69337733529557	8.04691389416951
H	3.65896778552514	3.63309939567075	8.88464558926716
H	1.94460408084461	3.91103347114651	8.46592710666478
H	3.23996544865314	4.55122041959935	7.39616359871612
C	2.93167256446831	1.86888099675887	0.34308836413994
C	1.90891454942649	1.30387059452133	1.17909818243070
N	6.49890284177178	2.48021143431455	2.32891458782943
N	7.38240143323154	4.90043380635894	3.62598524565812
N	3.16994980883423	0.64623338729835	5.07599381073112
N	2.91083112746915	2.42261347924562	7.33267174140001
Sb	3.98897114452915	2.15600871579098	3.05791517436356
O	3.98288418151590	2.44128537433088	0.94914818468789
O	2.07232297874077	1.38722911838572	2.50937868580317
C	0.78329380098293	0.71022183470321	0.58613785354022
C	2.79240920709334	1.82506157661374	-1.05511372671613
C	1.65569963947466	1.23277056660873	-1.63585283868511
C	0.64651242177924	0.68216242983175	-0.82332617889003
H	3.57335216012270	2.27669072162650	-1.67777361552459
H	1.55027391921323	1.22523407719421	-2.72936547510931
H	0.00066608628490	0.30357457820223	1.24141130487482
C	-0.54024024692465	-0.02077183511105	-1.45139674585924
H	-1.43893211678694	0.07871318752676	-0.80933901250366
H	-0.77959370308938	0.42833076095068	-2.43606915985616
C	-0.18132275701535	-1.49342416259519	-1.62356712523125
H	0.04160317797100	-1.97657225547309	-0.65794779775160
H	0.68085045525683	-1.62827137388623	-2.29716292367322
N	-1.34754129729925	-2.29139748817829	-2.24779467334912
H	-1.59789847610908	-1.89959792307042	-3.16764525278398
H	-2.18603638685168	-2.22828945664917	-1.65195774217894
H	-1.12180997295163	-3.28828771220245	-2.37683856931169

Table S24. Cartesian coordinates (Å) of **10**.

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Coordinates from ORCA-job Sbetg_opt

C	4.89460851697022	0.16519763935237	3.05063833112827
C	6.06417974329654	0.00662793645666	2.27754708594714
C	6.72006692787441	-1.23919000340695	2.24703865775204
H	7.63614970760871	-1.35703831522475	1.65240538990495
C	6.21722917976285	-2.32126349618842	2.98766199125045
H	6.73544221387963	-3.28797316441423	2.96729662006990
C	5.07177868736997	-2.15496709034109	3.78306148887941
H	4.69717887376147	-2.98948023180726	4.39132366380888
C	4.40871357936503	-0.91349095414486	3.81862461386039
C	6.59245464345549	1.19442296579208	1.49987441250438
H	7.64598158707622	1.02232649790240	1.18247079379440
H	5.97858037879930	1.34064991944044	0.59213409670791
C	7.39318822800402	2.45027778711776	3.43246896977012
H	8.44814921285130	2.40851809226980	3.07486369642993
H	7.20900071947283	1.55226778599439	4.04978477061574
C	7.18752209139683	3.71062601671799	4.26638961111038
H	6.17414944320296	3.67526880583362	4.74219727884444
H	7.93134529211479	3.73328484829341	5.08441504317597
C	6.61169859214417	3.63639367235710	1.46857349344635
H	5.84208615296375	3.59161199097151	0.67800914670504
H	7.61993693151602	3.66860814090921	0.99495505988568
C	6.41004839753118	4.88428321147946	2.32191577597671
H	6.57541998042568	5.78303937245287	1.69983408873585
H	5.35006405295904	4.91516997230134	2.67782611142520
C	7.21920989113984	6.12512053833983	4.23546116700601
H	7.97615697535758	6.13254938988975	5.04012443648377
H	6.21156289676712	6.23285616769059	4.70799794899079
H	7.39136234234460	7.00811256624554	3.59463165673624
C	3.17871746667388	-0.69940179402813	4.67508411673123
H	2.28017456083575	-0.72505340483755	4.03177221699168
H	3.08664553007644	-1.49929526707843	5.44405070580666
C	4.25595745408837	0.73407798798487	6.32691450438397
H	5.22734025432397	0.48503831919154	5.86252235622582
H	4.06540621273142	-0.00572356563423	7.13808548172689
C	4.30193752826517	2.13904483071361	6.91754854200847
H	5.05513238017308	2.17026163148157	7.72667134695898
H	4.63652412064913	2.85899995570301	6.12752751804466
C	1.90022572432500	1.03029967805419	5.83518568236010
H	1.57033302408717	0.31177357562765	6.62002231221456
H	1.18148054447078	1.01070485630462	4.99753294735398
C	1.97135293674971	2.43389460040201	6.42691817938703
H	2.16499277271299	3.16765838371201	5.60522702594305
H	0.99349634094537	2.69095375021930	6.87391526982539
C	3.03814640378679	3.82959092529591	8.09118604771344
H	3.79139368144247	3.83894371505863	8.89924650756760
H	2.05428302970012	4.06065214728776	8.53685708799603
H	3.29219392535247	4.64761144226243	7.37252117178976

C	2.84615760553405	1.41076147525445	0.50863289816264
H	3.26530617059722	0.37801859692445	0.45285101511147
H	2.58570242688114	1.73307578381038	-0.52042754819644
C	1.60408252704024	1.40493005892735	1.40833122175460
H	1.04407124524484	2.35787854079842	1.26466731885139
H	0.92809637303083	0.56725908038243	1.13457830106404
N	6.46622299785431	2.42686665854882	2.29192821520391
N	7.35015356866130	4.90886027617355	3.44535110692696
N	3.21110138316006	0.63520036337810	5.29546692282580
N	3.00055395361927	2.51454768646749	7.46653935594932
Sb	3.86521192618489	2.09604944867286	3.10189470402776
O	3.80306914350628	2.31392992969481	1.04781389435674
O	1.99966454788392	1.25515227096560	2.76511417198618

Table S25. Cartesian coordinates (Å) of **10**, one arm uncoordinated.

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Coordinates from ORCA-job Sbetg_opt_un1

C	4.79153858351987	-0.33111141764592	2.29751337822789
C	5.83142196778192	0.37336267540542	2.94295698053572
C	6.38798253166021	-0.14891141819482	4.13215377157616
H	7.21321164283042	0.39974435102602	4.60354786954062
C	5.90029554263519	-1.33743645693154	4.68929479365072
H	6.33844914267975	-1.73134676252380	5.61486307174943
C	4.82634579122146	-2.00824517204755	4.07901367898977
H	4.41599521318385	-2.92181752133234	4.53031187673064
C	4.27198155088353	-1.50877452859319	2.88879587588728
C	6.33977738125340	1.71499953600020	2.44165441023573
H	5.93130945302310	1.92382691342218	1.42595319373834
H	5.95402136884363	2.50855683739377	3.11388157942661
C	8.42840653376261	0.87556072084699	1.51509118604801
H	8.14450270144043	1.12127163570277	0.46636435725279
H	8.06577300582810	-0.14576326960696	1.72930555294610
C	9.94491170402624	0.92674965303404	1.66979863599033
H	10.22277449973263	0.54915056839839	2.68687948556886
H	10.41582594970736	0.25830446808041	0.92484246571623
C	8.27757933045545	3.16333175567629	2.23146232089628
H	7.80717115577783	3.83637069473781	2.97311782567478
H	7.99824673823414	3.52988705930651	1.21327797245734
C	9.79657995607650	3.21703819597114	2.38323706577654
H	10.15587073664651	4.24056739222168	2.16592949818072
H	10.06294352862202	2.98317353544690	3.44575727515731
C	11.89031584174980	2.35946942498693	1.53063301801047
H	12.33871707122206	1.68482537978272	0.77922178497976
H	12.29191977084961	2.07148554581795	2.53457699764464
H	12.22781099500237	3.38866070086381	1.31181530608593
C	3.11443618646509	-2.21305804835756	2.21610686494119
H	3.48605853762984	-2.82896299095110	1.37738249104713
H	2.58487182955357	-2.87878936116625	2.93218977901471
C	1.45765055023951	-0.47779594842045	2.67980283455384
H	2.20168129742782	0.03513618732028	3.31460892895644
H	0.88991794053669	-1.18760880369385	3.32127374578414

C	0.49909592629673	0.53525036585251	2.06265720708083
H	-0.06348585695998	1.03676190840739	2.87162624562159
H	1.08513352551366	1.32603034714168	1.53021844419261
C	1.22102155962606	-1.87592045112095	0.71096354726752
H	0.63529673999626	-2.64641161411211	1.25958427999999
H	1.80797341519786	-2.36072325549131	-0.08689000446725
C	0.27180829691118	-0.84462512805897	0.11328873175881
H	0.85270467270010	-0.14592000455710	-0.53982109957691
H	-0.46174280763401	-1.36029119624032	-0.53317815586495
C	-1.41770409330194	0.81357695518086	0.61608083834454
H	-1.97410568432502	1.29988337041907	1.43702975308037
H	-2.14377649373950	0.27297422958816	-0.01667012433130
H	-0.94716732998284	1.61473387235669	-0.00506004458141
C	6.19529826463706	-0.69502463531325	-0.87459104795802
H	6.63556876647750	-1.17615663340466	0.03023141545516
H	6.99936795618518	-0.58099614953751	-1.62945346530224
C	5.05871925208560	-1.57177955105082	-1.41220056706834
H	4.78078696627624	-1.23382325465874	-2.43504359019467
H	5.37090929961328	-2.63478468377144	-1.46811721662560
N	7.79811362923113	1.80144385704506	2.46413856601573
N	10.43933915526696	2.28804492617006	1.45414631450199
N	2.17905407815983	-1.22976701653833	1.63137541770669
N	-0.44808582168074	-0.12506359813920	1.16528817377579
Sb	3.87218613623682	0.32536406320976	0.41461955644758
O	5.66169304975808	0.58480835917941	-0.56251453603334
O	3.93275017895203	-1.48298785653281	-0.53901855721762

Table S26. Cartesian coordinates (Å) of **10**, two arms uncoordinated.

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Coordinates from ORCA-job Sbetg_opt_un2

C	4.92699785317124	-1.48339780297875	1.49069896294203
C	5.93927364724269	-0.51518775778400	1.27406204729776
C	5.90137809479058	0.70467631908415	1.97872397740592
H	6.71410570529981	1.42481647766121	1.82066676494036
C	4.85450271439124	0.97726000800293	2.87043473989567
H	4.83608484889009	1.92480431298790	3.42347336126557
C	3.81457092523573	0.05088327404717	3.02922528983455
H	2.97337234460743	0.25370976608240	3.70412811671782
C	3.83184465143038	-1.17545826406803	2.33363383412719
C	7.04724158706675	-0.71727075998982	0.25463885332980
H	7.01499776427384	-1.76330189186088	-0.14880130764154
H	6.85521236510073	-0.05439724310789	-0.61342657289489
C	8.78479227230488	-1.22202750200649	1.89909560466766
H	8.90478242949145	-2.28262254465418	1.58328303768517
H	7.99829147566532	-1.18770342089706	2.67387247519909
C	10.09777461607693	-0.69780586572173	2.47247235304470
H	9.92875718226009	0.32075083219737	2.90598451702164
H	10.43201518224185	-1.35897991140127	3.29375545122841
C	9.39333806212010	-0.36575632285561	-0.26562452566666
H	9.06060547317137	0.29809215912868	-1.08565974000402
H	9.55624440474588	-1.38423083601747	-0.69553480740017

C	10.71048078061143	0.15138623493554	0.31011440721114
H	11.49472302961479	0.11702513030318	-0.46920268654269
H	10.57823038006929	1.22211981339854	0.61046438530893
C	12.42286084104560	-0.24773222079645	1.97039838801904
H	12.73419614618747	-0.92485497918368	2.78601165220854
H	12.40856724280412	0.79500581437864	2.37534284918484
H	13.18930912935265	-0.29361020750212	1.17589714778251
C	2.62827036134791	-2.08931719317350	2.48062791994893
H	1.76118030677635	-1.60536874119897	1.98705616998766
H	2.80002101547538	-3.05163665952630	1.94084569168480
C	3.29270947493309	-3.00547660625384	4.64902823133860
H	4.24940257714454	-2.46659580777685	4.52774680344191
H	3.43872059592974	-4.04292100259708	4.27298800373173
C	2.89648905434088	-3.04033380591712	6.12185576554300
H	3.65649285729696	-3.60216619979334	6.69675437768418
H	2.87487029093759	-1.99465889340425	6.52180069186440
C	0.97156512927617	-2.97546297685709	4.02568444702218
H	0.99895044173330	-4.01640934073572	3.62037633323010
H	0.21013568594339	-2.41099182601983	3.45505065496188
C	0.57508385911170	-3.02136260833701	5.50052418219996
H	0.40929607613262	-1.97478696992682	5.86300786299414
H	-0.37938166363457	-3.56935470915934	5.61197020412626
C	1.22379670864437	-3.81995884101086	7.68886622863529
H	1.99818340583208	-4.38342394550933	8.23986476781822
H	0.27106055255627	-4.37281748461171	7.77563832097120
H	1.09442484230778	-2.82985975735061	8.19349718909269
C	6.86333049142218	-4.26918980074120	2.48911742942577
H	6.76425908650937	-3.36498075871530	3.13070159692231
H	7.79608926456784	-4.79715508425433	2.76617345264015
C	5.63895764107420	-5.16848224400948	2.66866441732256
H	5.83226016162908	-6.16619183725829	2.21878102587432
H	5.40508739124948	-5.30901105527457	3.74324861163036
N	8.36391438984612	-0.38095627479804	0.77247798786470
N	11.13601603830915	-0.67315554438790	1.44060567131488
N	2.26196447460286	-2.30555537379835	3.87538224339166
N	1.60164518783633	-3.70321323499450	6.28856428912356
Sb	5.10229658916923	-3.42213606742678	0.47733551955809
O	6.95967499523992	-3.89628066675645	1.10790182077009
O	4.50244535019495	-4.55308881480754	2.04691901171601

Table S27. Cartesian coordinates (Å) of **11**.

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Coordinates from ORCA-job Bietg_opt

C	4.93533088394912	0.15883896834195	3.08309827959348
C	6.09431301628407	0.00843032718887	2.29640011378944
C	6.75176170431995	-1.23691166745271	2.25867357156988
H	7.66138031097549	-1.35597998260971	1.65411320418584
C	6.25400508360654	-2.32046718363295	3.00196534889510
H	6.77264956278994	-3.28680841152352	2.97536548531270
C	5.10967056671051	-2.16070752568081	3.80151049333384
H	4.73628729560823	-3.00126052070623	4.40248528501751

C	4.44504824314352	-0.91955540421416	3.84498347488554
C	6.59588067997058	1.19540540981554	1.49773925050510
H	7.63961911404473	1.02585613213177	1.14874105352418
H	5.95188929682371	1.33305663219252	0.60944595885906
C	7.43649327418397	2.47445759273267	3.40307783263632
H	8.48619766546189	2.43937399547132	3.03004256469626
H	7.26899146052195	1.57965948270310	4.02942243756550
C	7.23156908461111	3.73924141163264	4.23029332782052
H	6.22269094347409	3.69914284045966	4.71990868571589
H	7.98231900702637	3.77499799834600	5.04130012208016
C	6.62322068835038	3.63840343916906	1.43927927212298
H	5.84305735583768	3.58357770534045	0.65945853207339
H	7.62491694021824	3.66848228085958	0.95215392107763
C	6.42940356583155	4.89461898835171	2.28232143085964
H	6.58840903074732	5.78806485437861	1.65130683347036
H	5.37002428937390	4.93283836123851	2.64472534731963
C	7.24476812690241	6.15443013113402	4.18063307047160
H	8.00771285398721	6.17190602509874	4.97925112308906
H	6.23999486915866	6.26125091342676	4.65987108329995
H	7.40747558820394	7.03261746488046	3.53104077432056
C	3.20027317412828	-0.71377482731159	4.68429912213727
H	2.31536733885990	-0.72563596349539	4.02147210990687
H	3.09068933478378	-1.52620290349360	5.43764314542794
C	4.24606537462342	0.70558256153235	6.37421684138603
H	5.22401326216168	0.46155103296744	5.92134716255387
H	4.04838821348771	-0.03628443339079	7.18177564895746
C	4.27926411440540	2.10980880882234	6.96761801201020
H	5.02371701493825	2.14631342804701	7.78444061608023
H	4.62197910577726	2.83419532801487	6.18206265869699
C	1.89417392045680	0.98704088165391	5.85958025281955
H	1.56288482971603	0.26119062430961	6.63700587741655
H	1.18346908066310	0.96694273673065	5.01475628566933
C	1.94732125551763	2.38807259576513	6.45944157680901
H	2.13238391638251	3.13003076581063	5.64086817745592
H	0.96529953005431	2.63408156055767	6.90309074419597
C	2.99451286395466	3.79531239662977	8.12634358524990
H	3.74135390875532	3.81080912154098	8.94006734691234
H	2.00549136275946	4.01970547231101	8.56354423944825
H	3.24821902708581	4.61445626041191	7.40846948725936
C	2.79726507312752	1.44463242775510	0.49707924920364
H	3.21910694853931	0.41088102010800	0.46446028448324
H	2.51130635891628	1.72912992365084	-0.53811283666837
C	1.55344728950339	1.44414193313899	1.39962368080773
H	1.01032031828255	2.40868557535809	1.25816470219736
H	0.86873569845429	0.62329847734955	1.09244215612905
N	6.49078720035858	2.43891991626924	2.27917525080424
N	7.37382520222128	4.93209752757433	3.40005954515329
N	3.21446679034045	0.61053219630050	5.33059438461737
N	2.97162848394896	2.48042265075644	7.50126245375737
Bi	3.86359472144011	2.16874898019182	3.14842538758153
O	3.75980882084789	2.36736899782088	0.98206612952265

O	1.91415296339097	1.26135666723850	2.75916484392678

Table S28. Cartesian coordinates (Å) of **11**, one arm uncoordinated.

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Coordinates from ORCA-job Bietg_opt_un1

C	4.78760190052229	-0.27743015722124	2.35029547967050
C	5.82721677234147	0.41840270845801	3.00020436679089
C	6.37625561678441	-0.11171435592461	4.18977332386331
H	7.20190992154331	0.42877714944242	4.66997713978534
C	5.88098596879408	-1.30350494653255	4.73407094755326
H	6.31204068813023	-1.70580376558888	5.65935623906794
C	4.81336171797669	-1.97169380642436	4.10865953026129
H	4.40519295894925	-2.89243498323285	4.54760933479552
C	4.26468931575258	-1.46362862548638	2.91840115327496
C	6.34933116640851	1.75186974086105	2.49214263791842
H	5.92765446801606	1.96462607789287	1.47942453991888
H	5.98616703873446	2.55604406517099	3.16407674560261
C	8.40828518606186	0.87304182388005	1.53634675639737
H	8.10878980877835	1.11498490130292	0.49156086890248
H	8.03388575714897	-0.14095614330662	1.76414291485634
C	9.92743457842812	0.90232248433863	1.66740576700814
H	10.21600058737937	0.52665650322320	2.68227159263830
H	10.37592351442446	0.22238282145204	0.91917139213185
C	8.30471470352960	3.16855525147651	2.24122237294117
H	7.85642924283176	3.85330183916198	2.98588110730786
H	8.01589231785642	3.53308754502670	1.22485578936636
C	9.82655220362321	3.19863806196450	2.36940784660405
H	10.19864926171437	4.21517384772521	2.14114514279032
H	10.10521070399344	2.96613872814511	3.42913721045733
C	11.89252202467855	2.30378433737412	1.48875270680357
H	12.31820421591014	1.61776422986579	0.73448450115501
H	12.30560995415954	2.01548573273432	2.48795476866325
H	12.24246316153236	3.32624939413177	1.25820482725129
C	3.12903237689974	-2.18266718198007	2.22097055880488
H	3.52761806057981	-2.76558311285205	1.37096207032206
H	2.61839908869303	-2.88250694513685	2.91867183125242
C	1.42188516013502	-0.49751242480339	2.69726446209151
H	2.15094255803751	0.01705286292026	3.34794779013408
H	0.85258340181346	-1.21976274086059	3.32414007398154
C	0.46086865387020	0.51120342555986	2.07719960391514
H	-0.11724315061732	1.00431149972277	2.88019428176018
H	1.04720361576561	1.31453727060962	1.55884293195039
C	1.22637192198092	-1.88181028190248	0.71688783830535
H	0.64688479659340	-2.66656154549458	1.25245383439336
H	1.82854512435354	-2.35036110562218	-0.07971410005111
C	0.26759453304399	-0.86094659620203	0.11583060950486
H	0.84355995401815	-0.15413393335162	-0.53572788396785
H	-0.45639140809017	-1.38173863182291	-0.53704005444903
C	-1.43726861589515	0.78547657983227	0.60541597238876
H	-2.00692857233459	1.26392472663298	1.42171961121518
H	-2.15112961453295	0.24266511544882	-0.03898614234670

H	-0.96467401516254	1.59298825264042	-0.00645281258749
C	6.22527173433767	-0.68581874423929	-0.92542410982430
H	6.64022674022943	-1.16407489949008	-0.00592888959264
H	7.04138855697519	-0.62677850542351	-1.67594574944510
C	5.07859441747531	-1.55403418345482	-1.46260770404683
H	4.80529548117770	-1.20287306205303	-2.48351845194948
H	5.40517765535554	-2.61302707538484	-1.53718096673537
N	7.80707725785380	1.81593290791229	2.48885190991501
N	10.43957956911480	2.25458814288285	1.43583588980190
N	2.16275331859599	-1.22314669219973	1.64782562726420
N	-0.46632579944868	-0.14747912692331	1.16093935936949
Bi	3.85421805510589	0.42090793750466	0.37813184987750
O	5.74702319530027	0.62035521811362	-0.65083358295335
O	3.94994000477154	-1.49679885249378	-0.59535670707616

Table S29. Cartesian coordinates (Å) of **11**, two arms uncoordinated.

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Coordinates from ORCA-job Bietg_opt_un2

C	4.88850772916527	-1.42506038482843	1.44803873232306
C	5.90705233181857	-0.46567622424991	1.23500229585952
C	5.87070423825901	0.75406752275215	1.94140594697909
H	6.68542925418970	1.47313011624784	1.78837087385514
C	4.82333661902783	1.02669301268062	2.83322080765522
H	4.80620248913443	1.97416659102033	3.38641364115957
C	3.78576774570712	0.09817662864615	2.99972707254618
H	2.95135155013762	0.29887146205963	3.68372389555295
C	3.80178006329351	-1.12746412627908	2.30229340142988
C	7.02786616900728	-0.68185882132307	0.23278595436997
H	6.98927346597742	-1.73007271644710	-0.16942573427734
H	6.86266279278908	-0.01926029843018	-0.64082381647692
C	8.72754893983346	-1.21725920879845	1.90586265754120
H	8.83196789069520	-2.27902042880777	1.58931077323203
H	7.92895465087449	-1.17066370041070	2.66736427079300
C	10.03967397382717	-0.71735441493227	2.50173664724975
H	9.88225728950211	0.30330980529844	2.93470973518232
H	10.34815452839513	-1.38621107938198	3.32676155219491
C	9.38742377165898	-0.36732778816788	-0.24695922100725
H	9.08043035213479	0.30385588929686	-1.07107711728194
H	9.53969722900381	-1.38807999919484	-0.67572913019486
C	10.70367757392449	0.12519633127150	0.35214408020885
H	11.49998481590708	0.07880249098038	-0.41421751707310
H	10.58534176639999	1.19756315089379	0.65274563793175
C	12.38090007916408	-0.30922483659790	2.03925050440397
H	12.66611102866765	-0.99432880969321	2.85772107840635
H	12.37930609859986	0.73245002237452	2.44721478361802
H	13.15933997030263	-0.36715709575441	1.25727782825820
C	2.61682173377815	-2.06153012894051	2.46891382966777
H	1.73221051896110	-1.60233412660232	1.98307109975450
H	2.80393960132171	-3.02507047314869	1.93140332343484
C	3.32825906754092	-2.95800604365689	4.63086658907153
H	4.27115782164912	-2.39770282910924	4.49991963067042

H	3.49476335512650	-3.98989824931281	4.24958462091793
C	2.94959694375484	-2.99970040023968	6.10798503246676
H	3.72757912946340	-3.54600642587589	6.67360062328805
H	2.91202011552917	-1.95452391830123	6.50836549682501
C	0.99823866282148	-2.97654367081411	4.03592436476900
H	1.04239554701534	-4.01773157330522	3.63279308378176
H	0.21856838481333	-2.42893910955894	3.47350819549049
C	0.62111274535208	-3.02676971578880	5.51559379743296
H	0.44013704617581	-1.98262322274661	5.87809634384916
H	-0.32152879653546	-3.59222252990309	5.63982919053820
C	1.31193039835440	-3.80878671268674	7.69670861667799
H	2.10357036159602	-4.35666689869170	8.23879813027241
H	0.37082225429510	-4.37914130061830	7.79634788834167
H	1.17051461402519	-2.82028977616549	8.20136435077323
C	6.86672980784948	-4.32249209719415	2.45940833469980
H	6.75341667412667	-3.41793200571966	3.09994641456433
H	7.79239180285224	-4.85088720456818	2.76428038433192
C	5.64602298835928	-5.23011130054206	2.64167420469565
H	5.84336724274194	-6.21622118079067	2.16558261971197
H	5.45510585130846	-5.40152799167387	3.72176840792591
N	8.34011563263215	-0.36693259472955	0.77322443382098
N	11.09530394654890	-0.70926390880094	1.48724973978378
N	2.27309785767212	-2.28131897239002	3.86754845304238
N	1.67002279160882	-3.68743241879878	6.29166112978968
Bi	5.05505858929108	-3.45258431288023	0.39213571556434
O	7.00030742493533	-3.95426842542532	1.08460735472757
O	4.48000926063754	-4.62091108624532	2.08057446487845

Table S30. Cartesian coordinates (Å) of **12**.

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Coordinates from ORCA-job Sbpin_opt

C	10.02546382736389	4.93313105614460	7.29279362169586
C	10.87074706157428	3.84853933781700	6.97773678655492
C	12.24050103549354	4.07351218241180	6.74286217716080
H	12.89807336187374	3.22632164576014	6.50505370263082
C	12.76775985123025	5.37262529600788	6.82451064097820
H	13.83658426862577	5.54313802474023	6.64572220637822
C	11.93269588047828	6.44836646293673	7.16775520926426
H	12.34931420171162	7.46022895183697	7.26427104391986
C	10.56164881137385	6.23282104308741	7.40458827828033
C	10.27571569952723	2.45926408657274	6.88308283376472
H	9.75807228834875	2.35291000228828	5.91196004769792
H	11.07249189161756	1.68293741916985	6.93727071516582
C	9.84331605597014	2.16881250270991	9.26661871113880
H	10.42440131131172	3.09044044411564	9.45261030399099
H	10.54492454285829	1.30494266098370	9.32771645619523
C	8.75222773747798	2.01632568870777	10.32172780677716
H	9.22087784436190	1.89432699491965	11.31596788883273
H	8.14100864769243	2.95396081366022	10.35702505340191
C	7.32581234352607	0.95176112508718	8.70931462178074
H	6.63057255398907	1.82495733081754	8.63895270259565

H	6.73128432820579	0.04069525275888	8.51268932495033
C	8.40432204718012	1.08918823247618	7.64046523280982
H	9.01594553595498	0.15828596286386	7.60640807945725
H	7.93622089845027	1.25475957606690	6.65449894760464
C	6.90878496797180	0.64975638062513	11.07317350003528
H	6.19068404967832	1.50356509202922	11.14859981853947
H	7.39441148790663	0.52400228874690	12.05749480059910
H	6.32895375110255	-0.26531583234445	10.85759471344228
C	9.63659925326195	7.37380656998506	7.77310394585894
H	10.21767950977136	8.25316027878064	8.13288854220981
H	9.06279218134470	7.67909713915759	6.87866959048746
C	9.27066977550603	6.68840481329050	10.08566335699999
H	9.73767094834808	7.62240085370388	10.47481914287710
H	10.07133873726958	5.93797125887646	9.95516616863187
C	8.23476074138814	6.18010232245224	11.08306619877983
H	7.87772750380056	5.16909255769583	10.75975439564514
H	8.71166538207115	6.05624364818397	12.07315858354837
C	6.50584170272651	7.35551339203934	9.89993231008178
H	5.69623600914111	8.09908099030919	10.01807210857218
H	6.04346006433075	6.42119184817173	9.49496195208351
C	7.52685705575589	7.87841380921239	8.89564648606586
H	7.06214559688049	7.96203274511357	7.89798416238755
H	7.89024678700737	8.88052133948077	9.21985657639217
C	6.15276626265539	6.68390052902461	12.19761704282233
H	5.35512528866530	7.44096044623833	12.30113936222653
H	6.64452782625252	6.56751874675143	13.18005439798492
H	5.67139405752307	5.70946326879506	11.93469425318889
C	7.34301136335876	4.33634945903556	4.75377029854186
C	6.58556324410831	5.63521512896009	5.24560515092161
C	8.70325738117461	4.69332733561953	4.12341866310725
H	9.27887906161725	5.37007940050800	4.77668224279090
H	8.58859151496916	5.17129005469310	3.13429360959883
H	9.28797503623230	3.76683319114494	3.98646122570210
C	6.51528481282226	3.49853451276907	3.76855439260232
H	7.11613559595933	2.63986680937192	3.41962563549758
H	6.21471756508746	4.08721946217000	2.88254804716193
H	5.61043991022183	3.10072975015347	4.25634844962371
C	6.58690949858140	6.76295560984416	4.20396856758982
H	6.00285296613976	7.61916255084161	4.58591161654024
H	6.13360978194130	6.43761586576266	3.24988530718861
H	7.61339259714104	7.11329236419083	4.00848202557224
C	5.13648813476328	5.31452107663831	5.66478358335759
H	5.10644992993222	4.43964254606613	6.33927492473608
H	4.48437646139087	5.10218219074961	4.79900039138207
H	4.72461833579794	6.18509012314810	6.20441719402055
N	9.25628880583673	2.25483588768293	7.92122108140058
N	7.92039260488944	0.84665265552948	10.04433794211278
N	8.65150952477592	6.93799324203458	8.77474482431866
N	7.12547356954629	7.12396969514126	11.20733577715080
O	7.29908109178658	6.13026003608415	6.38629206737759
O	7.56080684022933	3.51005374415419	5.90886702945165

Sb	7.89065140513986	4.59400572744578	7.62898914976524

Table S31. Cartesian coordinates (Å) of **13**.

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Coordinates from ORCA-job Bipin_opt

C	10.07373431108878	4.91615192288438	7.34461176769976
C	10.90499727680909	3.82623322454738	7.01913246633567
C	12.27708830836969	4.04403386005241	6.78779819039617
H	12.93053954672938	3.19604187098253	6.54082565484630
C	12.81148120458812	5.34032553768633	6.87992909296143
H	13.88177455546166	5.50498936026217	6.70438721164838
C	11.98214622564141	6.42236017835465	7.22002132730862
H	12.40506026194799	7.43224478826960	7.31188556770272
C	10.60855134621624	6.21462394025550	7.45286003469517
C	10.29084202788102	2.44643988611479	6.89013495043795
H	9.76148372446413	2.37839196617909	5.92175970831385
H	11.07775869593628	1.65870209768935	6.91082644680916
C	9.86863297595022	2.08714788740658	9.26901583387547
H	10.46754199191925	2.99302820373315	9.47384201757871
H	10.55312642808576	1.20857024190366	9.30965704764570
C	8.77573582232105	1.93154877243300	10.32152448692394
H	9.23944621312295	1.78521563272695	11.31463751394227
H	8.17860569598617	2.87989773186156	10.37602593048998
C	7.33681645642237	0.91092572232842	8.68803721222313
H	6.64195916829778	1.78759429068982	8.63214284356826
H	6.73592129226737	0.00780513735578	8.47586697536531
C	8.41542773862474	1.06245839646246	7.62090755285434
H	9.01779026351244	0.12680050471371	7.56386677797928
H	7.94668557838576	1.25618513925610	6.64003257274770
C	6.91053219775681	0.57854714454075	11.04601453100841
H	6.20117278581599	1.43880478950098	11.13273038465909
H	7.39252817907379	0.43252162635754	12.02914997240599
H	6.32159689422012	-0.32658133172025	10.81450698569343
C	9.67905756278013	7.36418039878553	7.78757557145755
H	10.25680563747657	8.25562646749013	8.12191554349715
H	9.10919848656316	7.63977891432257	6.88074644427414
C	9.28871747765304	6.74360437661776	10.11841153279024
H	9.75009157354105	7.68466146193976	10.49704196215170
H	10.09091074850937	5.99083823700336	10.01391369754905
C	8.23755933026219	6.25451148524793	11.10964824007936
H	7.88151805690738	5.23715818002861	10.79777489122563
H	8.69806244512043	6.14196964304437	12.10866193633197
C	6.53038697812878	7.42354663707755	9.88562726016589
H	5.72551968619211	8.17482696168626	9.98359945345406
H	6.06004216751259	6.48859659508140	9.48697920310426
C	7.56736526871005	7.92009759581374	8.88455793965336
H	7.11383486275024	7.98651002278833	7.88023386002501
H	7.93486224233763	8.92525839752812	9.19396617416232
C	6.14042419635298	6.78145185712262	12.18594014689028
H	5.34623625949054	7.54458983660449	12.26713319460307
H	6.61739371351033	6.67535805523821	13.17664837405781

H	5.65658325394849	5.80641693350701	11.92898990737872
C	7.29539745167386	4.33956597367957	4.74251422116057
C	6.53580645205603	5.64419351699462	5.23774680915889
C	8.66934702087371	4.70451429954445	4.14529886815893
H	9.23616167809171	5.35852731774080	4.82914876074455
H	8.57852775775590	5.21244132263929	3.16869860884632
H	9.24980378704320	3.77772613043095	3.99244875591192
C	6.47806391741396	3.53823706896484	3.71593908539720
H	7.07654147933795	2.68009863457919	3.36140744970643
H	6.20408458560160	4.14997988526895	2.83703952775201
H	5.55822722211567	3.13971119863536	4.17457683056335
C	6.51931664474118	6.75798516635961	4.17814633174511
H	5.92723806909755	7.61230714606757	4.55233314092612
H	6.06758947224851	6.41806614120802	3.22846330942643
H	7.54137693296161	7.11816210640825	3.97707470063928
C	5.08948713609890	5.31096179494994	5.66126091025521
H	5.06935750031555	4.43370776497819	6.33377445395524
H	4.43469421051616	5.09132497895579	4.79924414289607
H	4.67196440443036	6.17820222542922	6.20204586648698
N	9.27644860109847	2.21416375084887	7.92997827163398
N	7.92571295113234	0.78221695225956	10.02230770832326
N	8.68382206631691	6.96621869420389	8.79706104619812
N	7.12929059375481	7.20084704755852	11.20301310383332
O	7.24084901876553	6.16904666668987	6.36520616601173
O	7.48629124735549	3.47468620686920	5.86823850727804
Bi	7.85013068455964	4.57193242897925	7.70507003202307

Table S32. Cartesian coordinates (Å) of **14**.

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Coordinates from ORCA-job Sbcat_opt

C	4.84808373718883	0.21810556218915	3.02856401815753
C	6.00617426478038	0.02429818400217	2.24908477553599
C	6.59225596721885	-1.25340782983342	2.17642498081603
H	7.49991453938809	-1.40370018279945	1.57660291894763
C	6.02602765597610	-2.32969061938357	2.87894032069183
H	6.48814761962565	-3.32295515388292	2.82386259051976
C	4.88775971365014	-2.12961663459244	3.67706413401720
H	4.46316778137702	-2.96461238205405	4.25039790202215
C	4.29539910310214	-0.85530397085442	3.75585714910903
C	6.58822265939887	1.20755531054145	1.50570897852393
H	7.64767599097675	1.01796202616692	1.22380112096112
H	6.00944063850887	1.37540563853075	0.57925477979435
C	7.37685801717241	2.42200692147336	3.46967208798936
H	8.43229361716505	2.34285324714606	3.12373304736150
H	7.15110986778256	1.52710929649517	4.07743444986587
C	7.20838720820302	3.68490860577589	4.30789167956680
H	6.19012206640397	3.68642377843953	4.77559123700660
H	7.94320135586274	3.67317322934240	5.13411517814298
C	6.67053601589128	3.65042047835969	1.50098330008007
H	5.91728726751046	3.64002618757243	0.69460943728163
H	7.68807941808894	3.64573195137656	1.04933348905606

C	6.50085117413184	4.89780847764284	2.36113144286446
H	6.70733585888983	5.79347693188067	1.74734020421655
H	5.43748004652851	4.96736412396227	2.70161294221918
C	7.33325307268691	6.09679571672723	4.29277976776981
H	8.08124145053344	6.07029242249179	5.10521056712414
H	6.32563784674298	6.24105667222194	4.75494379497593
H	7.54687775251962	6.97541816190727	3.65879796130870
C	3.07095867506935	-0.60020993912041	4.60853819906305
H	2.17395506261482	-0.58654982269131	3.96314307703533
H	2.94107429789411	-1.40263111342597	5.36820734055052
C	4.18718122099116	0.76089695459637	6.29751989528756
H	5.15387032354915	0.47696603053131	5.84354320375980
H	3.95007220331082	0.01572545045698	7.09032233385891
C	4.28342229027548	2.15130128149252	6.91617544827947
H	5.02452100910996	2.13403978128733	7.73669064678776
H	4.66289729964290	2.87216461024345	6.14685402105705
C	1.85310823253814	1.16643304537468	5.78007978082289
H	1.48788195856612	0.44823280256002	6.54842201320185
H	1.14035108184527	1.18723552512865	4.93783190508428
C	1.97440761284924	2.55491057852411	6.39854081637953
H	2.20767288011526	3.29649156420778	5.59407059989192
H	1.00192917751677	2.84357513367203	6.83740891265022
C	3.07493867688360	3.87138530560167	8.10592027268176
H	3.81268264383941	3.83077444526504	8.92707240008032
H	2.09408444920022	4.13555538255596	8.53919789619044
H	3.37692378077051	4.69210084159748	7.40953805648206
C	2.84501462051688	1.70549998402472	0.49120296012393
C	1.84978435640296	1.19651363124068	1.37721183609979
N	6.46649760101957	2.43632441099281	2.31103161921617
N	7.42531646453557	4.88021057312138	3.49700715125656
N	3.15435028157984	0.72574546995241	5.24743909224476
N	2.99161831019215	2.57245755928276	7.45207591163173
Sb	3.92124097872108	2.18761022327863	3.12485936041987
O	3.87870418196358	2.40176263608753	1.04079404463595
O	2.00706927328417	1.44421819471800	2.70741506844764
C	0.75986495307967	0.47480677346100	0.86462607363382
C	2.73159705327216	1.48256151290980	-0.89043289872922
C	1.63235741718908	0.75997731146653	-1.39655352995428
C	0.65202789849856	0.25905291670142	-0.52407661413316
H	3.50498276251139	1.88424085318779	-1.55686631619688
H	1.54732696494236	0.59080426075571	-2.47710038125919
H	-0.20285912164714	-0.30332554970414	-0.91944695970216
H	0.00223453205047	0.09428683182000	1.56090518919367

Table S33. Cartesian coordinates (Å) of **15**.

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Coordinates from ORCA-job Bicat_opt

C	4.88163763808409	0.21454642965397	3.06776421960712
C	6.02505691529855	0.02413247146660	2.26934939417429
C	6.60555450675452	-1.25621174934468	2.18690222256688
H	7.50316082561545	-1.41154182917816	1.57306874686310

C	6.04187401632997	-2.33171765096749	2.89405559512798
H	6.49947066177286	-3.32657878121370	2.83091336959236
C	4.90718839420522	-2.13332424818944	3.69886821309586
H	4.48012965806054	-2.97261487104877	4.26438636767002
C	4.31993091810012	-0.85658882283009	3.78773902693234
C	6.58306382963263	1.20425568483423	1.49996747307185
H	7.63019997204896	1.01034429768389	1.17793094208107
H	5.96780638488466	1.36738457416314	0.59620195618353
C	7.43425587119317	2.43869059641936	3.43007211819868
H	8.48273419046117	2.36672387451498	3.06218126424901
H	7.22884545892684	1.54571337405322	4.04744877678236
C	7.27174399430617	3.70488170173263	4.26426044347044
H	6.25976790493198	3.70070079962332	4.75080824989346
H	8.01763416566715	3.70500296180537	5.08037184503053
C	6.68745382367652	3.64805377525148	1.46624299598783
H	5.91958893987605	3.62955735726344	0.67360542594529
H	7.69678826908409	3.63979022906707	0.99669737513960
C	6.53131147298246	4.90345458029126	2.31749129405991
H	6.73004058024122	5.79455065538772	1.69483565591308
H	5.46995548868923	4.98060954869129	2.66824192860607
C	7.37702126671655	6.11837612153046	4.23315199782761
H	8.13412443098880	6.10079081766481	5.03713185244332
H	6.37367790836324	6.26074635584037	4.70558644923936
H	7.57868518764084	6.99355865304010	3.59079145558738
C	3.08063211432135	-0.60416413147579	4.62204812113466
H	2.19866362354356	-0.57342377657175	3.95644319557270
H	2.92828889810405	-1.41774439130818	5.36544064245027
C	4.16688195478239	0.73962844988328	6.35040123927737
H	5.13970362083006	0.45603075212184	5.90989650388274
H	3.91838065049549	-0.00549385137510	7.13966706970153
C	4.25455402802223	2.13011983444057	6.97025126427870
H	4.98634676248941	2.11687370065092	7.79898529751207
H	4.64564963720530	2.85276208327355	6.20502159799043
C	1.83836823217995	1.13826469408553	5.80730920835920
H	1.46921633140001	0.41475384559355	6.56863750077562
H	1.13465821672101	1.15919657947847	4.95722446149287
C	1.94571575092041	2.52508134596794	6.43206660827384
H	2.17485238477036	3.27311245521337	5.62995725947632
H	0.96925403177534	2.80750633426112	6.86567732851097
C	3.02985781806955	3.85218502140437	8.14152423422149
H	3.76285055791485	3.81717203184183	8.96696791681706
H	2.04501211851860	4.11239760334814	8.56771071892503
H	3.33192866743901	4.67265435965699	7.44455924975720
C	2.80504102977400	1.74867790846067	0.48170529618069
C	1.80710676075007	1.23688434681060	1.37305945502037
N	6.49697482183037	2.44472792010584	2.29455401455477
N	7.46434441733587	4.89683972858849	3.44490071718967
N	3.14882001577541	0.71152688103069	5.28697663518013
N	2.95759342270467	2.55223494601285	7.48886611012643
Bi	3.92745938950975	2.26971753739737	3.18834698513484
O	3.83439094393342	2.47169447744805	0.99681678157160

O	1.92445091654278	1.49188256600587	2.70303766161720
C	0.73591771658162	0.48628961589730	0.85531415446633
C	2.69821532900471	1.49224461670303	-0.89732519685543
C	1.61623266337600	0.74509399217391	-1.40269687514758
C	0.63768497971630	0.24355443581297	-0.52878443992475
H	3.47068369859535	1.89515230144683	-1.56462329425631
H	1.54396381560320	0.55725533733120	-2.48120975260185
H	-0.20603761419505	-0.33963198903120	-0.91830360317912
H	-0.02047726887461	0.10570713210845	1.55342195917252

Table S34. Cartesian coordinates (Å) of **CO_2**.

3

Coordinates from ORCA-job CO2_opt

C	0.00000077979583	0.21999945483071	0.07333285931746
O	0.55189324941734	0.08334730797605	1.10156747529757
O	-0.55189404921317	0.35665324119324	-0.95490032161503

Table S35. Cartesian coordinates (Å) of **H_2O**.

3

Coordinates from ORCA-job H2O

O	-0.00136624200000	-0.00000000022727	-0.39289243579087
H	-0.00136624200000	0.76683446176300	0.20605260348462
H	-0.00136624200000	-0.76683446153574	0.20605260330625

Table S36. Cartesian coordinates (Å) of **$C_2O_4H_2$**.

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Coordinates from ORCA-job opt_oxa

C	3.15762300140725	1.59042041058895	0.93386059931226
C	1.90214005630671	1.56641207614788	1.84021290886703
O	3.28398310155892	2.80808570711072	0.35681493161145
O	1.77498007193959	0.34836302642947	2.41620821237249
O	3.90965305471490	0.65378306247861	0.77125314944711
O	1.15080178181181	2.50347958114862	2.00362932065213
H	4.09093974794739	2.76136194979328	-0.20054297751463
H	0.96821840931344	0.39517351530248	2.97384566825216

Table S37. Cartesian coordinates (Å) of the cation **$[1,2\text{-}O_2\text{-}C_6H_3\text{-}3\text{-}(CH_2)_2NH_3]^+$**.

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Coordinates from ORCA-job opt_dop

C	2.85658863532383	1.38871033244400	0.46843306125693
C	1.76668621861132	1.31485500735583	1.37779283438274
O	4.11025084398468	1.67741474732344	0.90768999429692
O	2.10576269753625	1.55453548738247	2.68512259783034
C	0.47868673096672	1.02457099835263	0.91150416663131
C	2.62974355439600	1.16710303957859	-0.89605964706991
C	1.33183840027994	0.87606753595130	-1.36870309795171
C	0.26012041718428	0.80097614895352	-0.45989459606429
H	3.48531209401490	1.25220355038736	-1.57819865294416
H	-0.75636469572380	0.58794686584157	-0.81363905604341
H	-0.35998354385302	0.97967390994363	1.61813381306326

H	4.06878180545955	1.82057148374916	1.87580341524625
H	1.31843488205592	1.52706388282240	3.25801772496945
C	1.11891300866262	0.58358529978012	-2.84290212161012
H	1.77100015562123	1.23349122552474	-3.45993078155958
H	0.07039379929232	0.79981365624765	-3.12560675073479
C	1.44261431008138	-0.88585055045660	-3.11077202223032
H	2.48458512479455	-1.13182559319379	-2.84674130999689
H	0.76972377210291	-1.56252304499859	-2.55847288430325
N	1.28178238564603	-1.23201992074587	-4.59822622620692
H	0.31723175540888	-1.05084999371287	-4.91500132983422
H	1.49793501435669	-2.22081190444507	-4.79386107053007
H	1.90666812079681	-0.65146451008562	-5.17804841559755

Table S38. Cartesian coordinates (Å) of **1,2-$(HO)_2C_2H_4$**.

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Coordinates from ORCA-job opt_etg

C	2.90305086766871	1.44068954136938	0.46587225913170
H	3.40723395140833	0.44882502806124	0.47421753474365
H	2.50457708400376	1.60863083788062	-0.55134796676595
C	1.76102723488716	1.42457997915351	1.47270553610183
H	1.22340459494965	2.39460060348128	1.43866043461532
H	1.04433548946723	0.61197022672562	1.22436624695836
O	3.83014694127081	2.49279361756133	0.73311562589092
O	2.35971135503785	1.21415845651453	2.76592242100300
H	4.04770616720050	2.41145097964790	1.68198264494115
H	1.71091423410600	1.45094536160462	3.44949062938004

Table S39. Cartesian coordinates (Å) of **1,2-$(HO)_2C_2Me_4$**.

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Coordinates from ORCA-job opt_pin

C	7.33480738890041	4.26397645186106	4.73003980560142
C	6.63806005126631	5.57513403277088	5.25492134356247
C	8.74605245652545	4.55999631304086	4.18501725013477
H	9.34002227225367	5.13356045815695	4.91694143408594
H	8.71623196951001	5.12816935438820	3.23848070680950
H	9.25661562218464	3.60079029653493	3.99388517695103
C	6.50088545886384	3.53495287247169	3.67180056944951
H	7.04334496646706	2.63088281573144	3.34584680328191
H	6.32767599401864	4.16812360183970	2.78474365031652
H	5.52887169693900	3.21350295716144	4.08016771768636
C	6.62194922013345	6.71061513549773	4.22126065434312
H	6.09852208720899	7.59230557869511	4.63509277941820
H	6.09072991290151	6.41248859647721	3.29996942602378
H	7.64594261049879	7.01851437744225	3.95546754725013
C	5.22035947509566	5.29414414758572	5.77284963792063
H	5.22027418662671	4.43067178551459	6.45860342874146
H	4.52111663291977	5.08696413429518	4.94461351052458
H	4.83130876974464	6.18077865165772	6.30954099082064
O	7.48695001472004	5.96663263111663	6.37826028523353
O	7.44186397998981	3.35084556202594	5.84269106456491
H	7.78847609416190	3.89876183246172	6.57684387251646

H	6.97557311906977	6.58213231827305	6.93190916676316

Table S40. Cartesian coordinates (Å) of **1,2-$(HO)_2C_6H_4$**.

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Coordinates from ORCA-job opt_cat

C	2.76374595802018	1.86739565536600	0.48511965535784
C	1.80691218118750	1.32868544406787	1.37889797584846
O	3.73509724381432	2.65581143000619	1.08114557575674
O	1.88348622260947	1.59880000154968	2.72088852880248
C	0.77900969035931	0.51552175806382	0.87983617918949
C	2.68827418544302	1.59339680531012	-0.88619174735686
C	1.65419199457701	0.77651173811541	-1.38089135122102
C	0.70358491047812	0.24059488224742	-0.49710976076121
H	3.43827896987051	2.01891887572753	-1.56728379097655
H	1.59809477576184	0.56404922983927	-2.45461679288526
H	-0.10384039131856	-0.39617252823377	-0.87699600729505
H	0.04720311039588	0.10711629091589	1.58622931036401
H	4.34861052636819	2.98274046615034	0.40056472398352
H	2.66199950743322	2.17559158987423	2.85478001019342