

Supplementary materials

Polyfunctional sterically hindered catechols with additional phenolic group and their triphenylantimony(V) catecholates: Synthesis, structure and redox properties

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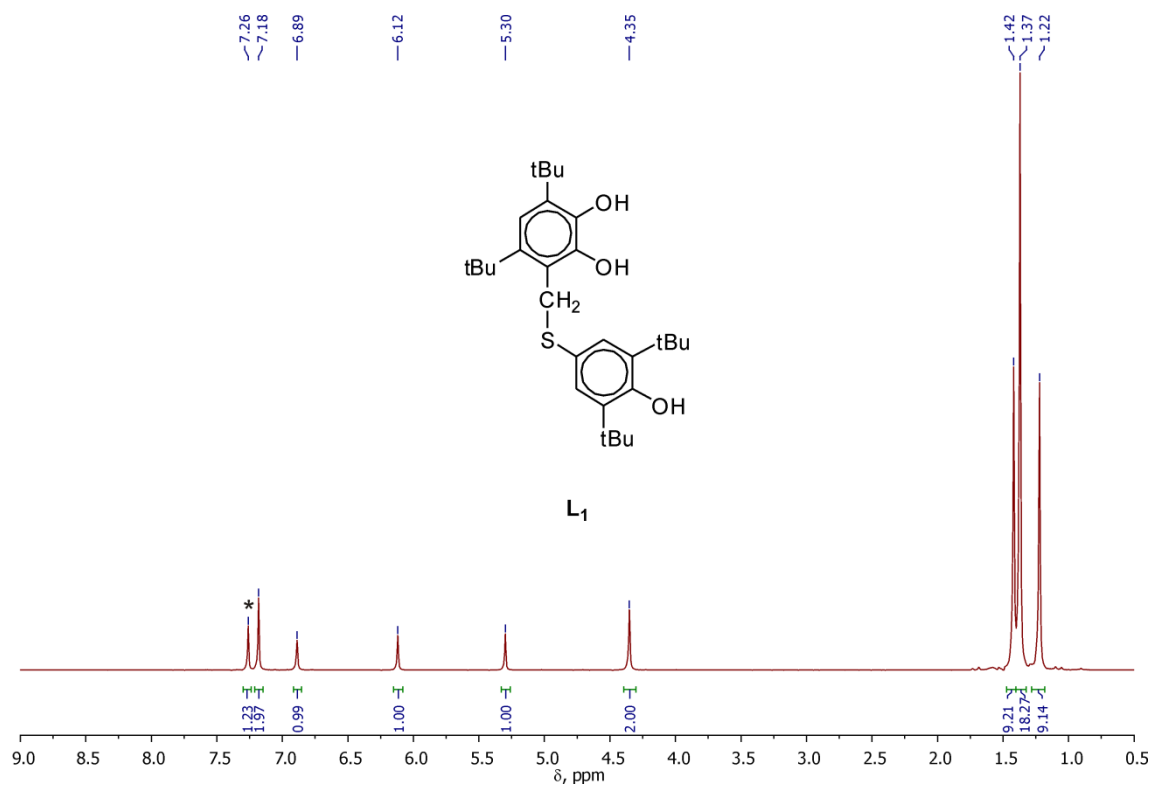


Figure S1. The ¹H NMR spectrum of **L₁** (CDCl₃, 200 MHz).

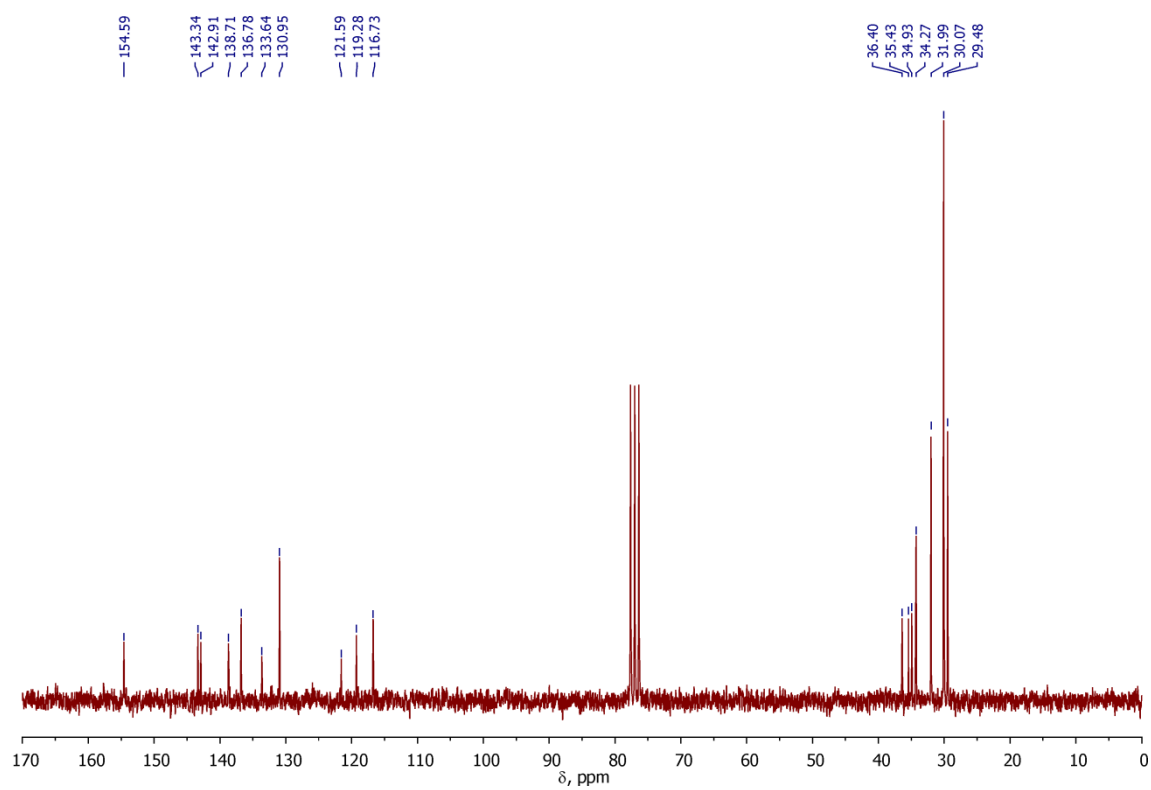


Figure S2. The ¹³C{¹H} NMR spectrum of **L₁** (CDCl₃, 50 MHz).

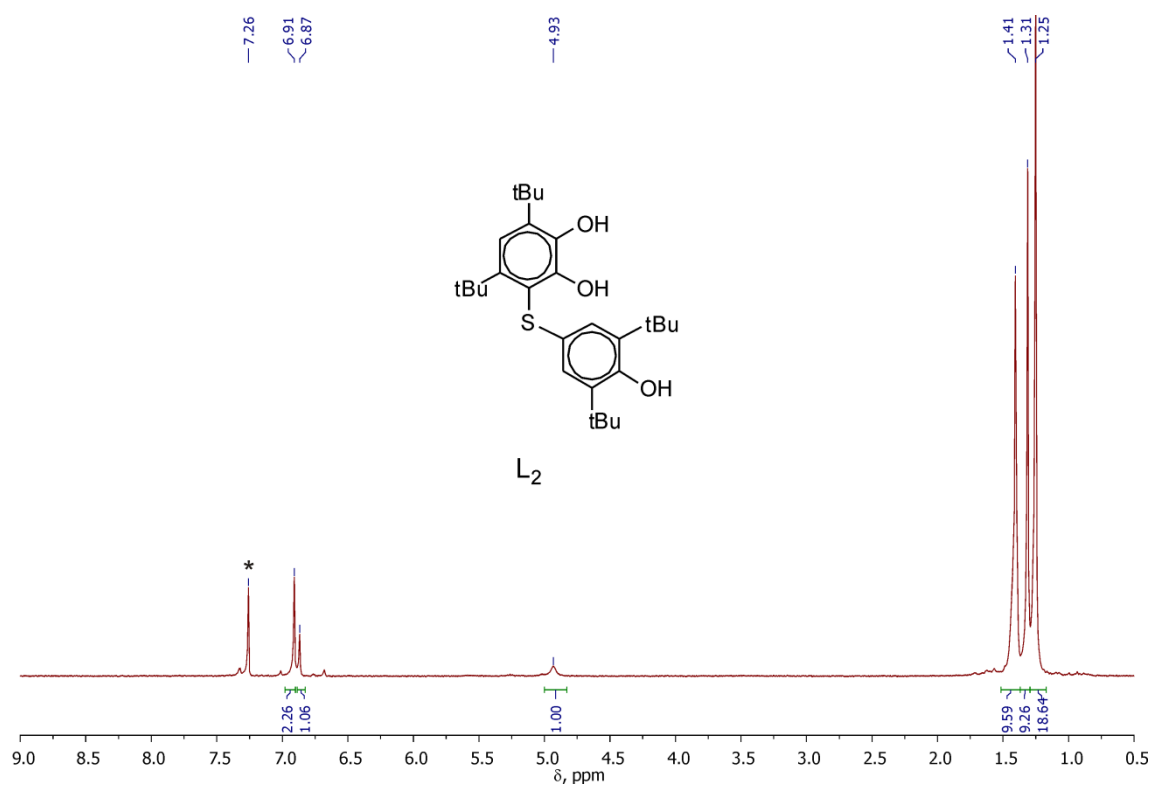


Figure S3. The ¹H NMR spectrum of **L₂** (CDCl₃, 200 MHz).

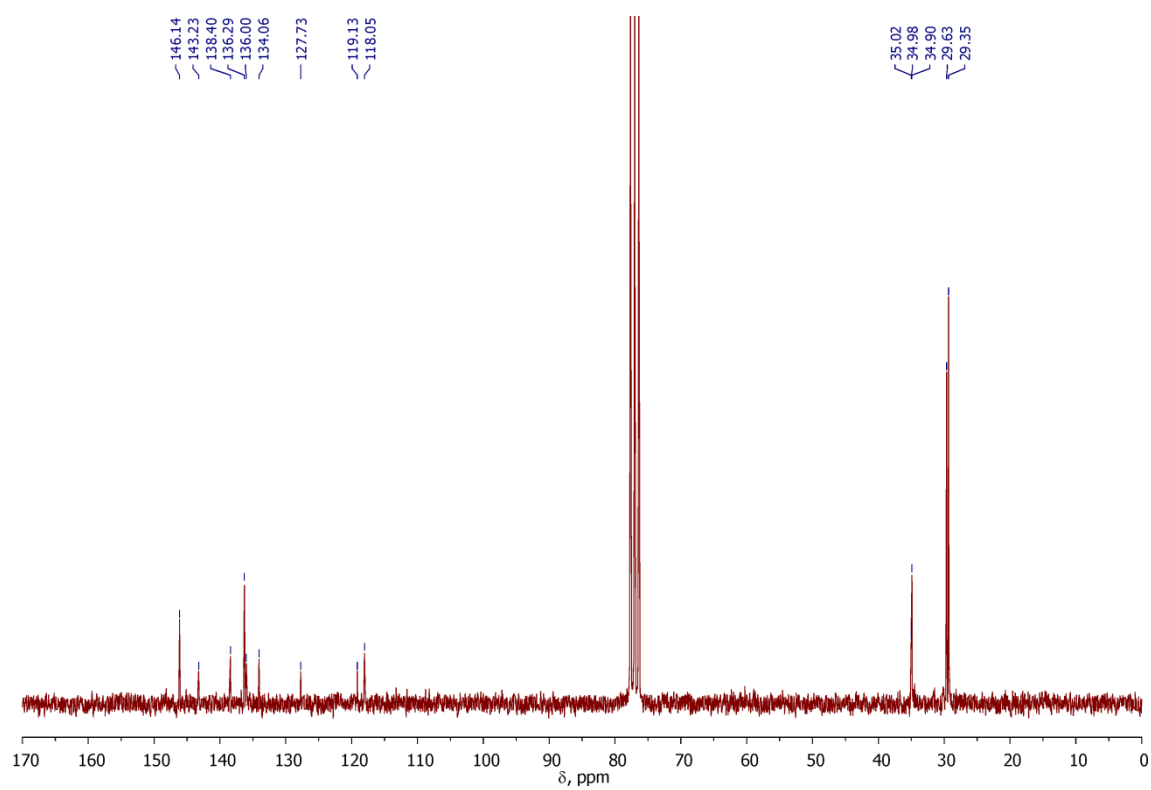


Figure S4. The ¹³C{¹H} NMR spectrum of **L₂** (CDCl₃, 50 MHz).

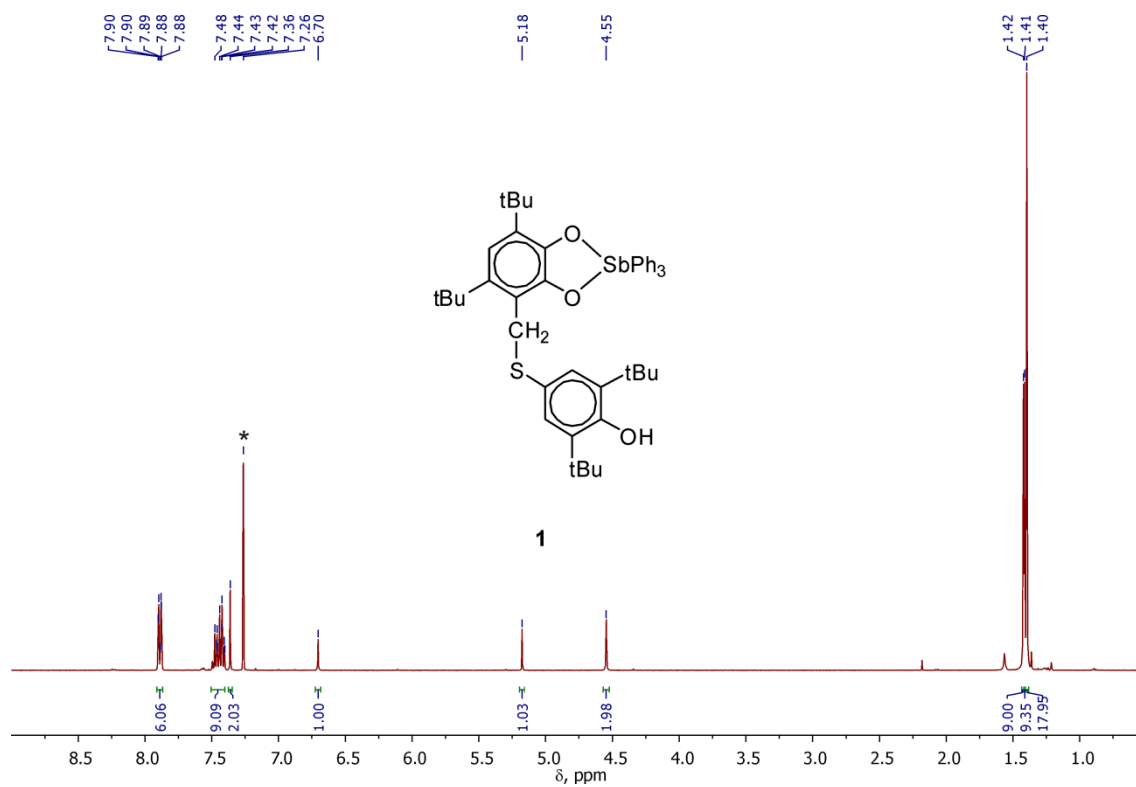


Figure S5. The ¹H NMR spectrum of **1** (CDCl₃, 400 MHz).

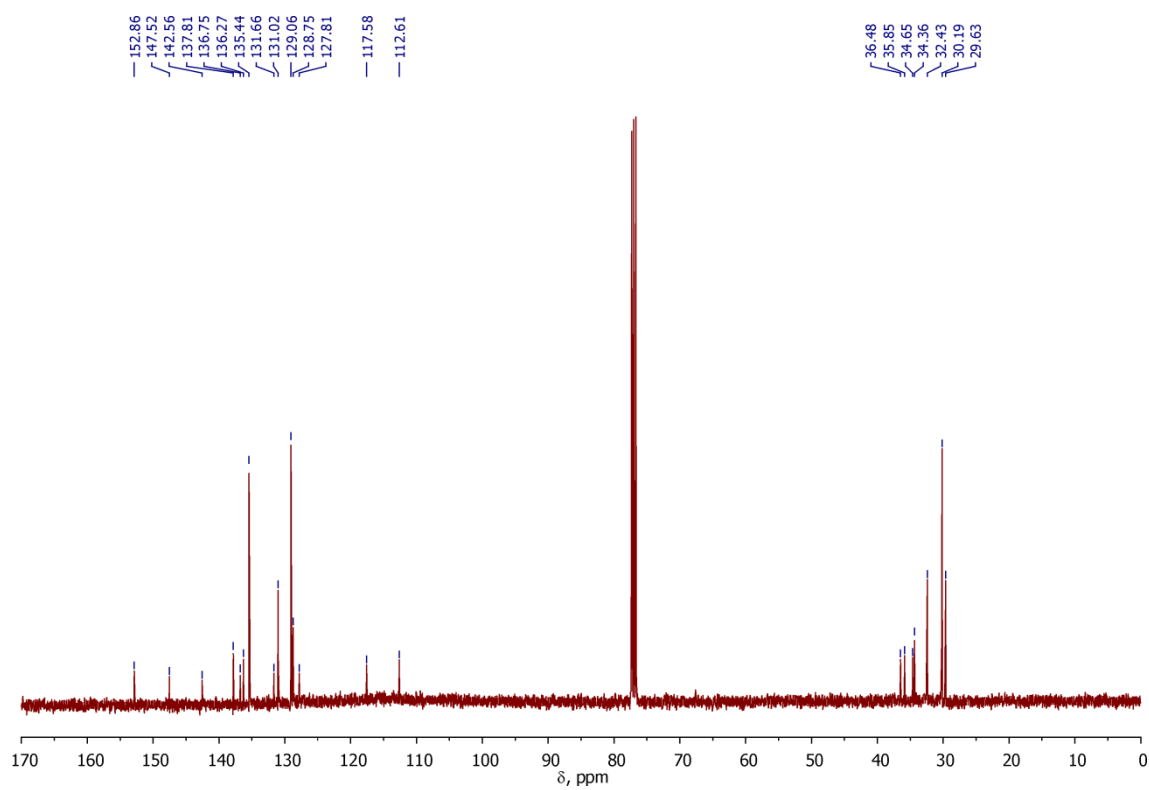


Figure S6. The ¹³C{¹H} NMR spectrum of **1** (CDCl₃, 100 MHz).

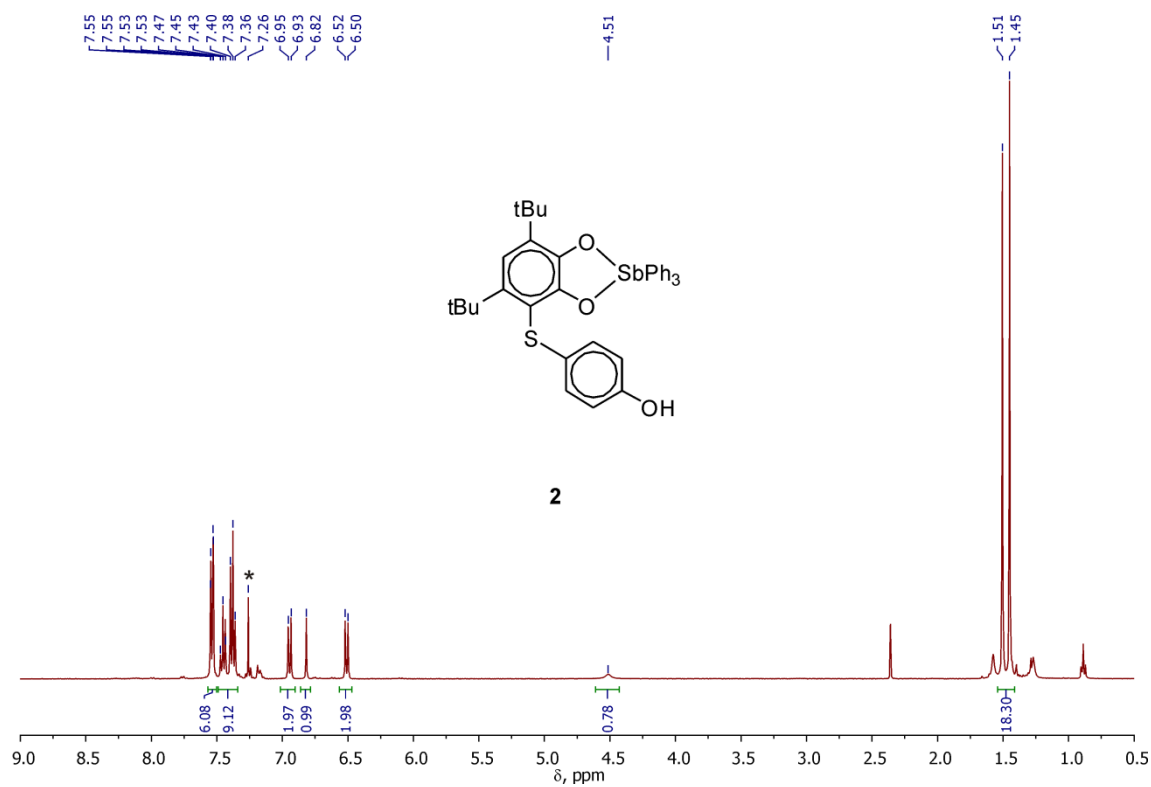


Figure S7. The ¹H NMR spectrum of **2** (CDCl₃, 400 MHz).

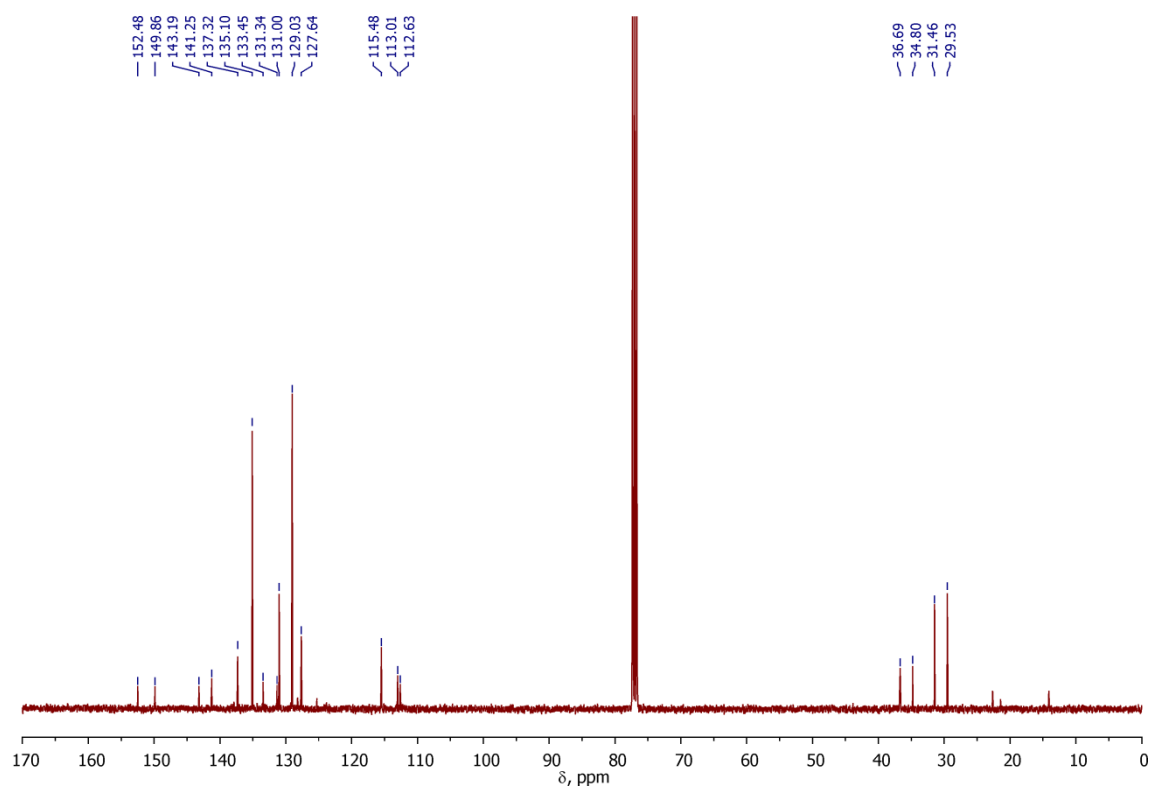


Figure S8. The ¹³C{¹H} NMR spectrum of **2** (CDCl₃, 100 MHz).

Table S1. Crystal data and structure refinement for **L1** and **1**.

	L1	1
Empirical formula	C ₂₉ H ₄₄ O ₃ S	C ₄₇ H ₅₇ O ₃ SSb
Formula weight	472.70	823.73
Temperature, K	100(2)	100(2)
Crystal system	Triclinic	Monoclinic
Space group	P-1	P2(1)/n
Unit cell dimensions		
a, Å	10.8864(5)	14.9452(8)
b, Å	11.5220(5)	11.5228(6)
c, Å	12.6870(5)	25.0515(14)
alpha, °	84.5080(10)	90
beta, °	69.6320(10)	90.9770(10)
gamma, °	63.2450(10)	90
Volume, Å ³	1328.61(10)	4313.5(4)
Z, Calculated density, Mg/m ³	2, 1.182	4, 1.268
Absorption coefficient mm ⁻¹	0.149	0.726
F(000)	516	1720
Crystal size, mm	0.420 x 0.350 x 0.320	1.000 x 0.710 x 0.600
Θ range, deg.	1.717 - 29.127	1.945 - 25.999
Limiting indices	-14 ≤ h ≤ 14 -15 ≤ k ≤ 15 -17 ≤ l ≤ 17	18 ≤ h ≤ 18 -14 ≤ k ≤ 14 -30 ≤ l ≤ 30
Reflections collected / unique	19531 / 7116 [R(int) = 0.0195]	36556 / 8456 [R(int) = 0.0230]
Completeness to Θ = 25.242°, %	100.0 %	99.7
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	7116 / 0 / 322	8456 / 0 / 485
Goodness-of-fit on F ²	1.030	1.050
Final R indices [I > 2σ(I)]	R ₁ = 0.0439, wR ₂ = 0.1128	R ₁ = 0.0281, wR ₂ = 0.0678
R indices (all data)	R ₁ = 0.0506, wR ₂ = 0.1204	R ₁ = 0.0310, wR ₂ = 0.0692
Larg.diff. peak and hole, e.Å ⁻³	0.472 and -0.212	0.918 and -0.298

Table S2. The selected bond lengths for **L₁**.

bond	distance, Å
Sb(1)-O(1)	2.0402(13)
Sb(1)-O(2)	2.0256(13)
Sb(1)-C(30)	2.1328(19)
Sb(1)-C(36)	2.1383(19)
Sb(1)-C(42)	2.1054(19)
O(1)-C(1)	1.358(2)
O(2)-C(2)	1.366(2)
O(3)-C(19)	1.376(2)
O(3)-H(1)	0.73(3)
S(1)-C(7)	1.8365(18)
S(1)-C(16)	1.7772(19)
C(1)-C(2)	1.398(3)
C(1)-C(6)	1.393(3)
C(2)-C(3)	1.392(3)
C(3)-C(4)	1.415(3)
C(4)-C(5)	1.400(3)
C(5)-C(6)	1.401(3)
C(16)-C(17)	1.385(3)
C(16)-C(21)	1.389(3)
C(17)-C(18)	1.394(3)
C(18)-C(19)	1.408(3)
C(19)-C(20)	1.390(3).
C(20)-C(21)	

Table S3. The selected bond lengths for **1**.

bond	distance, Å
Sb(1)-O(1)	2.0402(13)
Sb(1)-O(2)	2.0256(13)
Sb(1)-C(30)	2.1328(19)
Sb(1)-C(36)	2.1383(19)
Sb(1)-C(42)	2.1054(19)
O(1)-C(1)	1.358(2)
O(2)-C(2)	1.366(2)
O(3)-C(19)	1.376(2)
O(3)-H(1)	0.73(3)
S(1)-C(7)	1.8365(18)
S(1)-C(16)	1.7772(19)
C(1)-C(2)	1.398(3)
C(1)-C(6)	1.393(3)
C(2)-C(3)	1.392(3)
C(3)-C(4)	1.415(3)
C(4)-C(5)	1.400(3)
C(5)-C(6)	1.401(3)
C(16)-C(17)	1.385(3)
C(16)-C(21)	1.389(3)
C(17)-C(18)	1.394(3)
C(18)-C(19)	1.413(3)
C(19)-C(20)	1.408(3)
C(20)-C(21)	1.390(3)

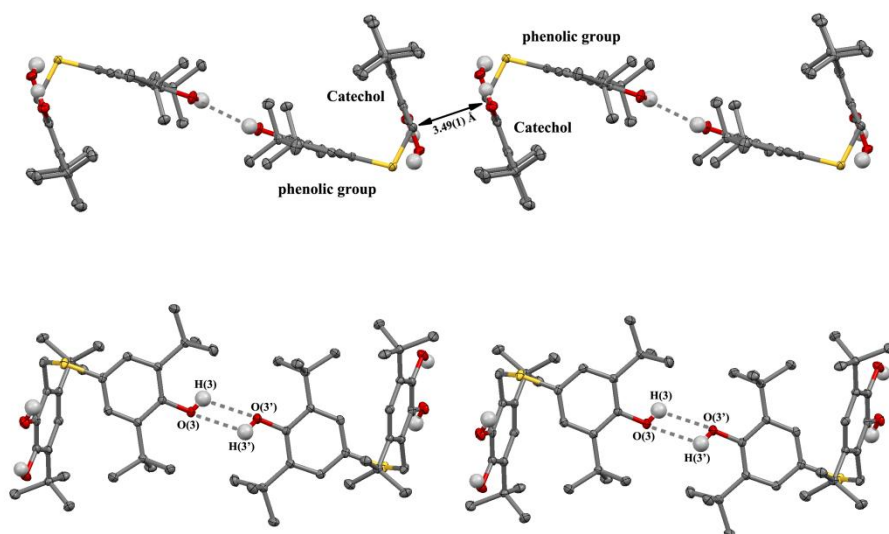


Figure S9. The intermolecular hydrogen bonds in crystals of **L₁**.

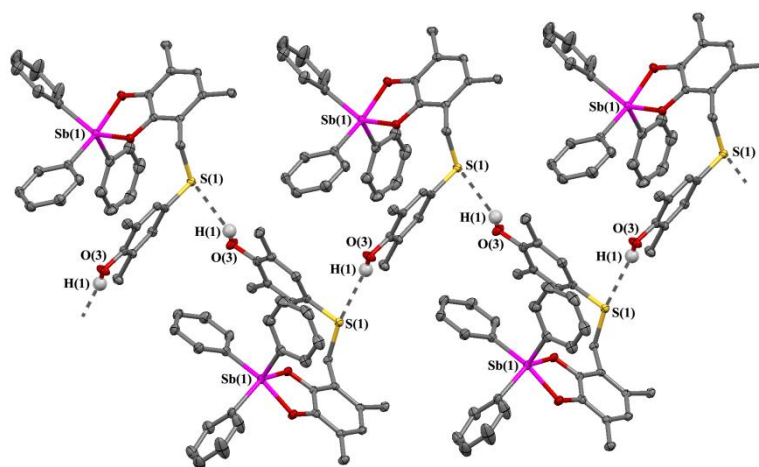


Figure S10. The order of complex **1** molecules in crystal cell with the indication of intermolecular hydrogen bonding. The methyl groups of tert-butyls and hydrogen atoms excepting atoms H(1) are omitted for clarity. The ellipsoids of 50% probability.

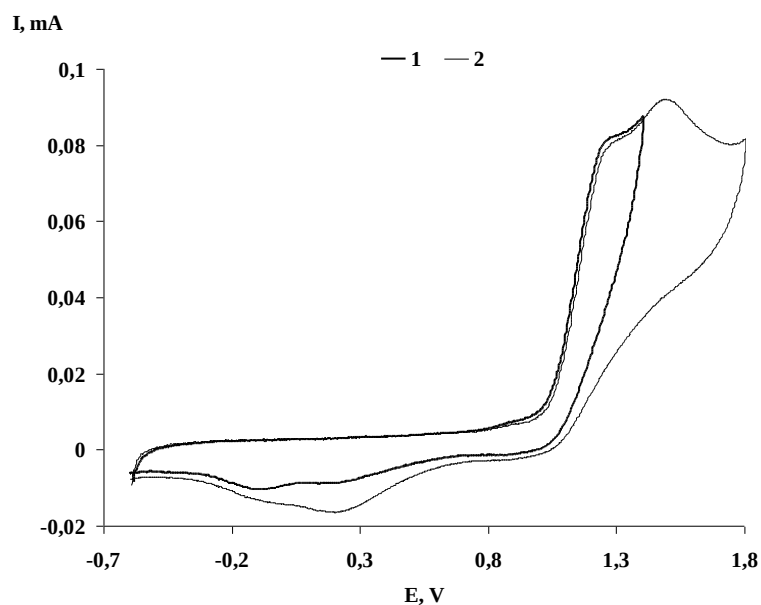


Figure S11. The CVs of compound **L**₁ (in the potential switch from -0.6 to 1.4 V – curve 1; in the potential switch from -0.6 to 1.8 V – curve 2) (CH₂Cl₂, C = 3 mM, 0.15 M TBAP, scan rate 200 mV·s⁻¹).

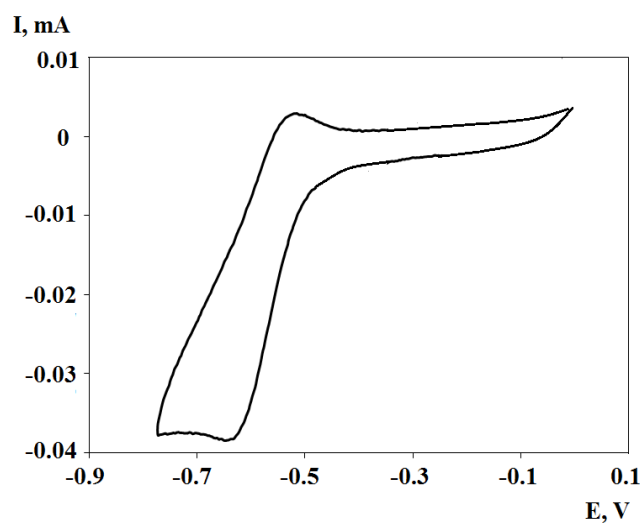


Figure S12. The CV of the electrolysis products of compound **L**₁ in the potential switch from 0.0 to - 0.78 V (MeCN, 90 min, E = 1.2 V, C = 2 mM, 0.15 M TBAP, scan rate 200 mV·s⁻¹).

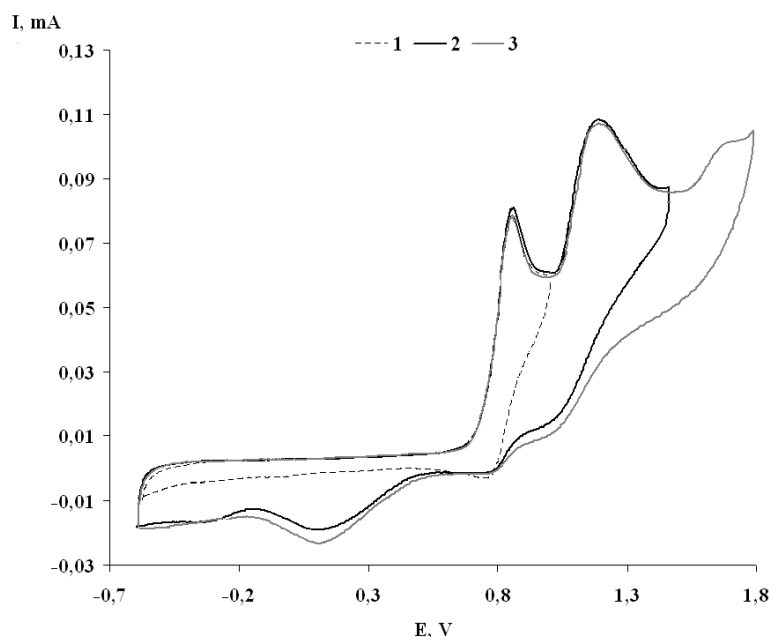


Figure S13. The CVs of compound **1** (in the potential switch from -0.5 to 1.0 V – curve 1; in the potential switch from -0.5 to 1.5 V – curve 2; in the potential switch from -0.5 to 1.8 V – curve 3) (CH_3CN , $C = 3 \text{ mM}$, 0.15 M TBAP , scan rate $200 \text{ mV}\cdot\text{s}^{-1}$).

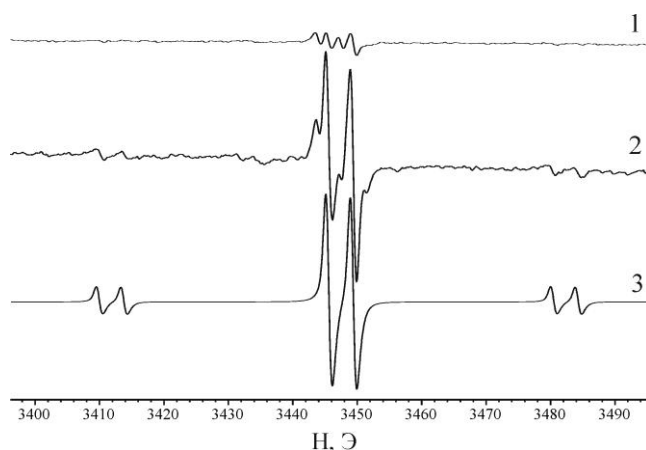


Figure S14. The EPR spectrum of the mixture “**L**₁ + PbO_2 ” in toluene immediately after mixing the reagents (spectrum 1), after heating at 60°C for 15 minutes (spectrum 2), and simulated EPR spectrum (WinEPR SimFonia 1.25) with parameters $g_i = 2.0009$, $a_i(^1\text{H}) = 3.85 \text{ G}$, $a_i(^{207}\text{Pb}) = 70.5 \text{ G}$ (spectrum 3).