Synthesis and structures of lead(II) complexes with hydroxy-substituted *closo*-decaborate anions

SUPPORTING INFORMATION

Table S1. Crystal data and structure refinement for compounds 1–3.

Compound	**1**·CH_3CN	**2**·0.5bipy·CH_3CN	**3**
Empirical formula	$C_{22}H_{29}B_{10}N_5OPb$	$C_{31}H_{41}B_{10}N_6O_3Pb$	$C_{17}H_{32}B_{10}N_2O_3Pb$
Formula weight	694.79	860.99	627.73
Temperature/K	100.00	100.00	100.00
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	P-1	$P2_1/c$
a/Å	12.196(4)	9.332(3)	16.444(4)
b/Å	12.397(5)	12.312(4)	9.9311(17)
c/Å	19.739(4)	16.170(4)	15.580(6)
α/°	90	98.931(12)	90
β/°	106.015(12)	95.893(10)	106.575(16)
γ/°	90	97.553(13)	90
Volume/Å^3	2868.5(15)	1805.0(10)	2438.5(12)
Z	4	2	4
ϱ_{calc}g/cm^3	1.609	1.584	1.710
μ/mm^{-1}	5.908	4.716	6.942
F(000)	1344.0	850.0	1216.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.924 to 57.996	2.57 to 54.996	4.848 to 57.298
Index ranges	-12 ≤ h ≤ 16, -16 ≤ k ≤ 13, -26 ≤ l ≤ 26	-12 ≤ h ≤ 11, -15 ≤ k ≤ 13, -20 ≤ l ≤ 20	-22 ≤ h ≤ 22, -13 ≤ k ≤ 13, -20 ≤ l ≤ 20
Reflections collected	14166	13308	23410
Independent reflections	7477 R_{int} = 0.0365, R_{sigma} = 0.0665	8109 R_{int} = 0.0354, R_{sigma} = 0.0747	6250 R_{int} = 0.0331, R_{sigma} = 0.0318
Data/restraints/parameters	7477/3/302	8109/0/444	6250/3/301
Goodness-of-fit on F^2	1.057	1.038	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.1188	R_1 = 0.0424, wR_2 = 0.0871	R_1 = 0.0215, wR_2 = 0.0399
Final R indexes [all data]	R_1 = 0.0761, wR_2 = 0.1274	R_1 = 0.0547, wR_2 = 0.0913	R_1 = 0.0283, wR_2 = 0.0415

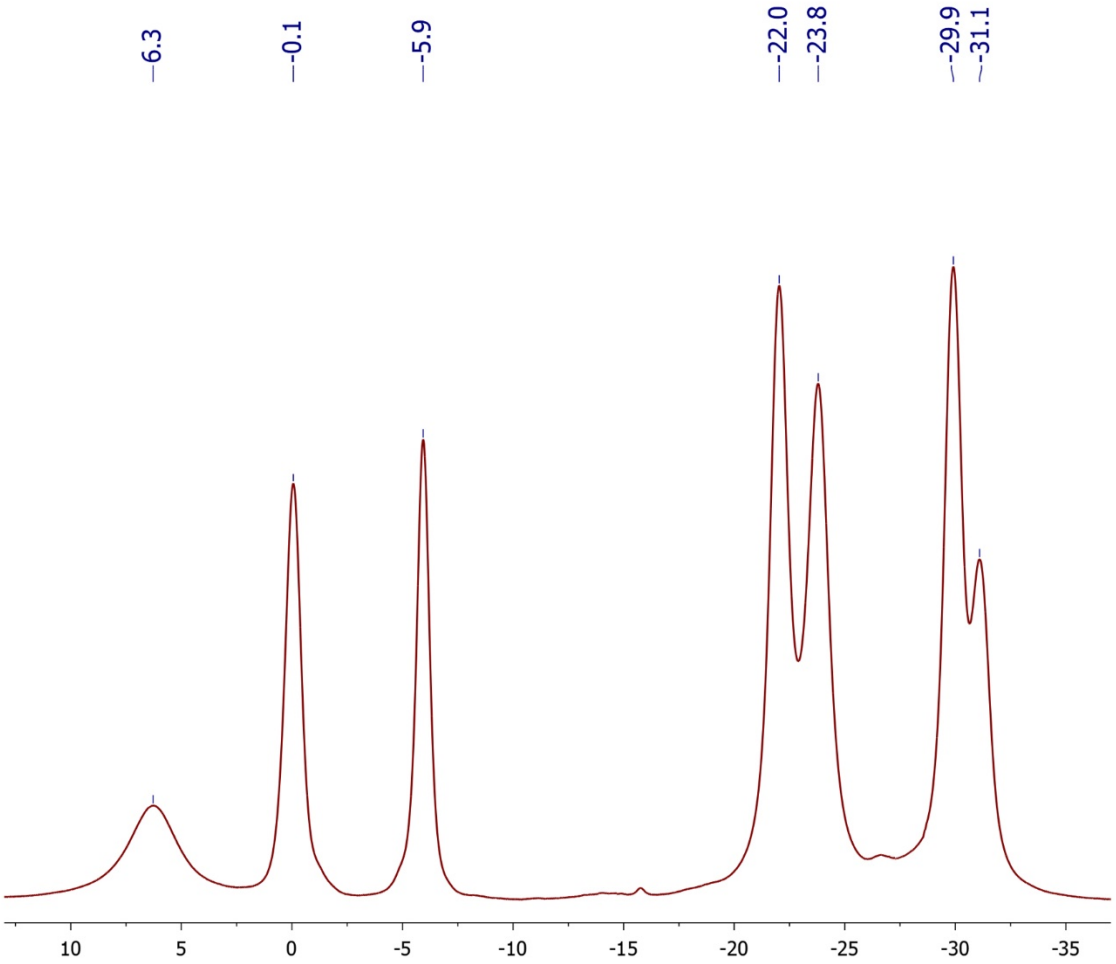

Figure S1. ^{11}B {^{1}H} NMR spectrum of $K[B_{10}H_9OC_5H_{10}]$ in CD_3CN

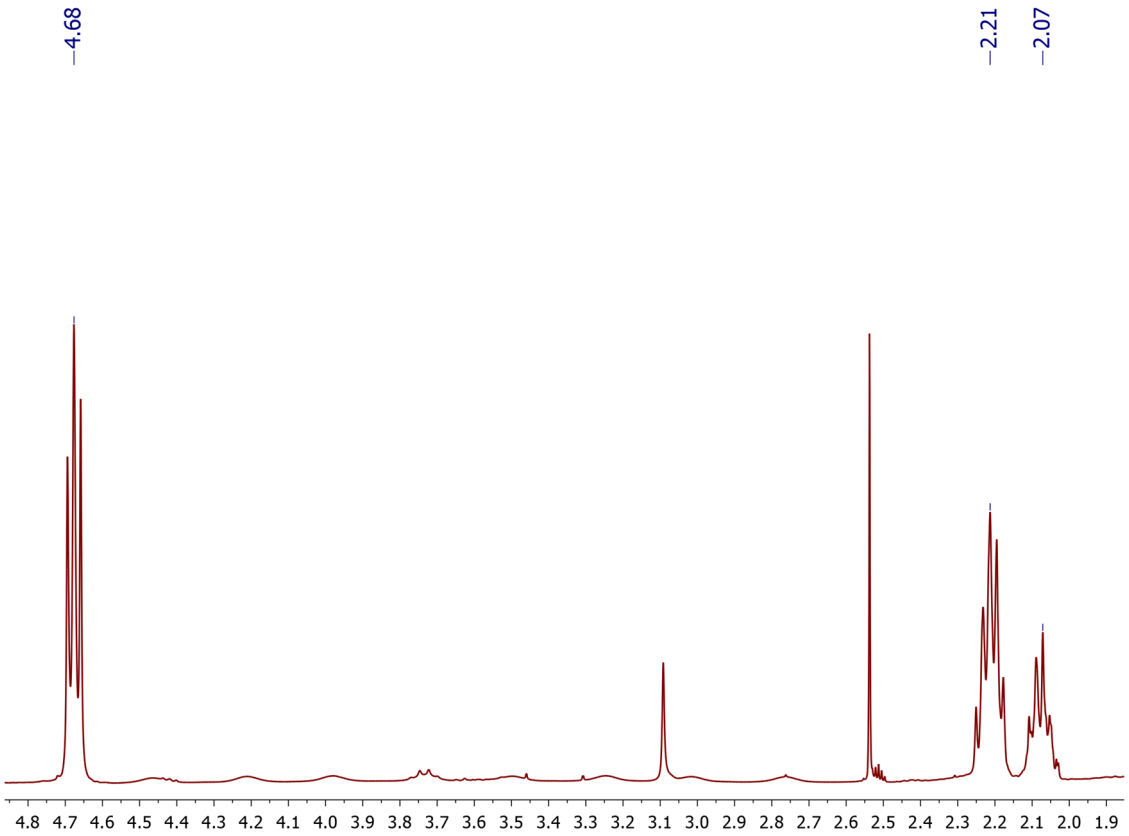

Figure S2. ^{1}H NMR spectrum of $K[B_{10}H_9OC_5H_{10}]$ in CD_3CN

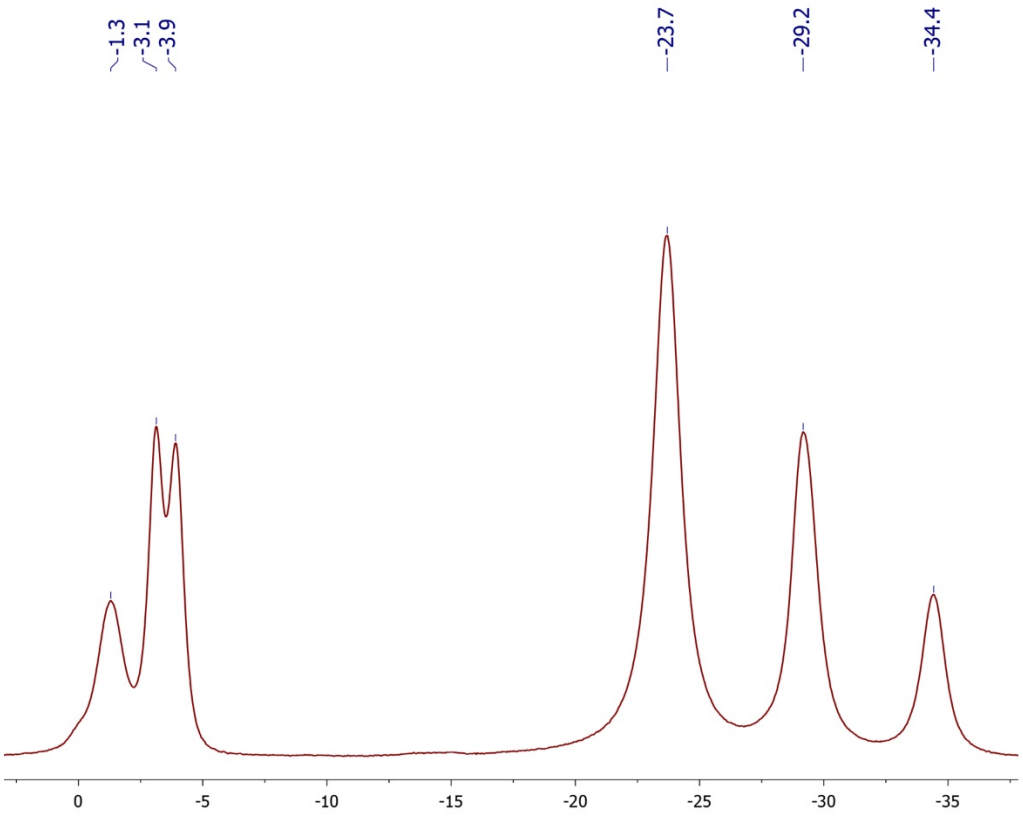

Figure S3. ^{11}B {^{1}H} NMR spectrum of $Cs_2[B_{10}H_9OCH_2CH_2CH_2CH_2CH_2OCH_2CH_2OH]$ in D_2O

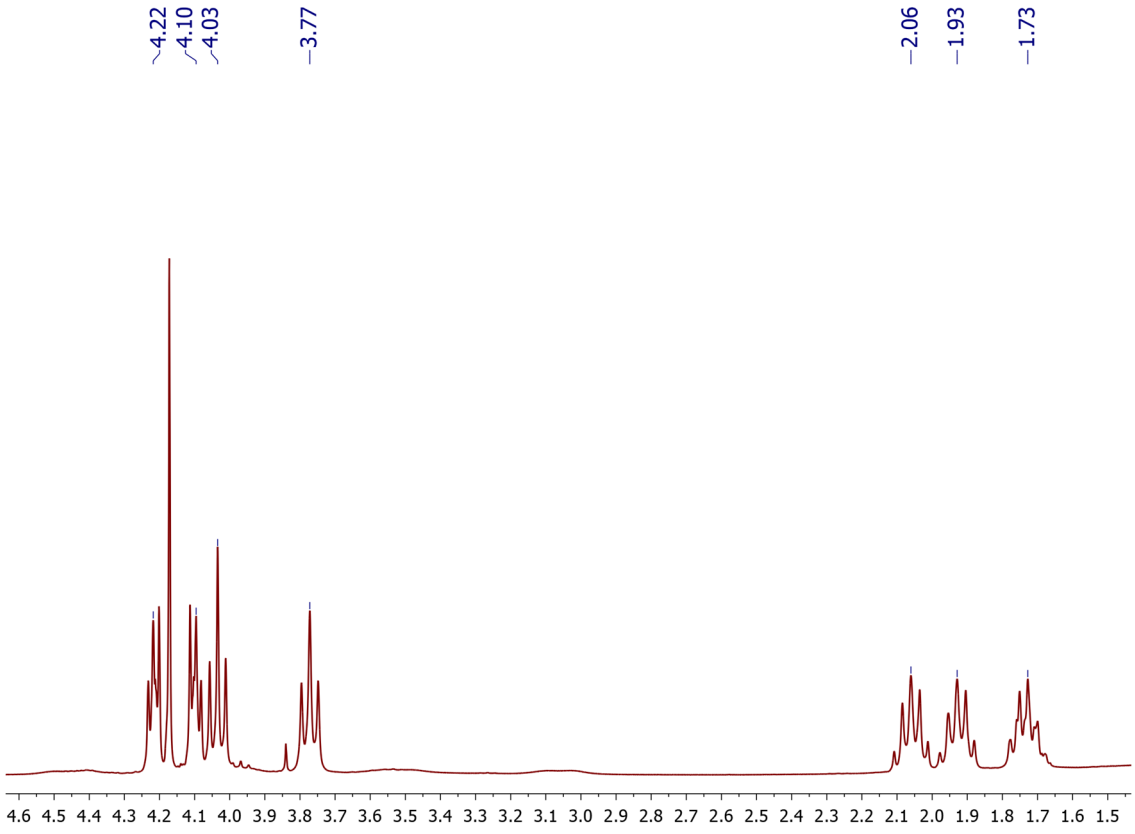

Figure S4. ^{1}H NMR spectrum of $Cs_2[B_{10}H_9OCH_2CH_2CH_2CH_2CH_2OCH_2CH_2OH]$ in D_2O

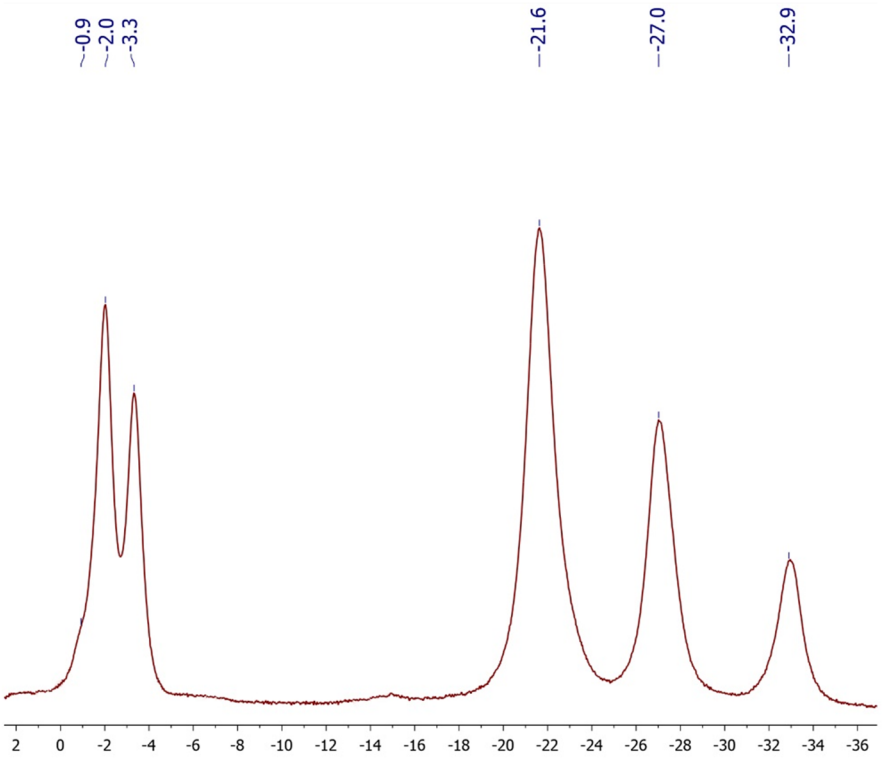

Figure S5. ^{11}B {^{1}H} NMR spectrum of [Pb(bipy)$_2$[$B_{10}H_9OH$]] in D_2O

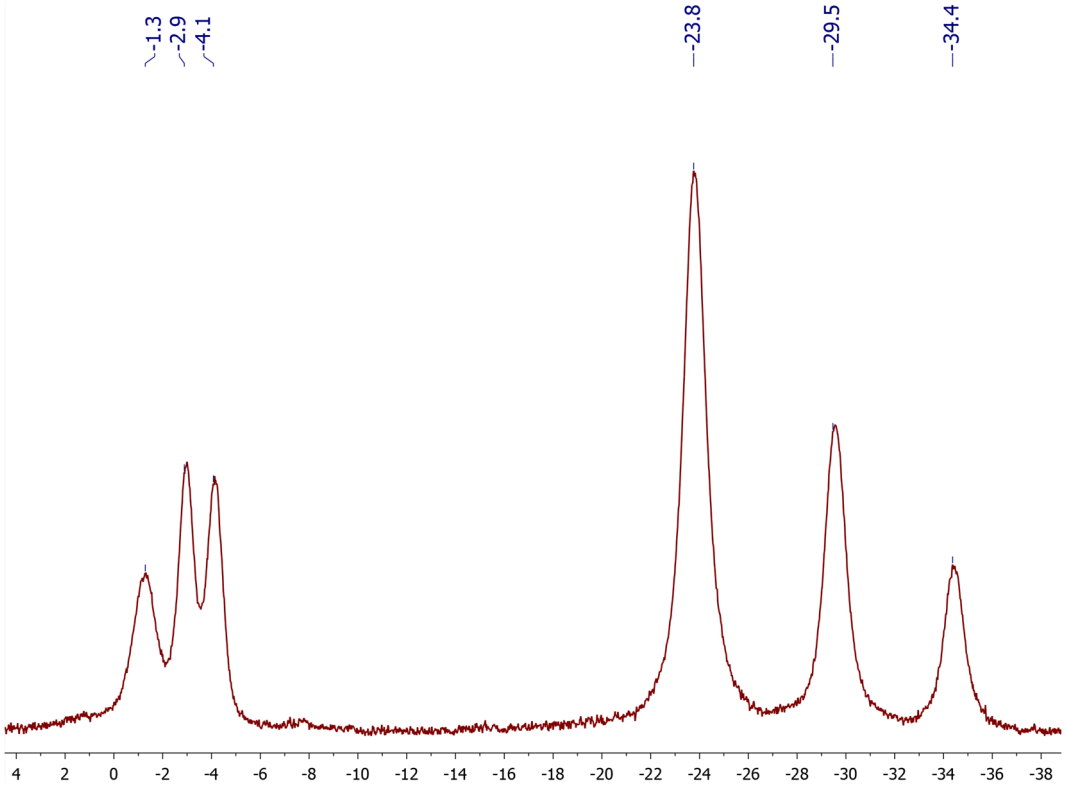

Figure S6. ^{11}B {^{1}H} NMR spectrum of [Pb(bipy)$_2$[$B_{10}H_9O(CH_2)_2O(CH_2)_2OH$]] in D_2O

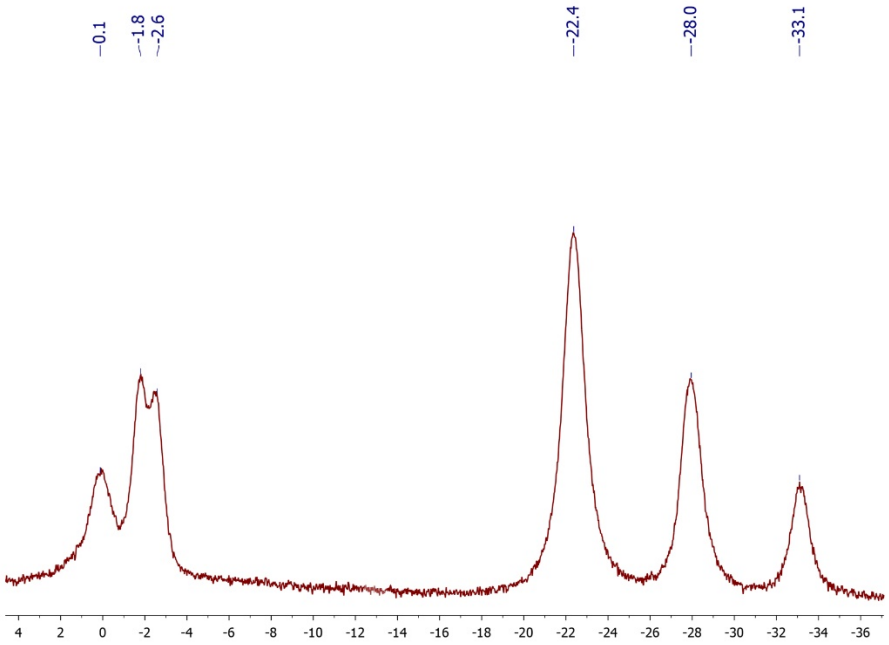

Figure S7. ^{11}B {^{1}H} NMR spectrum of $[Pb(bipy)_2[B_{10}H_9O(CH_2)_5O(CH_2)_2OH]]_n$ in D_2O