Phosphido-Bis(Borane) Complexes of the Alkaline Earth Metals

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SUPPORTING INFORMATION

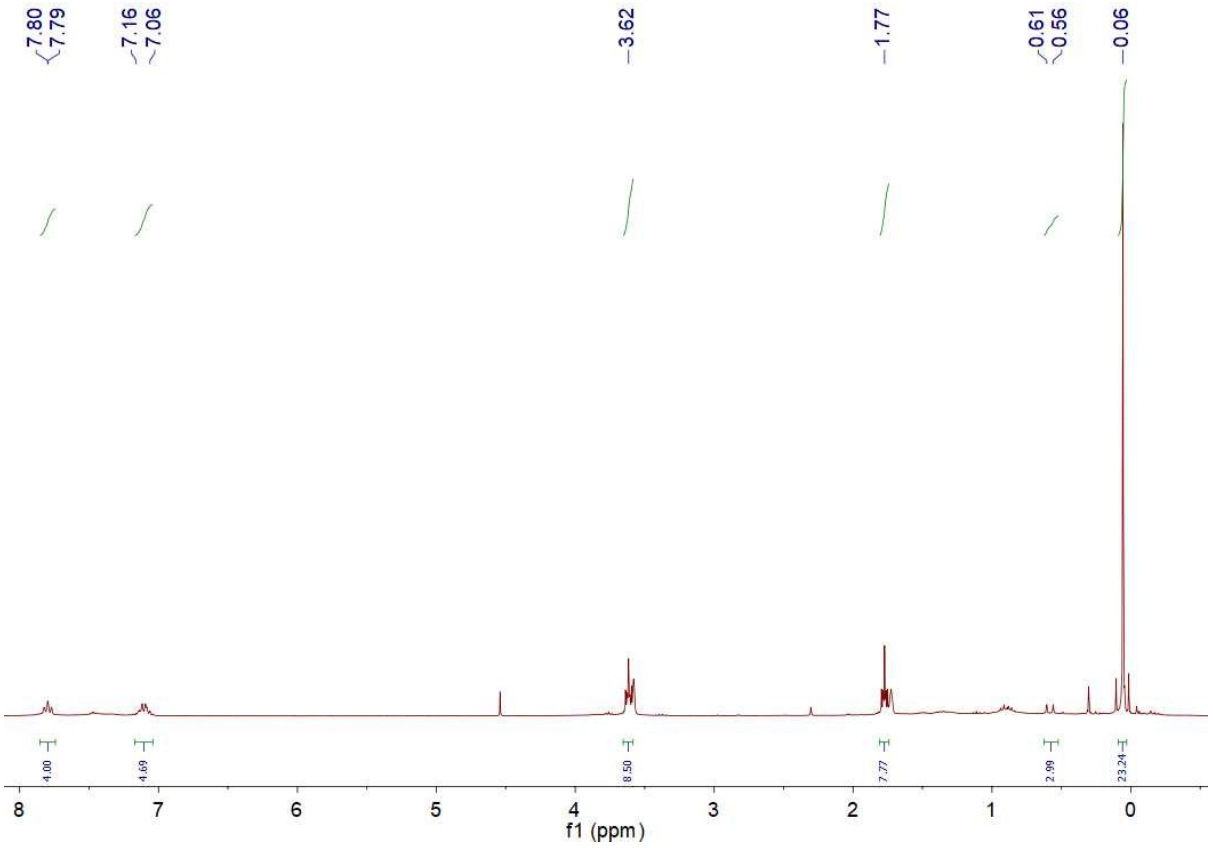

Figure S1. ^{1}H NMR spectrum of **2a** in d_8-THF.

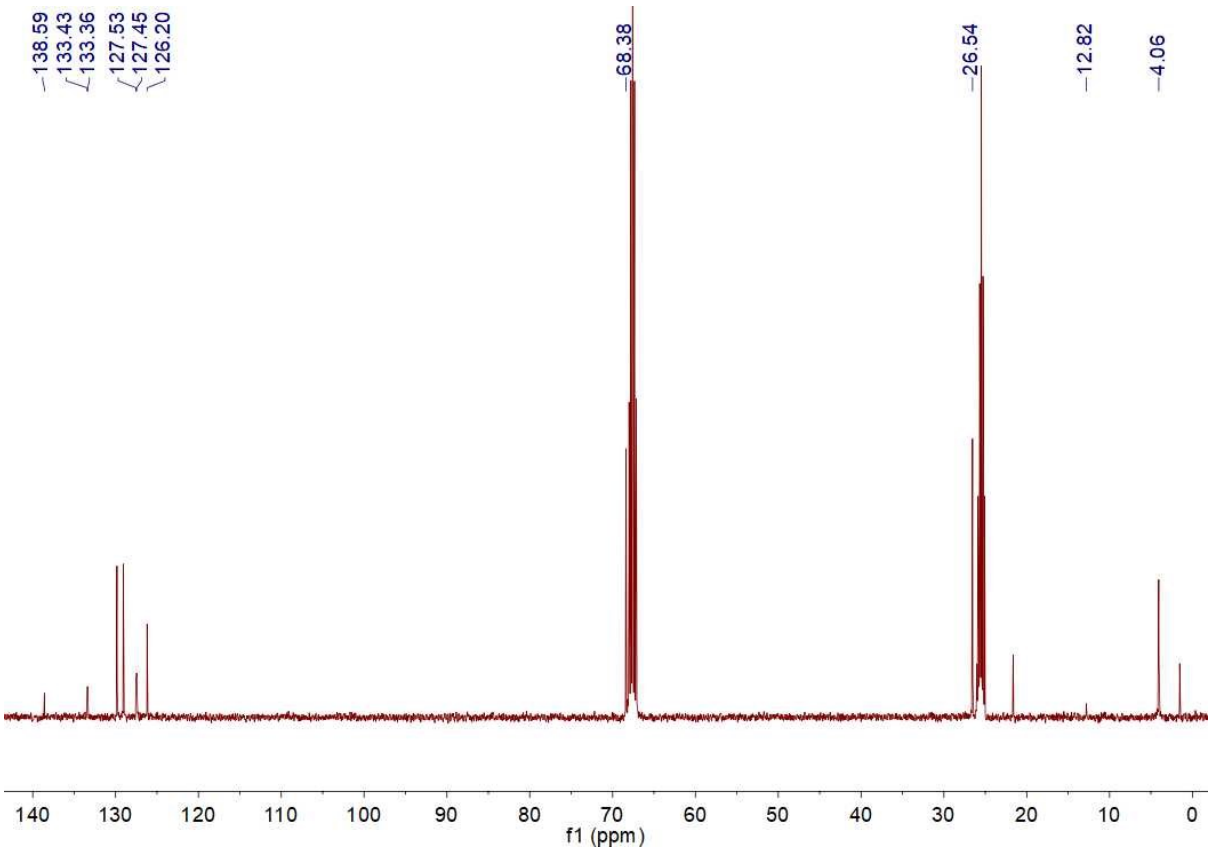

Figure S2. ^{13}C{^{1}H} NMR spectrum of **2a** in d_8-THF.

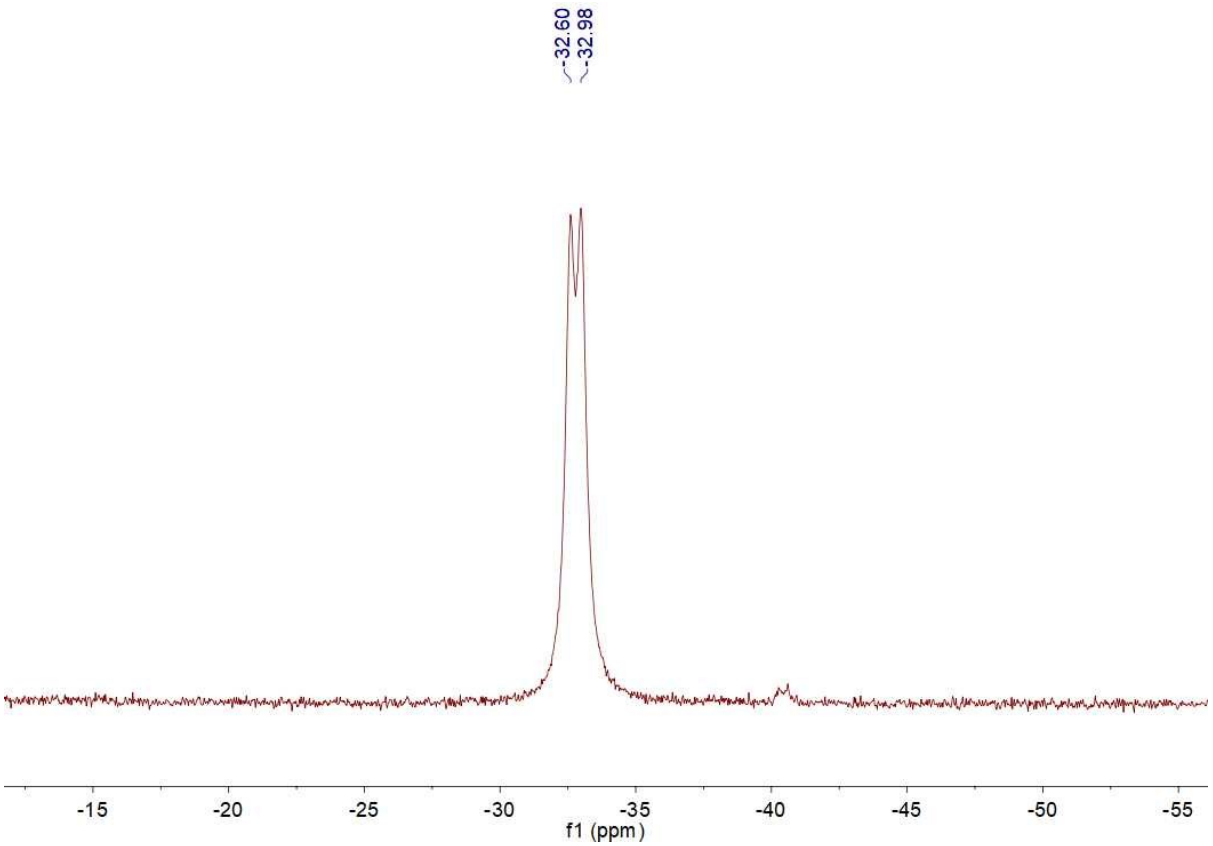

Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum of **2a** in d_8-THF.

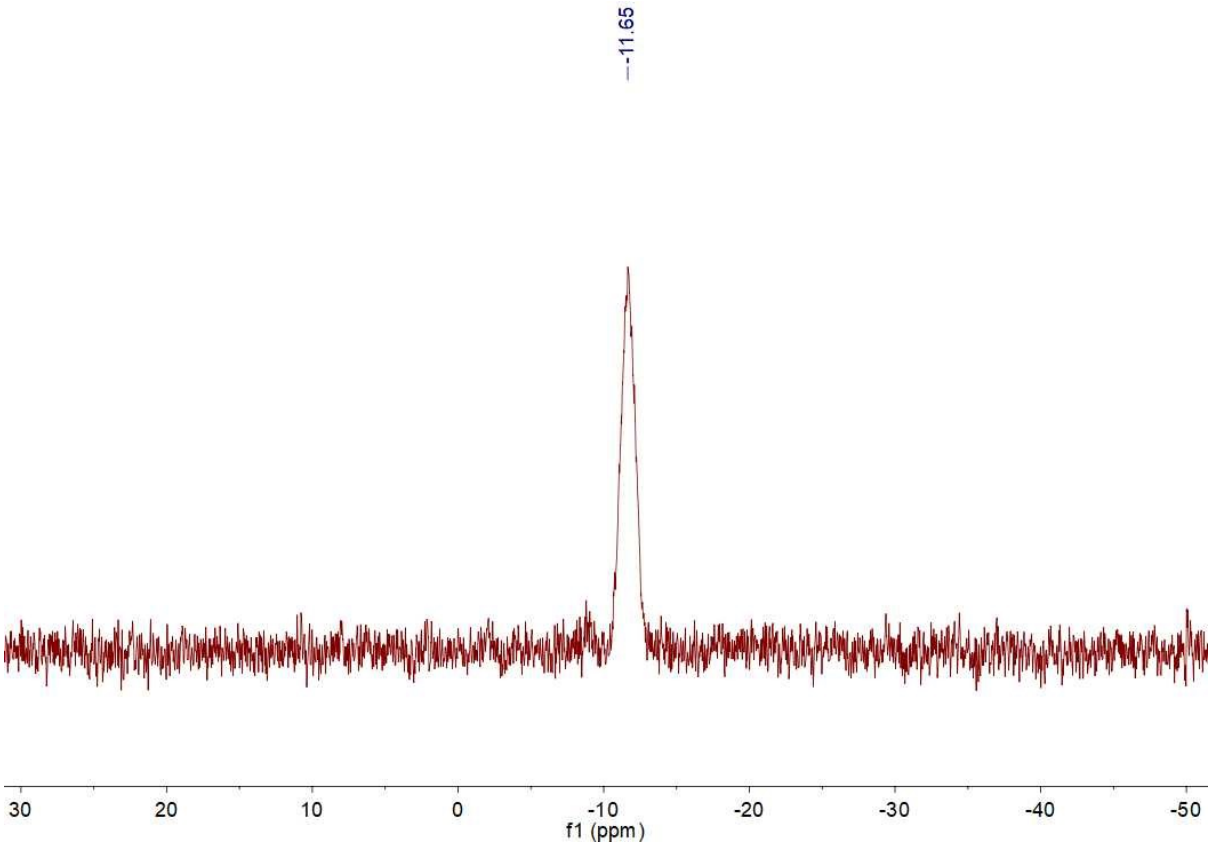

Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum of **2a** in d_8-THF.

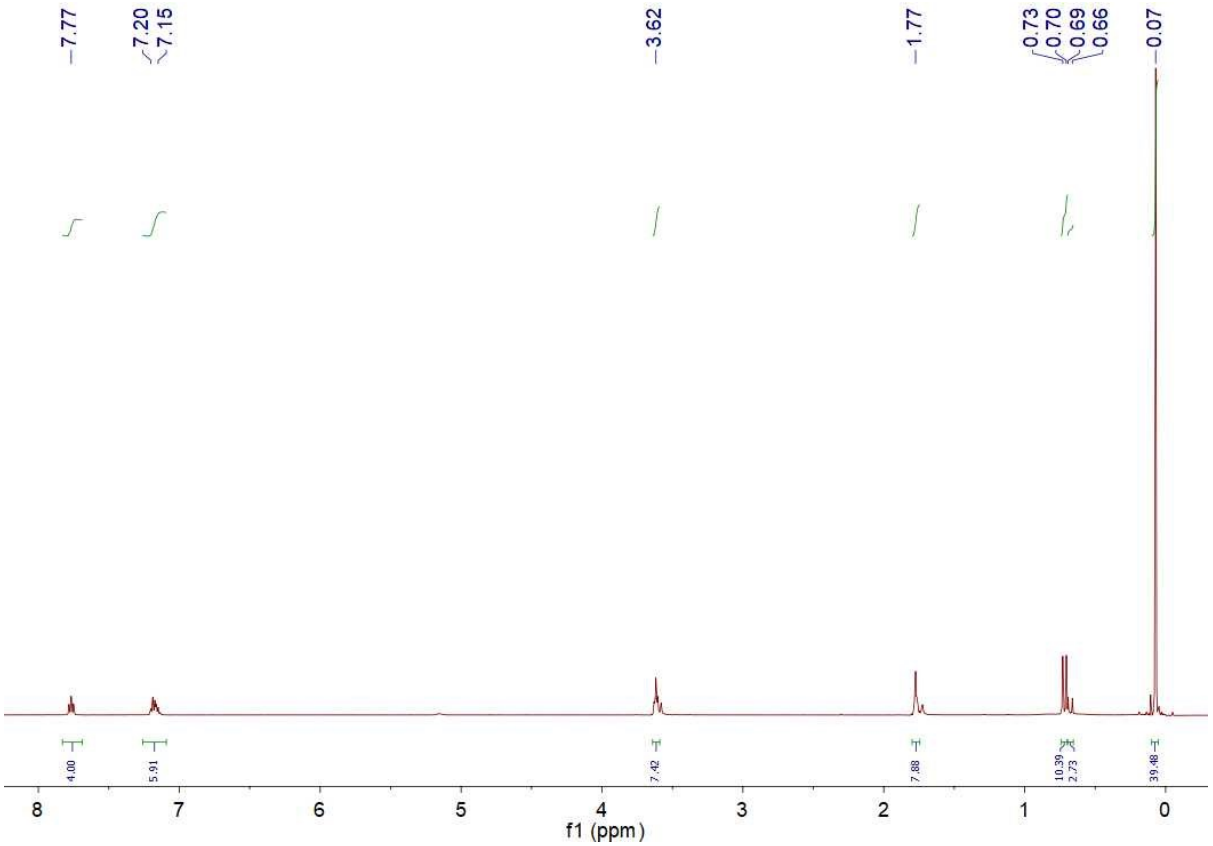

Figure S5. $^{1}H\{^{11}B\}$ NMR spectrum of **3** in d_8-THF.

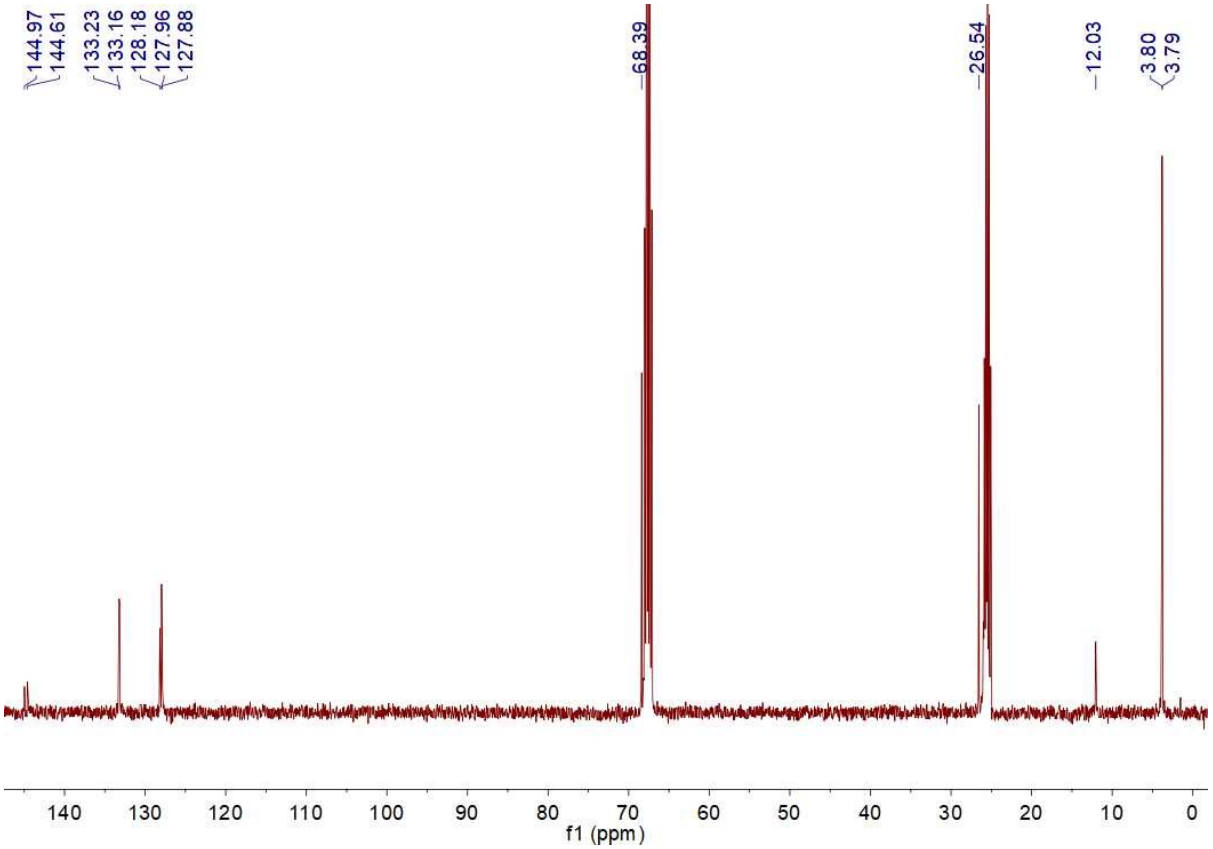

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in d_8-THF.

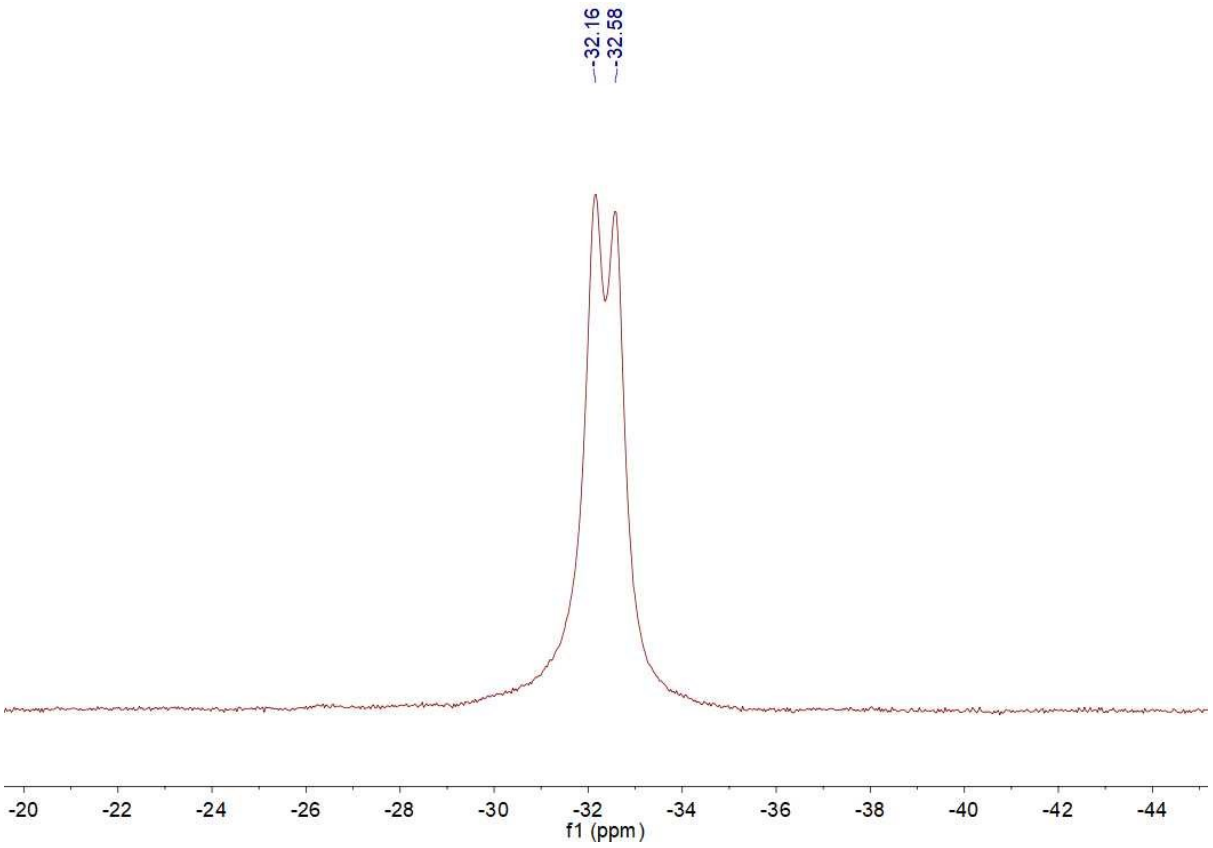

Figure S7. $^{11}B\{^{1}H\}$ NMR spectrum of **3** in d_8-THF.

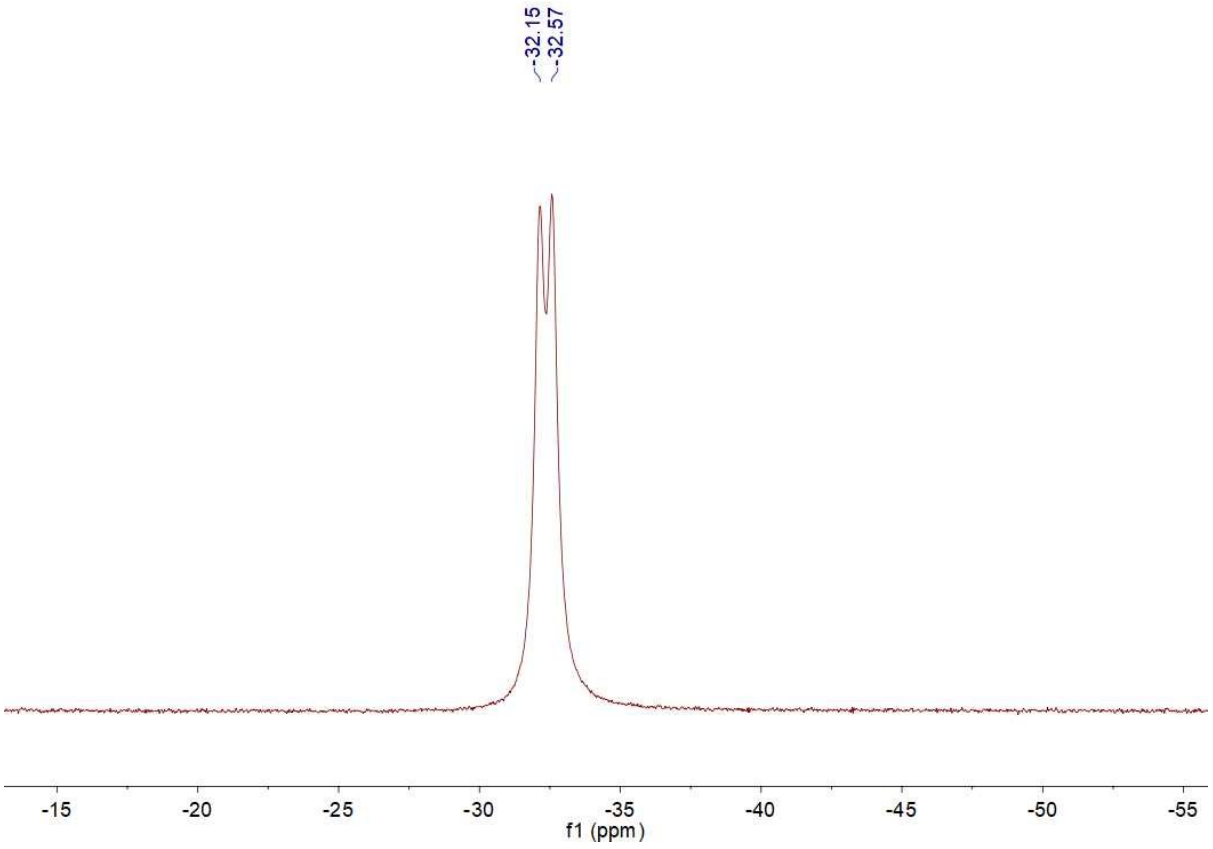

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in d_8-THF.

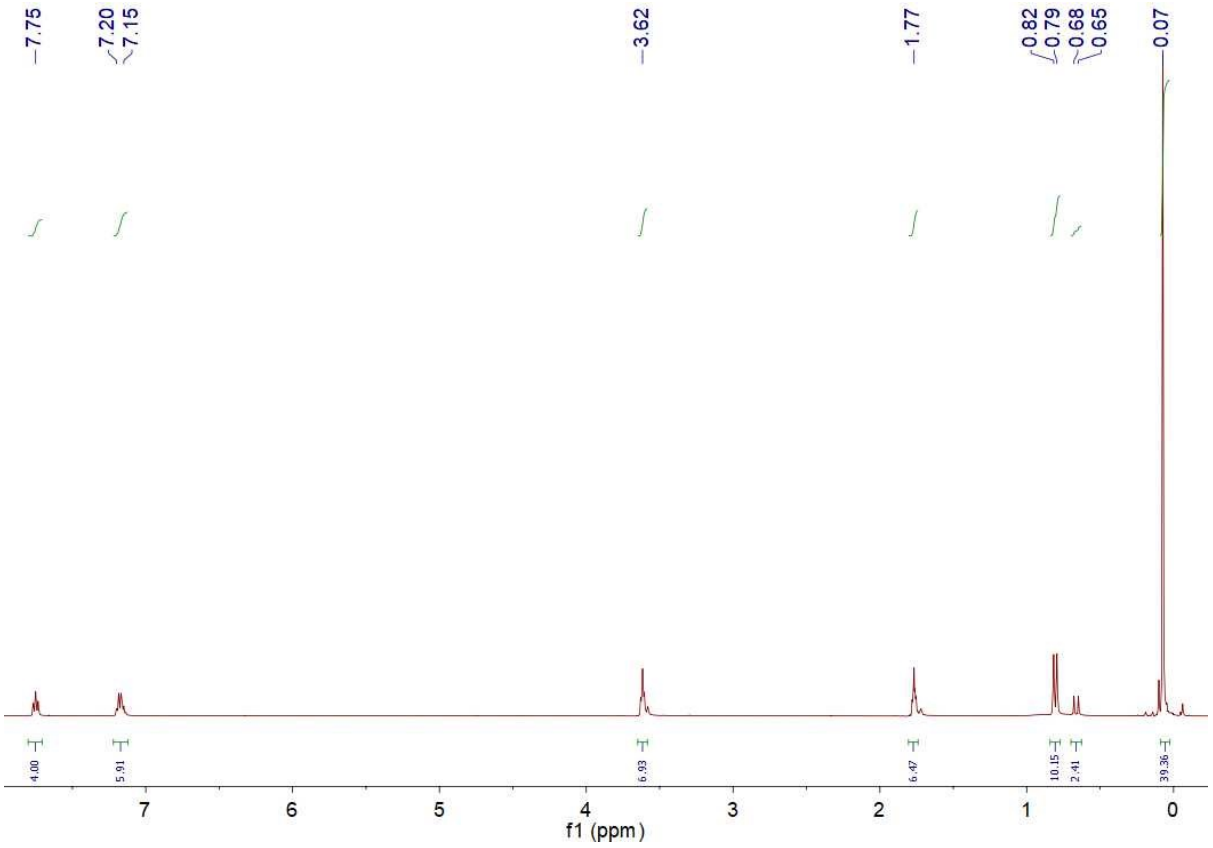

Figure S9. $^{1}H\{^{11}B\}$ NMR spectrum of **4** in d_8-THF.

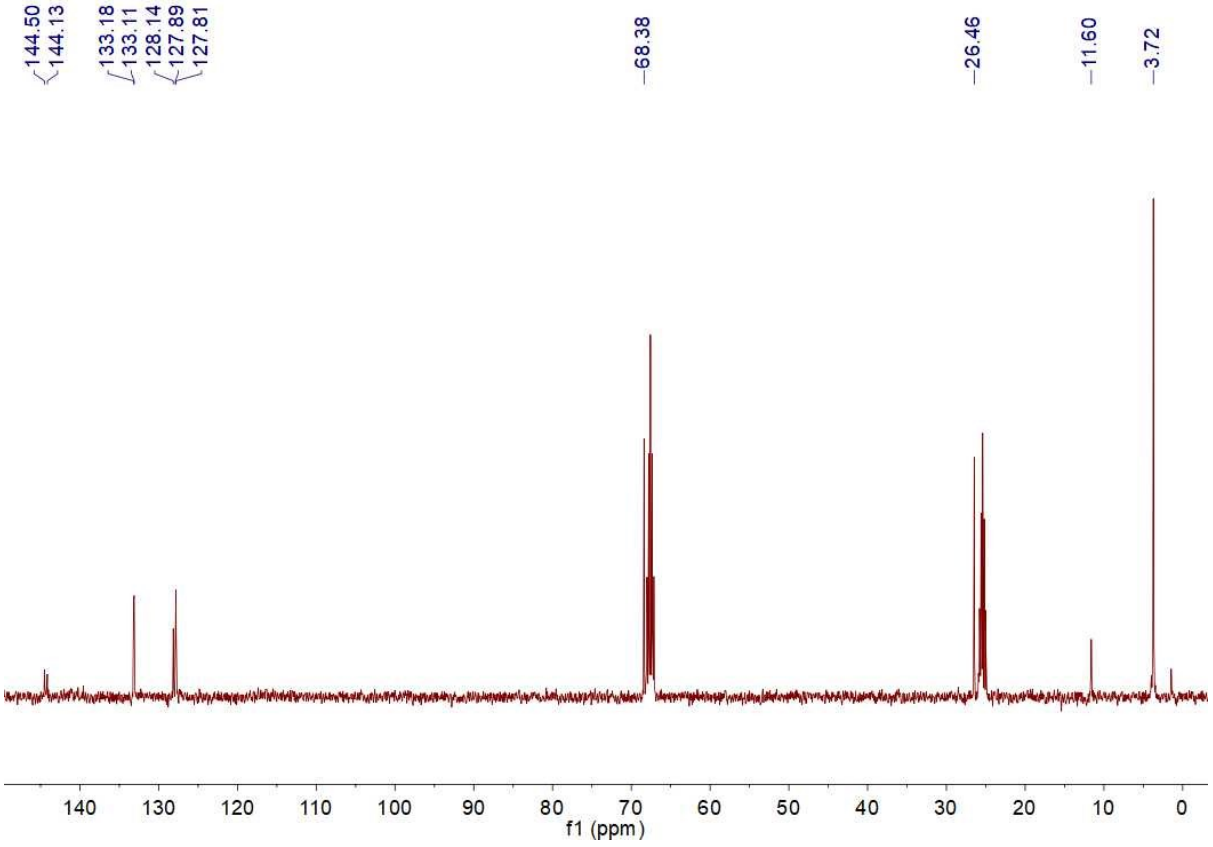

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in d_8-THF.

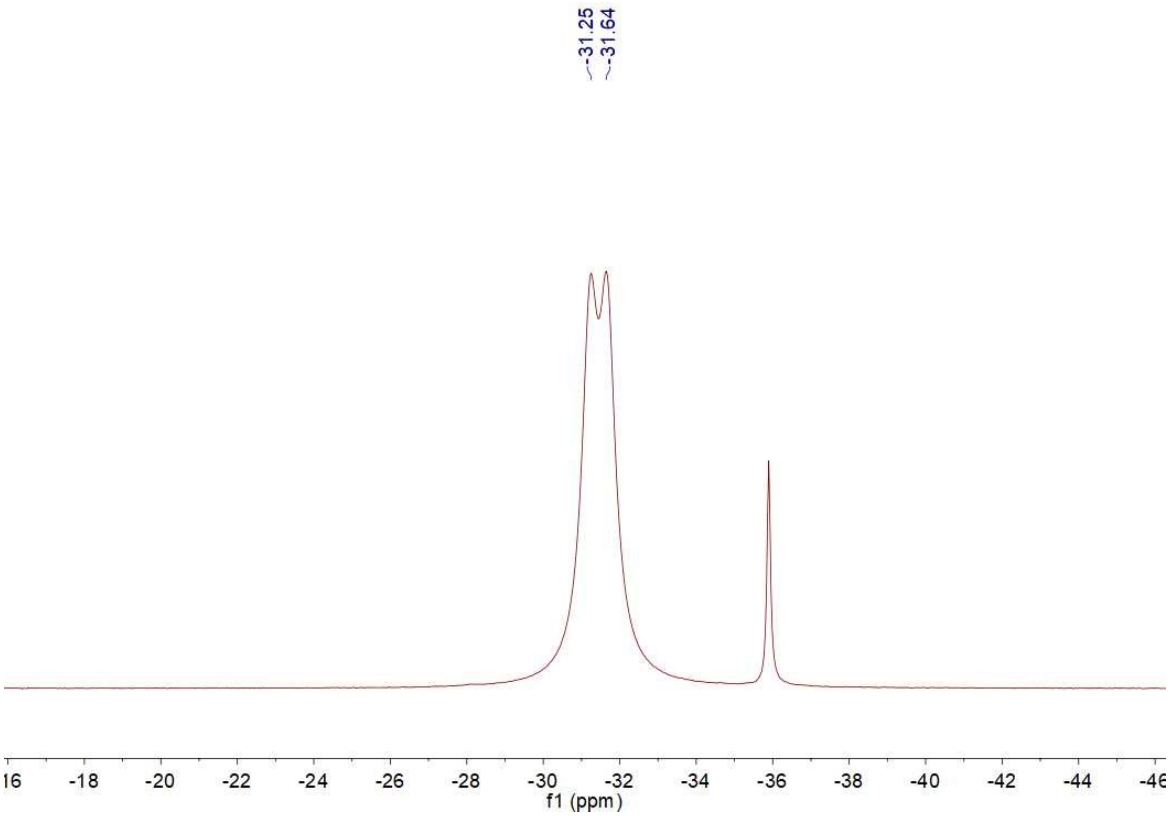

Figure S11. $^{11}B\{^{1}H\}$ NMR spectrum of **4** in d_8-THF (the signal at -36 ppm is due to a minor impurity).

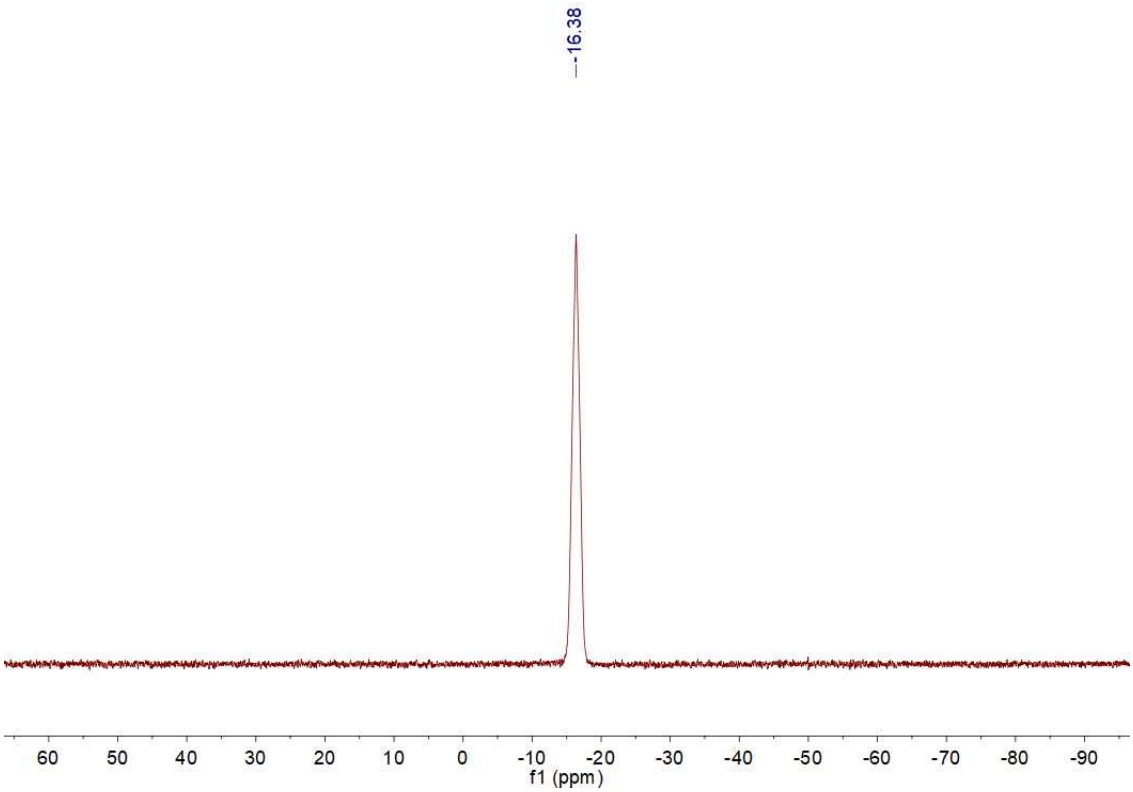

Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in d_8-THF.

Table S1. Crystallographic data for 2a, 2b, 2c, 3, and 4.

Compound	**2a**	**2b**	**2c**	**3**	**4**
CCDC reference	2023940	2023941	2023942	2023944	2023943
formula	$C_{42}H_{92}B_4MgO_4P_2Si_4$ ·C_4H_8O	$C_{24}H_{48}MgO_6^{2+}$ ·$2C_{13}H_{30}B_2PSi_2^-$·C_4H_8O	$C_{24}H_{48}MgO_6^{2+}$ ·$2C_{13}H_{30}B_2PSi_2^-$·$2C_4H_8O$	$C_{42}H_{92}B_4CaO_4P_2Si_4$	$C_{42}H_{92}B_4O_4P_2Si_4Sr$
M_w	975.10	1119.31	1191.41	918.77	966.31
cryst. size /mm^3	0.30 × 0.10 × 0.10	0.30 × 0.27 × 0.24	0.25 × 0.22 × 0.20	0.42 × 0.20 × 0.05	0.10 × 0.02 × 0.005
crystal system	monoclinic	monoclinic	triclinic	orthorhombic	orthorhombic
space group	*C*2/*c*	$P2_1/c$	$P\bar{1}$	*Pbca*	*Pbca*
a /Å	19.5728(3)	13.2927(5)	11.1332(7)	15.9886(5)	16.342(10)
b /Å	25.8266(3)	11.0851(4)	11.8801(10)	11.9737(4)	12.080(7)
c /Å	14.1712(2)	23.1860(9)	15.3074(13)	29.3298(8)	30./005(19)
α /°			71.516(7)		
β /°	121.729(2)	91.103(4)	85.080(6)		
γ /°			70.545(7)		
V /Å^3	6092.90(18)	3415.8(2)	1810.1(3)	5615.0(3)	5923(6)

Z	4	2	1	4	4
μ /mm^{-1}	1.782	0.186	0.180	0.288	1.084
reflections measured	8741	13948	10838	26273	14418
unique reflections	4732	6567	6867	6252	4839
R_{int}	0.0162	0.0246	0.0255	0.0482	0.1191
refined parameters	289	425	425	375	375
R (on F, $F^2>2\sigma$)	0.0342	0.0344	0.0425	0.0391	0.0767
R_w (on F^2, all data)	0.0959	0.0861	0.1079	0.0905	0.2032
goodness of fit on F^2	1.054	0.970	1.035	0.884	1.024
max, min electron density /e Å^{-3}	0.29, –0.26	0.36, –0.26	0.39, –0.25	0.29, –0.26	0.50, –0.34