Supporting information for

Formation of a Zwitterionic Boronium Species from the Reaction of a Stable Carbenoid with Borane: CO2 Reduction.

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1. Synthetic procedures
   a. General procedures

All reactions were done under an inert atmosphere of argon using Schlenk and glovebox techniques with dry and deoxygenated solvents. Tetrahydrofuran, diethyl ether, toluene, and pentane were purified on an MBraun SPS-800 Solvent Purifying System. Nuclear magnetic resonance spectra were recorded on a Bruker Advance 300 MHz spectrometer operating at 300 MHz for ^{1}H, 75.5 MHz for ^{13}C, and 121.5 MHz for ^{31}P. Solvent peaks are used as internal references relative to Me_4Si for ^{1}H (C_6D_6; δ = 7.16 ppm) and ^{13}C (C_6D_6; δ = 128.1 ppm) chemical shifts (ppm); ^{31}P chemical shifts are relative to a 85% H_3PO_4 external reference; ^{11}B chemical shifts are relative to a BF_3 etherate external reference. Coupling constants are given in hertz (Hz). The following abbreviations are used: s=singlet; d=doublet; t=triplet; q=quartet; m=multiplet; br = broad singlet. Elemental analyses were performed by the in-house service of Laboratoire de Chimie de Coordination (205, route de Narbonne, 31077 Toulouse, France) on a PerkinElmer 2400 Series II system. $Li_2C(PPh2NMes)_2$ (**1**, Mes = 2,4,6-$Me_3C_6H_2$) was prepared according to literature procedures.[1] All other reagents and chemicals were obtained commercially and used as received.

The crystal data of compounds **2** and **4** were collected on a Bruker-AXS Quazar APEX II diffractometer using a 30 W air-cooled microfocus source (ImS) with focusing multilayer optics with MoKα radiation (wavelength = 0.71073 Å) by using phi- and omega-scans. Crystals were mounted in inert oil and crystal structure determinations were effected at 193 K. The structures were solved by direct methods, using SHELXTL Software Package and refined using the least-squares method on F^2.[2] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were assigned to idealized geometric positions and included in structure factors calculations. The 2 H of BH_2 in **4** were located by difference Fourier maps and refined without using restraints. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication: CCDC-1034939 (**2**) and CCDC-1034940 (**4**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

   b. Synthesis and characterization of compounds.

Synthesis of compound **2**. To **1** (0.133 g, 0.2 mmol) in ether (10 ml), hexachloroethane (0.0474 g, 0.2 mmol) was added at -78 °C. The reaction was warmed up to room temperature and stirred for 30 mins. The colour changed from bright orange to dark brown. After 30 mins, the mixture was filtered and the filtrate was concentrated to afford crystals of **2** (0.122 g, 73 %). ^{1}H NMR (C_6D_6, 298 K): δ 0.712 (t, $^{3}J_{H-H}$ = 7.11 Hz, 6H, Ether-CH_3), 2.10 (s, 6H, Mes *p*-CH_3), 2.24 (s, 12H, Mes *o*-CH_3), 2.82 (q, $^{3}J_{H-H}$ = 7.11 Hz, 4H, Ether-CH_2), 6.68 (s, 4H, Mes C*H*), 7.12 (m, 12H, *m*,*p*-Ph C*H*), 7.92 (m, 8H, *o*-Ph C*H*). ^{7}Li NMR (C_6D_6, 298 K): δ 1.7 (s). ^{13}C{^{1}H} NMR (C_6D_6, 298 K): δ 14.5 (s, ether *C*H_3), 20.8 (s, Mes *p*-CH_3), 21.2 (s, Mes *o*-CH_3), 64.9 (s, ether *C*H_2), 127.4 (t, J_{P-C} = 5.69 Hz, Ph *o*-C), 133.4 (t, J_{P-C} = 4.41 Hz, Mes *ipso*-C), 129.1 (s, Mes *o*-C), 129.3 (t, J_{P-C} = 2.20 Hz, Ph *p*-C), 129.8 (s, Ph *m*-C), 134.9 (t, J_{P-C} = 3.32 Hz, Mes *m*-C), 135.3 (d, J_{P-C} = 96.6 Hz, Ph *ipso*-C), 146.2 (t, J_{P-C} = 3.72 Hz, Mes *o*-C). ^{31}P{^{1}H} NMR (C_6D_6, 298 K): δ 27.2 (s). Anal. Calc for $C_{47}H_{52}ClLiN_2OP_2$: C, 73.77; H, 6.85; N, 3.66 %. Found: C, 73.77; H, 6.67; N, 3.56 %.

Synthesis of compound **3**. A sample of **2** in C_6D_6 (0.5 ml) was opened in air to allow the hydrolysis of the compound. The colour changed from a clear orange solution to a cloudy orange solution. ^{1}H NMR (C_6D_6, 298 K): δ 2.06 (s, 6H, Mes *p*-C*H*$_3$), 2.29 (s, 12H, Mes *o*-C*H*$_3$), 5.49 (s, 1H, $^2J_{H\text{-}P}$ = 9.05 Hz, PC(*H*)P), 6.61 (s, 4H, Mes C*H*), 7.08 (m, 12H, *m*,*p*-Ph C*H*), 7.88 (m, 8H, *o*-Ph C*H*). ^{31}P NMR (C_6D_6, 298 K): δ 31.0 (s).

Synthesis of compound **4**. **2** (0.168 g, 0.2 mmol) was dissolved in ether (10 ml). The solution was cooled to -78 ^{o}C and 2 equivalents of borane dimethyl sufide complex (2 M in toluene, 0.2 ml, 0.4 mmol) was added drop wise. The mixture was warmed to room temperature and stirred overnight to afford a cloudy yellow solution. The mixture was filtered to get a clear yellow solution. The solution was concentrated to afford yellow crystals of **4** (0.095 g, 68 %). ^{1}H NMR (C_6D_6, 298 K): δ 2.06 (s, 6H, Mes *p*-C*H*$_3$), 2.13 (s, 12H, Mes *o*-C*H*$_3$), 4.49 (br, 2H, B*H*$_2$), 6.61 (s, 4H, Mes C*H*), 7.08 (m, 12H, *m*,*p*-Ph C*H*), 8.10 (m, 8H, *o*-Ph C*H*). ^{11}B{^{1}H} NMR (C_6D_6, 298 K): δ -4.6 (br). ^{13}C{^{1}H} NMR (C_6D_6, 298 K): δ 20.7 (s, Mes *p*-CH_3), 21.2 (s, Mes *o*-CH_3), 127.8 (s, Ph *o*-C), 129.6 (s, Mes *o*-C), 131.4 (s, Ph *p*-C), 131.7 (d, $J_{P\text{-}C}$ = 100 Hz, Ph *ipso*-C), 134.0 (s, Ph *m*-C), 134.6 (t, $J_{P\text{-}C}$ = 4.47 Hz, Mes *ipso*-C) 138.1 (s, Mes *m*-C), 142.6 (s, Mes *p*-C). ^{31}P{^{1}H} NMR (C_6D_6, 298 K): δ 37.0 (s). Anal. Calc for $C_{43}H_{44}BClN_2P_2$: C, 74.09; H, 6.36; N, 4.02 %. Found: C, 73.60; H, 6.10; N, 3.75 %.

c. X-ray structures of 2 and 4

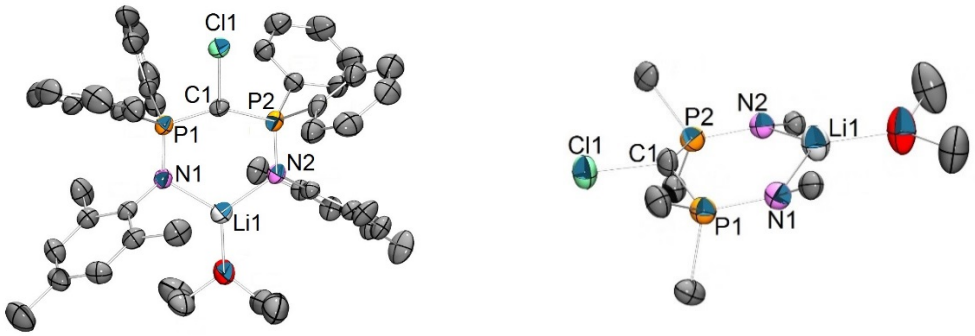


Figure S1. Molecular structure of **2**.

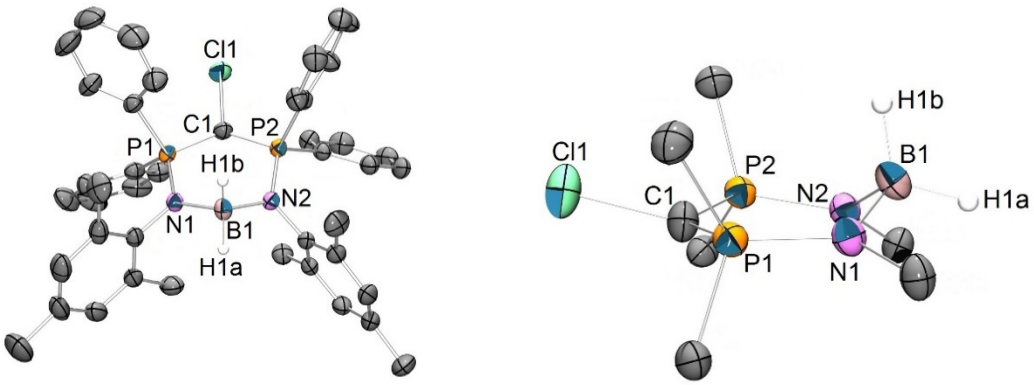


Figure S2. Molecular structure of **4**.

d. General procedure for carbon dioxide reduction.

0.01 mmol of the base catalyst was dissolved in C_6D_6 (~ 0.5 ml) in a J-Young NMR tube. The required amount of $BH_3.SMe_2$ was then added. The NMR tube was frozen in a liquid nitrogen bath under vacuum and 1 bar of CO_2 was added. The reaction was followed by NMR spectroscopy. The yields reported using ^1H NMR are according to the integration of both $B(OMe)_3$ at 3.44 ppm and $(MeOBO)_3$ at 3.34 ppm and compared to the –Mes CH of the catalyst at 6.59 ppm.[3, 4]

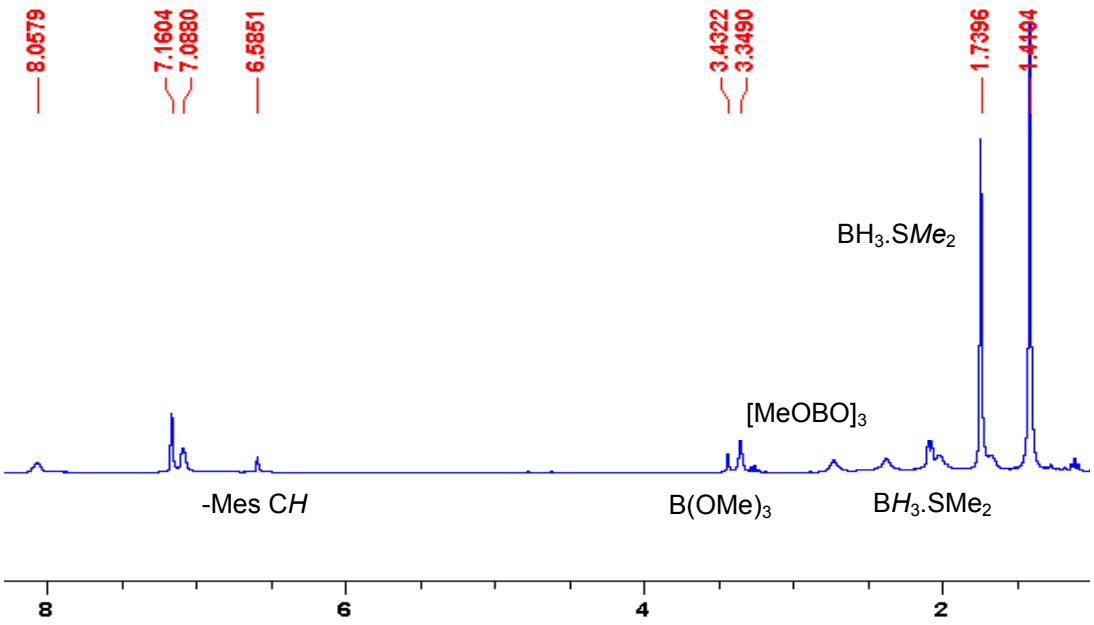


Figure S3. Typical ^1H NMR spectrum of the carbon dioxide reduction using $BH_3.SMe_2$. Incomplete reaction with 5 mol% catalyst loading of **2** (300 MHz, C_6D_6).

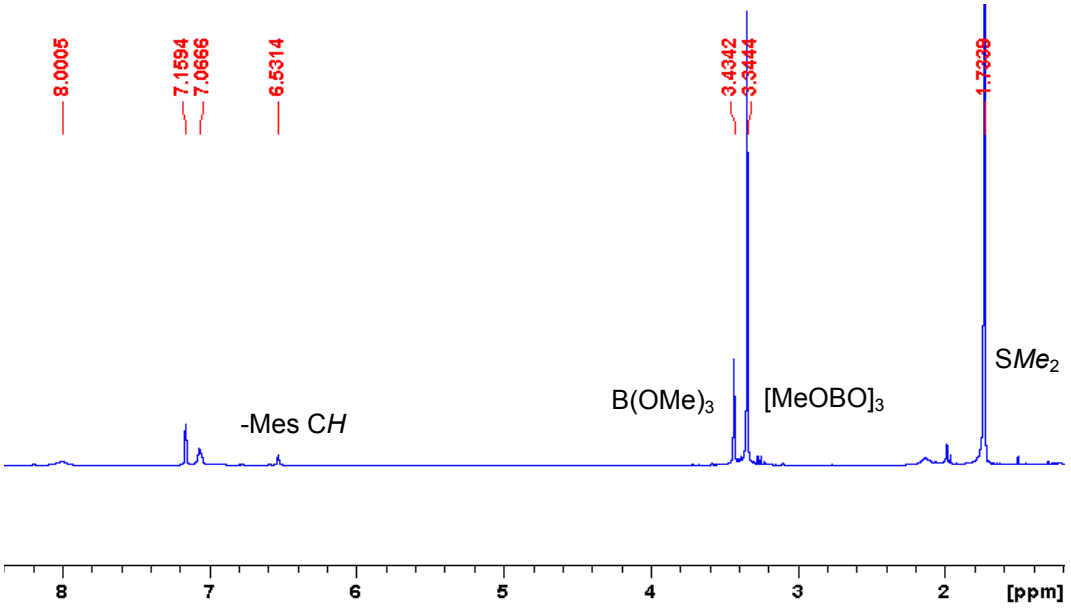
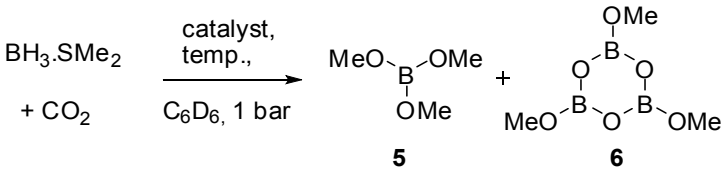


Figure S4. Typical ^1H NMR spectrum of the carbon dioxide reduction using $BH_3.SMe_2$. Spectrum recorded after full conversion with 5 mol% catalyst loading of **2** (300 MHz, C_6D_6).

Table 1. Catalyst result.



Entry	Cat. (mol%)	*T* (°C)	*t* (h)	Yield **5** (%)	Yield **6** (%)	Total yield (%)	TON	TOF (h^{-1})
1	**4** (10)	80	2	8	91	99	35	17
2	**2** (10)	80	2	9	67	76	28	14
3	**2** (5)	80	2	9	71	80	58	29
4	**2** (5)	25	40	6	77	83	58	1.4
5[a]	**2** (5)	80	4	4	85	89	118	30
6	**2** (1)	80	24	5	78	83	278	12
7[b]	**2** (1)	80	2	6	78	84	286	143
8[b]	**4** (1)	80	2	3	96	99	313	157
9[b,c]	**2** (0.1)	80	4	1	70	71	2213	553
10[b,c]	**4** (0.1)	80	4	2	84	86	2646	661
11	**2** (0.01)	80	?	?	?	?	?	?

Conditions: 0.01 mmol of catalyst in C_6D_6 (~0.5 ml), amount of $BH_3.SMe_2$ is calculated then added to obtain the desired catalytic loading, 1 bar of CO_2. The yield was obtained by ^1H NMR using the -Mes C*H* of the ligand as an internal standard. TON and TOF are given to the number of hydride transferred. [a] Additional $BH_3.SMe_2$ and CO_2 was added after 2h. [b] Reactions are done in a schlenk tube to increase the volume of CO2. [c] Hexamethylbenzene is used as an internal standard. 2 times 1 bar of CO_2.

2. Crystallographic details.

Table 2. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C51 H62 Cl Li N2 O2 P2	
Formula weight	839.36	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.3879(18) Å	α = 63.721(6)°.
	b = 14.2429(19) Å	β = 84.210(6)°.
	c = 15.839(2) Å	γ = 63.061(7)°.
Volume	2395.3(5) $Å^3$	
Z	2	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.186 mm^{-1}	
F(000)	896	
Crystal size	0.35 x 0.19 x 0.16 mm^3	
Theta range for data collection	3.17 to 25.68°.	
Index ranges	-14<=h<=16, -17<=k<=17, -18<=l<=19	
Reflections collected	32345	
Independent reflections	8943 [R(int) = 0.0927]	
Completeness to theta = 25.68°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9712 and 0.9377	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8943 / 337 / 617	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0580, wR2 = 0.1208	
R indices (all data)	R1 = 0.1387, wR2 = 0.1520	
Largest diff. peak and hole	0.460 and -0.259 $e.Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6042(1)	3973(1)	1801(1)	44(1)
C(1)	7298(2)	2618(3)	2068(2)	33(1)
P(1)	7001(1)	1502(1)	2177(1)	32(1)
N(1)	8100(2)	255(2)	2545(2)	33(1)
N(2)	9562(2)	1721(2)	1942(2)	32(1)
Li(1)	9587(5)	191(5)	2556(4)	49(2)
O(1)	10940(9)	-1213(8)	2845(10)	65(2)
C(44)	11008(8)	-2465(7)	3259(6)	71(2)
C(45)	11102(12)	-2600(11)	2382(7)	102(4)
C(46)	12046(10)	-1404(14)	3040(10)	80(3)
C(47)	11968(9)	-1121(11)	3832(9)	85(3)
O(1')	10864(9)	-1358(9)	3049(10)	67(3)
C(44')	10753(9)	-1843(8)	2317(7)	82(2)
C(45')	10892(11)	-3007(9)	2971(10)	111(4)
C(46')	11921(11)	-1533(16)	3308(10)	89(3)
C(47')	12347(10)	-1897(11)	4277(8)	89(3)
C(2)	5919(2)	1485(3)	2961(2)	37(1)
C(3)	5818(3)	1861(3)	3643(2)	49(1)
C(4)	5005(4)	1803(3)	4264(3)	67(1)
C(5)	4307(3)	1354(4)	4190(3)	69(1)
C(6)	4420(3)	967(3)	3526(3)	61(1)
C(7)	5213(3)	1025(3)	2909(2)	49(1)
C(8)	6325(3)	1912(3)	1041(2)	36(1)
C(9)	5206(3)	2771(3)	709(2)	49(1)
C(10)	4758(4)	3171(3)	-196(3)	63(1)
C(11)	5401(5)	2750(4)	-797(3)	72(1)
C(12)	6503(4)	1897(4)	-482(3)	61(1)
C(13)	6965(3)	1473(3)	441(2)	46(1)
C(14)	8128(2)	-782(3)	3327(2)	32(1)
C(15)	8489(3)	-1087(3)	4256(2)	38(1)
C(16)	8584(3)	-2140(3)	4993(2)	44(1)
C(17)	8341(3)	-2902(3)	4854(2)	46(1)
C(18)	7987(3)	-2589(3)	3937(2)	47(1)

C(19)	7890(3)	-1559(3)	3171(2)	38(1)
C(20)	8780(3)	-304(3)	4469(2)	51(1)
C(21)	8434(4)	-4042(3)	5671(3)	77(1)
C(22)	7558(3)	-1300(3)	2183(2)	57(1)
C(23)	8194(3)	3849(3)	371(2)	38(1)
C(24)	7267(3)	4145(3)	-194(2)	44(1)
C(25)	7116(3)	4821(3)	-1163(2)	56(1)
C(26)	7897(4)	5215(4)	-1585(3)	71(1)
C(27)	8829(4)	4916(4)	-1037(3)	74(1)
C(28)	8984(3)	4241(3)	-74(3)	55(1)
P(2)	8414(1)	2911(1)	1643(1)	33(1)
C(29)	8377(19)	3770(12)	2259(9)	42(2)
C(30)	8321(15)	4884(11)	1807(8)	46(2)
C(31)	8452(10)	5386(8)	2340(8)	51(2)
C(32)	8638(8)	4775(9)	3325(8)	52(2)
C(33)	8693(11)	3661(10)	3776(8)	52(2)
C(34)	8563(16)	3159(10)	3244(9)	44(2)
C(29')	8405(17)	3900(11)	2090(9)	39(2)
C(30')	8345(15)	5000(10)	1510(7)	49(2)
C(31')	8435(10)	5656(8)	1910(8)	59(2)
C(32')	8584(7)	5212(9)	2891(8)	52(2)
C(33')	8644(9)	4112(9)	3472(7)	55(2)
C(34')	8554(14)	3456(8)	3071(8)	50(2)
C(35)	10551(2)	1647(3)	1481(2)	31(1)
C(36)	11388(3)	1780(3)	1812(2)	35(1)
C(37)	12366(3)	1628(3)	1382(2)	43(1)
C(38)	12572(3)	1313(3)	651(2)	48(1)
C(39)	11746(3)	1175(3)	340(2)	45(1)
C(40)	10740(3)	1334(3)	734(2)	36(1)
C(41)	11245(3)	2077(3)	2636(2)	50(1)
C(42)	13665(3)	1113(4)	206(3)	75(1)
C(43)	9887(3)	1160(3)	352(3)	54(1)
C(48)	4398(5)	5032(4)	3575(4)	113(2)
C(49)	5281(4)	5383(4)	3583(3)	85(1)
O(2)	4753(2)	6612(3)	3288(2)	72(1)
C(50)	5501(4)	7055(5)	3260(4)	95(2)
C(51)	4911(5)	8342(5)	2906(5)	135(2)

Table 4. Bond lengths [Å] and angles [°] for **2**.

Cl(1)-C(1)	1.792(3)
C(1)-P(2)	1.724(3)
C(1)-P(1)	1.740(3)
P(1)-N(1)	1.596(3)
P(1)-C(2)	1.812(3)
P(1)-C(8)	1.821(3)
P(1)-Li(1)	3.066(6)
N(1)-C(14)	1.434(4)
N(1)-Li(1)	1.953(6)
N(2)-C(35)	1.429(4)
N(2)-P(2)	1.593(2)
N(2)-Li(1)	1.939(6)
Li(1)-O(1)	1.887(10)
Li(1)-O(1')	1.930(10)
Li(1)-C(14)	2.776(6)
Li(1)-C(35)	2.778(6)
Li(1)-C(44')	2.779(11)
Li(1)-P(2)	3.091(6)
O(1)-C(46)	1.420(10)
O(1)-C(44)	1.564(12)
C(44)-C(45)	1.470(11)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.459(12)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
O(1')-C(46')	1.392(11)
O(1')-C(44')	1.636(13)
C(44')-C(45')	1.447(11)
C(44')-H(44C)	0.9900

C(44')-H(44D)	0.9900
C(45')-H(45D)	0.9800
C(45')-H(45E)	0.9800
C(45')-H(45F)	0.9800
C(46')-C(47')	1.468(11)
C(46')-H(46C)	0.9900
C(46')-H(46D)	0.9900
C(47')-H(47D)	0.9800
C(47')-H(47E)	0.9800
C(47')-H(47F)	0.9800
C(2)-C(3)	1.376(4)
C(2)-C(7)	1.397(4)
C(3)-C(4)	1.396(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.387(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.357(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.375(5)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(13)	1.380(4)
C(8)-C(9)	1.395(4)
C(9)-C(10)	1.370(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.370(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.375(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.396(5)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(19)	1.400(4)
C(14)-C(15)	1.405(4)
C(15)-C(16)	1.391(4)
C(15)-C(20)	1.505(4)
C(16)-C(17)	1.372(5)
C(16)-H(16)	0.9500

C(17)-C(18)	1.380(5)
C(17)-C(21)	1.521(5)
C(18)-C(19)	1.387(4)
C(18)-H(18)	0.9500
C(19)-C(22)	1.505(4)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.391(4)
C(23)-C(28)	1.401(4)
C(23)-P(2)	1.819(3)
C(24)-C(25)	1.379(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.384(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.378(6)
C(26)-H(26)	0.9500
C(27)-C(28)	1.370(5)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
P(2)-C(29')	1.830(5)
P(2)-C(29)	1.855(5)
C(29)-C(30)	1.3900
C(29)-C(34)	1.3900
C(30)-C(31)	1.3900
C(30)-H(30)	0.9500
C(31)-C(32)	1.3900
C(31)-H(31)	0.9500
C(32)-C(33)	1.3900
C(32)-H(32)	0.9500
C(33)-C(34)	1.3900
C(33)-H(33)	0.9500

C(34)-H(34)	0.9500
C(29')-C(30')	1.3900
C(29')-C(34')	1.3900
C(30')-C(31')	1.3900
C(30')-H(30')	0.9500
C(31')-C(32')	1.3900
C(31')-H(31')	0.9500
C(32')-C(33')	1.3900
C(32')-H(32')	0.9500
C(33')-C(34')	1.3900
C(33')-H(33')	0.9500
C(34')-H(34')	0.9500
C(35)-C(40)	1.402(4)
C(35)-C(36)	1.402(4)
C(36)-C(37)	1.386(4)
C(36)-C(41)	1.511(4)
C(37)-C(38)	1.378(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.377(5)
C(38)-C(42)	1.521(5)
C(39)-C(40)	1.392(4)
C(39)-H(39)	0.9500
C(40)-C(43)	1.504(4)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(48)-C(49)	1.480(7)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-O(2)	1.416(5)
C(49)-H(49A)	0.9900

C(49)-H(49B)	0.9900
O(2)-C(50)	1.393(5)
C(50)-C(51)	1.472(7)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800

P(2)-C(1)-P(1)	130.92(17)
P(2)-C(1)-Cl(1)	109.60(16)
P(1)-C(1)-Cl(1)	112.14(16)
N(1)-P(1)-C(1)	112.36(13)
N(1)-P(1)-C(2)	112.27(14)
C(1)-P(1)-C(2)	107.08(15)
N(1)-P(1)-C(8)	111.28(14)
C(1)-P(1)-C(8)	109.08(14)
C(2)-P(1)-C(8)	104.37(15)
C(1)-P(1)-Li(1)	79.33(15)
C(2)-P(1)-Li(1)	132.10(15)
C(8)-P(1)-Li(1)	118.47(15)
C(14)-N(1)-P(1)	122.17(19)
C(14)-N(1)-Li(1)	109.1(2)
P(1)-N(1)-Li(1)	119.2(2)
C(35)-N(2)-P(2)	123.4(2)
C(35)-N(2)-Li(1)	110.2(2)
P(2)-N(2)-Li(1)	121.9(2)
O(1)-Li(1)-O(1')	9.9(9)
O(1)-Li(1)-N(2)	121.7(5)
O(1')-Li(1)-N(2)	129.3(5)
O(1)-Li(1)-N(1)	122.5(5)
O(1')-Li(1)-N(1)	116.3(5)
N(2)-Li(1)-N(1)	114.1(3)
O(1)-Li(1)-C(14)	98.8(5)
O(1')-Li(1)-C(14)	90.7(5)
N(2)-Li(1)-C(14)	139.4(3)
N(1)-Li(1)-C(14)	29.23(13)
O(1)-Li(1)-C(35)	94.2(5)

O(1')-Li(1)-C(35)	102.9(5)
N(2)-Li(1)-C(35)	28.86(12)
N(1)-Li(1)-C(35)	136.2(3)
C(14)-Li(1)-C(35)	165.3(2)
O(1)-Li(1)-C(44')	32.9(5)
O(1')-Li(1)-C(44')	35.2(4)
N(2)-Li(1)-C(44')	133.1(3)
N(1)-Li(1)-C(44')	96.5(3)
C(14)-Li(1)-C(44')	82.4(3)
C(35)-Li(1)-C(44')	105.5(3)
O(1)-Li(1)-P(1)	149.2(4)
O(1')-Li(1)-P(1)	143.3(5)
N(2)-Li(1)-P(1)	87.3(2)
N(1)-Li(1)-P(1)	27.03(11)
C(14)-Li(1)-P(1)	53.75(12)
C(35)-Li(1)-P(1)	111.87(19)
C(44')-Li(1)-P(1)	119.8(3)
O(1)-Li(1)-P(2)	147.5(5)
O(1')-Li(1)-P(2)	155.1(5)
N(2)-Li(1)-P(2)	25.95(11)
N(1)-Li(1)-P(2)	88.6(2)
C(14)-Li(1)-P(2)	113.62(19)
C(35)-Li(1)-P(2)	53.62(12)
C(44')-Li(1)-P(2)	148.1(3)
P(1)-Li(1)-P(2)	61.57(11)
C(46)-O(1)-C(44)	105.8(8)
C(46)-O(1)-Li(1)	126.7(8)
C(44)-O(1)-Li(1)	124.4(8)
C(45)-C(44)-O(1)	99.2(9)
C(45)-C(44)-H(44A)	111.9
O(1)-C(44)-H(44A)	111.9
C(45)-C(44)-H(44B)	111.9
O(1)-C(44)-H(44B)	111.9
H(44A)-C(44)-H(44B)	109.6
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5

H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
O(1)-C(46)-C(47)	103.8(9)
O(1)-C(46)-H(46A)	111.0
C(47)-C(46)-H(46A)	111.0
O(1)-C(46)-H(46B)	111.0
C(47)-C(46)-H(46B)	111.0
H(46A)-C(46)-H(46B)	109.0
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46')-O(1')-C(44')	119.1(10)
C(46')-O(1')-Li(1)	120.8(9)
C(44')-O(1')-Li(1)	102.1(7)
C(45')-C(44')-O(1')	101.4(10)
C(45')-C(44')-Li(1)	126.5(8)
C(45')-C(44')-H(44C)	111.5
O(1')-C(44')-H(44C)	111.5
Li(1)-C(44')-H(44C)	69.8
C(45')-C(44')-H(44D)	111.5
O(1')-C(44')-H(44D)	111.5
Li(1)-C(44')-H(44D)	118.2
H(44C)-C(44')-H(44D)	109.3
C(44')-C(45')-H(45D)	109.5
C(44')-C(45')-H(45E)	109.5
H(45D)-C(45')-H(45E)	109.5
C(44')-C(45')-H(45F)	109.5
H(45D)-C(45')-H(45F)	109.5
H(45E)-C(45')-H(45F)	109.5
O(1')-C(46')-C(47')	124.2(10)
O(1')-C(46')-H(46C)	106.3
C(47')-C(46')-H(46C)	106.3
O(1')-C(46')-H(46D)	106.3
C(47')-C(46')-H(46D)	106.3
H(46C)-C(46')-H(46D)	106.4

C(46')-C(47')-H(47D)	109.5
C(46')-C(47')-H(47E)	109.5
H(47D)-C(47')-H(47E)	109.5
C(46')-C(47')-H(47F)	109.5
H(47D)-C(47')-H(47F)	109.5
H(47E)-C(47')-H(47F)	109.5
C(3)-C(2)-C(7)	119.1(3)
C(3)-C(2)-P(1)	121.0(3)
C(7)-C(2)-P(1)	119.8(3)
C(2)-C(3)-C(4)	120.3(4)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	119.4(4)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	120.2(4)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.8(4)
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-H(6)	119.6
C(6)-C(7)-C(2)	120.1(4)
C(6)-C(7)-H(7)	120.0
C(2)-C(7)-H(7)	120.0
C(13)-C(8)-C(9)	118.6(3)
C(13)-C(8)-P(1)	119.4(3)
C(9)-C(8)-P(1)	121.5(3)
C(10)-C(9)-C(8)	120.4(4)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(11)-C(10)-C(9)	120.9(4)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(10)-C(11)-C(12)	119.6(4)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	120.0(4)
C(11)-C(12)-H(12)	120.0

C(13)-C(12)-H(12)	120.0
C(8)-C(13)-C(12)	120.4(4)
C(8)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(19)-C(14)-C(15)	118.8(3)
C(19)-C(14)-N(1)	120.7(3)
C(15)-C(14)-N(1)	120.3(3)
C(19)-C(14)-Li(1)	131.8(2)
C(15)-C(14)-Li(1)	92.4(2)
C(16)-C(15)-C(14)	119.1(3)
C(16)-C(15)-C(20)	119.3(3)
C(14)-C(15)-C(20)	121.5(3)
C(17)-C(16)-C(15)	122.7(3)
C(17)-C(16)-H(16)	118.6
C(15)-C(16)-H(16)	118.6
C(16)-C(17)-C(18)	117.3(3)
C(16)-C(17)-C(21)	122.0(3)
C(18)-C(17)-C(21)	120.6(3)
C(17)-C(18)-C(19)	122.6(3)
C(17)-C(18)-H(18)	118.7
C(19)-C(18)-H(18)	118.7
C(18)-C(19)-C(14)	119.4(3)
C(18)-C(19)-C(22)	119.9(3)
C(14)-C(19)-C(22)	120.7(3)
C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(17)-C(21)-H(21A)	109.5
C(17)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(17)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5

H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(28)	118.1(3)
C(24)-C(23)-P(2)	120.8(3)
C(28)-C(23)-P(2)	120.9(3)
C(25)-C(24)-C(23)	121.2(3)
C(25)-C(24)-H(24)	119.4
C(23)-C(24)-H(24)	119.4
C(24)-C(25)-C(26)	119.7(4)
C(24)-C(25)-H(25)	120.2
C(26)-C(25)-H(25)	120.2
C(27)-C(26)-C(25)	119.9(4)
C(27)-C(26)-H(26)	120.1
C(25)-C(26)-H(26)	120.1
C(28)-C(27)-C(26)	120.6(4)
C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(27)-C(28)-C(23)	120.5(4)
C(27)-C(28)-H(28)	119.7
C(23)-C(28)-H(28)	119.7
N(2)-P(2)-C(1)	110.73(13)
N(2)-P(2)-C(23)	111.19(13)
C(1)-P(2)-C(23)	113.85(15)
N(2)-P(2)-C(29')	114.5(6)
C(1)-P(2)-C(29')	105.9(6)
C(23)-P(2)-C(29')	100.3(4)
N(2)-P(2)-C(29)	112.4(6)
C(1)-P(2)-C(29)	100.2(6)
C(23)-P(2)-C(29)	108.0(4)
C(1)-P(2)-Li(1)	78.77(14)
C(23)-P(2)-Li(1)	123.84(15)
C(29')-P(2)-Li(1)	129.9(5)
C(29)-P(2)-Li(1)	123.9(5)
C(30)-C(29)-C(34)	120.0
C(30)-C(29)-P(2)	124.6(7)
C(34)-C(29)-P(2)	114.9(7)

C(31)-C(30)-C(29)	120.0
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.0
C(30)-C(31)-H(31)	120.0
C(32)-C(31)-H(31)	120.0
C(33)-C(32)-C(31)	120.0
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	120.0
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(29)	120.0
C(33)-C(34)-H(34)	120.0
C(29)-C(34)-H(34)	120.0
C(30')-C(29')-C(34')	120.0
C(30')-C(29')-P(2)	123.7(6)
C(34')-C(29')-P(2)	116.1(6)
C(31')-C(30')-C(29')	120.0
C(31')-C(30')-H(30')	120.0
C(29')-C(30')-H(30')	120.0
C(30')-C(31')-C(32')	120.0
C(30')-C(31')-H(31')	120.0
C(32')-C(31')-H(31')	120.0
C(33')-C(32')-C(31')	120.0
C(33')-C(32')-H(32')	120.0
C(31')-C(32')-H(32')	120.0
C(32')-C(33')-C(34')	120.0
C(32')-C(33')-H(33')	120.0
C(34')-C(33')-H(33')	120.0
C(33')-C(34')-C(29')	120.0
C(33')-C(34')-H(34')	120.0
C(29')-C(34')-H(34')	120.0
C(40)-C(35)-C(36)	118.9(3)
C(40)-C(35)-N(2)	119.6(3)
C(36)-C(35)-N(2)	121.3(3)
C(40)-C(35)-Li(1)	96.6(2)
C(36)-C(35)-Li(1)	126.6(2)

C(37)-C(36)-C(35)	119.5(3)
C(37)-C(36)-C(41)	119.5(3)
C(35)-C(36)-C(41)	121.1(3)
C(38)-C(37)-C(36)	122.6(3)
C(38)-C(37)-H(37)	118.7
C(36)-C(37)-H(37)	118.7
C(39)-C(38)-C(37)	117.2(3)
C(39)-C(38)-C(42)	120.8(3)
C(37)-C(38)-C(42)	122.0(3)
C(38)-C(39)-C(40)	122.8(3)
C(38)-C(39)-H(39)	118.6
C(40)-C(39)-H(39)	118.6
C(39)-C(40)-C(35)	119.1(3)
C(39)-C(40)-C(43)	119.1(3)
C(35)-C(40)-C(43)	121.8(3)
C(36)-C(41)-H(41A)	109.5
C(36)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(36)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(38)-C(42)-H(42A)	109.5
C(38)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(38)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(40)-C(43)-H(43A)	109.5
C(40)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(40)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(49)-C(48)-H(48A)	109.5
C(49)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(49)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5

H(48B)-C(48)-H(48C)	109.5
O(2)-C(49)-C(48)	108.4(4)
O(2)-C(49)-H(49A)	110.0
C(48)-C(49)-H(49A)	110.0
O(2)-C(49)-H(49B)	110.0
C(48)-C(49)-H(49B)	110.0
H(49A)-C(49)-H(49B)	108.4
C(50)-O(2)-C(49)	114.0(4)
O(2)-C(50)-C(51)	111.5(4)
O(2)-C(50)-H(50A)	109.3
C(51)-C(50)-H(50A)	109.3
O(2)-C(50)-H(50B)	109.3
C(51)-C(50)-H(50B)	109.3
H(50A)-C(50)-H(50B)	108.0
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	30(1)	38(1)	60(1)	-23(1)	9(1)	-13(1)
C(1)	23(2)	31(2)	43(2)	-20(2)	7(1)	-8(2)
P(1)	28(1)	36(1)	34(1)	-16(1)	7(1)	-16(1)
N(1)	31(1)	35(2)	35(2)	-16(1)	7(1)	-17(1)
N(2)	27(1)	39(2)	34(2)	-18(1)	9(1)	-17(1)
Li(1)	35(3)	46(3)	60(4)	-21(3)	9(3)	-17(3)
O(1)	39(3)	46(3)	100(5)	-27(3)	25(3)	-21(3)
C(44)	62(4)	46(4)	97(4)	-34(4)	21(4)	-19(3)
C(45)	128(8)	71(7)	81(6)	-22(6)	9(6)	-38(6)
C(46)	42(4)	64(4)	98(6)	-10(4)	20(4)	-23(3)

C(47)	64(6)	77(6)	121(8)	-47(6)	18(5)	-37(6)
O(1')	40(3)	48(3)	97(5)	-25(3)	25(3)	-19(3)
C(44')	69(4)	54(4)	96(5)	-32(4)	27(4)	-14(4)
C(45')	99(7)	66(6)	149(9)	-35(6)	26(7)	-39(6)
C(46')	39(4)	76(5)	102(6)	-10(5)	18(4)	-18(4)
C(47')	74(7)	79(7)	107(8)	-47(6)	17(5)	-27(6)
C(2)	25(2)	37(2)	40(2)	-14(2)	6(2)	-11(2)
C(3)	49(2)	48(2)	51(2)	-24(2)	20(2)	-24(2)
C(4)	67(3)	57(3)	65(3)	-30(2)	31(2)	-21(2)
C(5)	40(2)	59(3)	75(3)	-11(2)	28(2)	-19(2)
C(6)	38(2)	66(3)	63(3)	-12(2)	10(2)	-28(2)
C(7)	31(2)	50(2)	53(2)	-14(2)	4(2)	-17(2)
C(8)	39(2)	36(2)	33(2)	-8(2)	-1(2)	-22(2)
C(9)	54(2)	42(2)	47(2)	-12(2)	-7(2)	-25(2)
C(10)	63(3)	47(2)	60(3)	-1(2)	-24(2)	-26(2)
C(11)	107(4)	69(3)	36(2)	3(2)	-22(3)	-54(3)
C(12)	94(3)	70(3)	38(2)	-19(2)	10(2)	-58(3)
C(13)	55(2)	53(2)	38(2)	-18(2)	5(2)	-32(2)
C(14)	23(2)	37(2)	37(2)	-22(2)	8(1)	-11(2)
C(15)	32(2)	44(2)	39(2)	-24(2)	9(2)	-14(2)
C(16)	48(2)	47(2)	28(2)	-16(2)	7(2)	-17(2)
C(17)	45(2)	41(2)	45(2)	-15(2)	16(2)	-19(2)
C(18)	57(2)	40(2)	49(2)	-21(2)	14(2)	-27(2)
C(19)	36(2)	41(2)	39(2)	-22(2)	6(2)	-16(2)
C(20)	59(2)	62(2)	42(2)	-31(2)	7(2)	-27(2)
C(21)	96(3)	63(3)	57(3)	-10(2)	17(2)	-42(3)
C(22)	81(3)	60(2)	47(2)	-27(2)	6(2)	-43(2)
C(23)	33(2)	37(2)	42(2)	-17(2)	8(2)	-16(2)
C(24)	43(2)	47(2)	38(2)	-15(2)	7(2)	-23(2)
C(25)	49(2)	65(3)	41(2)	-19(2)	4(2)	-21(2)
C(26)	68(3)	75(3)	39(2)	-7(2)	13(2)	-29(3)
C(27)	50(3)	71(3)	64(3)	2(2)	12(2)	-31(2)
C(28)	40(2)	53(2)	56(3)	-5(2)	2(2)	-26(2)
P(2)	29(1)	38(1)	38(1)	-19(1)	7(1)	-17(1)
C(29)	30(3)	45(4)	64(5)	-31(4)	3(4)	-20(3)
C(30)	36(3)	50(4)	63(5)	-34(4)	8(5)	-21(3)
C(31)	54(3)	47(4)	66(5)	-42(4)	12(5)	-20(3)
C(32)	50(4)	45(5)	75(5)	-42(4)	5(4)	-17(4)

C(33)	46(4)	52(5)	69(5)	-39(4)	5(4)	-20(4)
C(34)	38(3)	56(4)	63(4)	-44(4)	9(4)	-25(4)
C(29')	24(3)	48(4)	55(4)	-30(4)	15(4)	-19(3)
C(30')	42(3)	50(3)	67(5)	-34(4)	8(5)	-22(3)
C(31')	54(3)	56(4)	71(5)	-37(4)	11(5)	-21(3)
C(32')	50(3)	52(4)	69(6)	-44(4)	13(4)	-18(4)
C(33')	49(3)	52(5)	66(5)	-39(4)	7(4)	-12(4)
C(34')	41(3)	50(4)	64(4)	-33(4)	9(4)	-19(4)
C(35)	26(2)	33(2)	31(2)	-14(2)	6(1)	-11(2)
C(36)	29(2)	40(2)	34(2)	-18(2)	2(2)	-13(2)
C(37)	32(2)	57(2)	50(2)	-30(2)	8(2)	-23(2)
C(38)	39(2)	59(2)	53(2)	-32(2)	18(2)	-24(2)
C(39)	47(2)	55(2)	43(2)	-32(2)	17(2)	-24(2)
C(40)	37(2)	39(2)	34(2)	-19(2)	8(2)	-19(2)
C(41)	36(2)	76(3)	47(2)	-36(2)	4(2)	-24(2)
C(42)	54(3)	115(4)	89(3)	-67(3)	45(2)	-50(3)
C(43)	58(2)	72(3)	57(2)	-43(2)	13(2)	-35(2)
C(48)	132(5)	85(4)	150(5)	-72(4)	60(4)	-62(4)
C(49)	76(3)	76(3)	80(3)	-38(3)	4(3)	-12(3)
O(2)	56(2)	73(2)	92(2)	-46(2)	12(2)	-26(2)
C(50)	68(3)	127(5)	126(4)	-77(4)	20(3)	-54(3)
C(51)	92(4)	110(5)	240(8)	-95(5)	49(4)	-65(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2**.

	x	y	z	U(eq)
H(44A)	11680	-3073	3735	85
H(44B)	10319	-2482	3542	85
H(45A)	10346	-2248	2057	153
H(45B)	11499	-3439	2539	153
H(45C)	11526	-2202	1967	153
H(46A)	12263	-882	2483	96
H(46B)	12605	-2234	3221	96
H(47A)	11456	-282	3622	127

H(47B)	12719	-1299	4054	127
H(47C)	11677	-1592	4350	127
H(44C)	10005	-1347	1928	98
H(44D)	11353	-1881	1895	98
H(45D)	11696	-3547	3189	166
H(45E)	10585	-3288	2649	166
H(45F)	10488	-2974	3517	166
H(46C)	11955	-786	2902	107
H(46D)	12481	-2126	3113	107
H(47D)	11783	-1384	4529	133
H(47E)	13049	-1838	4270	133
H(47F)	12493	-2714	4681	133
H(3)	6302	2162	3693	59
H(4)	4931	2068	4732	80
H(5)	3749	1318	4607	83
H(6)	3945	652	3487	74
H(7)	5282	753	2446	59
H(9)	4751	3081	1112	59
H(10)	3992	3748	-409	76
H(11)	5086	3046	-1427	87
H(12)	6950	1595	-893	74
H(13)	7726	879	658	56
H(16)	8828	-2339	5619	53
H(18)	7803	-3098	3826	57
H(20A)	8526	-318	5075	77
H(20B)	8403	504	3963	77
H(20C)	9599	-587	4509	77
H(21A)	8940	-4270	6208	116
H(21B)	8736	-4666	5466	116
H(21C)	7684	-3925	5865	116
H(22A)	7446	-1945	2208	85
H(22B)	8158	-1223	1791	85
H(22C)	6855	-563	1907	85
H(24)	6728	3877	93	52
H(25)	6479	5015	-1539	67
H(26)	7792	5691	-2251	85
H(27)	9369	5179	-1330	89
H(28)	9632	4039	295	67

H(30)	8194	5302	1134	55
H(31)	8414	6147	2031	61
H(32)	8727	5118	3689	62
H(33)	8820	3243	4449	62
H(34)	8600	2398	3552	53
H(30')	8243	5303	839	59
H(31')	8394	6408	1514	70
H(32')	8645	5660	3165	63
H(33')	8746	3808	4142	66
H(34')	8595	2704	3467	60
H(37)	12916	1747	1598	52
H(39)	11869	962	-166	54
H(41A)	11970	1952	2862	75
H(41B)	10983	1569	3151	75
H(41C)	10688	2903	2428	75
H(42A)	13527	1794	-409	113
H(42B)	13939	404	113	113
H(42C)	14233	1013	626	113
H(43A)	10233	786	-66	81
H(43B)	9238	1925	-9	81
H(43C)	9636	654	880	81
H(48A)	3917	5133	4068	169
H(48B)	4756	4204	3698	169
H(48C)	3938	5526	2953	169
H(49A)	5690	4956	4230	102
H(49B)	5831	5185	3147	102
H(50A)	6077	6851	2842	114
H(50B)	5895	6683	3905	114
H(51A)	4544	8714	2258	202
H(51B)	5457	8624	2908	202
H(51C)	4340	8546	3318	202

Table 7. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C43 H44 B Cl N2 P2	
Formula weight	697.00	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.7251(15) Å	α = 90°.
	b = 18.239(2) Å	β = 102.121(6)°.
	c = 16.632(2) Å	γ = 90°.
Volume	3774.1(8) $Å^3$	
Z	4	
Density (calculated)	1.227 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	1472	
Crystal size	0.24 x 0.16 x 0.10 mm^3	
Theta range for data collection	5.13 to 27.88°.	
Index ranges	-16<=h<=16, -23<=k<=23, -21<=l<=15	
Reflections collected	55433	
Independent reflections	8921 [R(int) = 0.0567]	
Completeness to theta = 27.88°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9784 and 0.9493	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8921 / 0 / 456	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1042	
R indices (all data)	R1 = 0.0770, wR2 = 0.1199	
Largest diff. peak and hole	0.473 and -0.313 $e.Å^{-3}$	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3480(1)	2850(1)	2464(1)	44(1)
C(1)	2832(2)	3717(1)	2398(1)	30(1)
P(1)	3330(1)	4340(1)	1798(1)	25(1)
P(2)	2187(1)	3910(1)	3181(1)	24(1)
N(1)	2934(1)	5158(1)	1994(1)	26(1)
N(2)	1825(1)	4766(1)	3081(1)	25(1)
B(1)	2655(2)	5348(1)	2855(1)	29(1)
C(2)	4777(1)	4186(1)	2014(1)	32(1)
C(3)	5299(2)	4236(2)	2837(2)	50(1)
C(4)	6382(2)	4072(2)	3072(2)	66(1)
C(5)	6956(2)	3865(2)	2490(2)	69(1)
C(6)	6461(2)	3828(2)	1676(2)	64(1)
C(7)	5364(2)	3979(1)	1434(2)	45(1)
C(8)	2861(2)	4157(1)	712(1)	30(1)
C(9)	3248(2)	4533(1)	105(1)	40(1)
C(10)	2818(2)	4388(1)	-717(2)	53(1)
C(11)	1997(2)	3890(1)	-932(2)	56(1)
C(12)	1601(2)	3527(1)	-346(2)	49(1)
C(13)	2030(2)	3654(1)	478(1)	37(1)
C(14)	3062(1)	3682(1)	4164(1)	29(1)
C(15)	3743(2)	4200(1)	4616(1)	37(1)
C(16)	4445(2)	4003(1)	5341(1)	46(1)
C(17)	4473(2)	3294(2)	5622(1)	48(1)
C(18)	3816(2)	2774(1)	5177(2)	53(1)
C(19)	3110(2)	2968(1)	4451(1)	42(1)
C(20)	1043(1)	3311(1)	3161(1)	28(1)
C(21)	773(2)	2771(1)	2566(1)	36(1)
C(22)	-112(2)	2316(1)	2558(2)	44(1)
C(23)	-729(2)	2411(1)	3141(2)	44(1)
C(24)	-468(2)	2941(1)	3736(2)	40(1)
C(25)	423(2)	3388(1)	3760(1)	33(1)
C(26)	2990(2)	5760(1)	1435(1)	30(1)
C(27)	2072(2)	5949(1)	847(1)	34(1)

C(28)	2116(2)	6538(1)	329(2)	46(1)
C(29)	3040(2)	6960(1)	386(2)	51(1)
C(30)	3929(2)	6773(1)	976(2)	52(1)
C(31)	3932(2)	6182(1)	1512(1)	39(1)
C(32)	1034(2)	5545(1)	797(2)	44(1)
C(33)	3050(3)	7616(2)	-174(2)	84(1)
C(34)	4926(2)	6034(1)	2159(2)	53(1)
C(35)	804(1)	5031(1)	3220(1)	27(1)
C(36)	802(2)	5445(1)	3930(1)	33(1)
C(37)	-158(2)	5753(1)	4042(1)	40(1)
C(38)	-1121(2)	5652(1)	3484(1)	41(1)
C(39)	-1104(2)	5221(1)	2809(1)	38(1)
C(40)	-158(1)	4907(1)	2652(1)	30(1)
C(41)	1804(2)	5552(1)	4583(1)	45(1)
C(42)	-2150(2)	6008(2)	3611(2)	63(1)
C(43)	-254(2)	4442(1)	1892(1)	37(1)

Table 9. Bond lengths [Å] and angles [°] for **4**.

Cl(1)-C(1)	1.7763(19)
C(1)-P(2)	1.715(2)
C(1)-P(1)	1.720(2)
P(1)-N(1)	1.6291(16)
P(1)-C(8)	1.810(2)
P(1)-C(2)	1.8226(18)
P(2)-N(2)	1.6265(16)
P(2)-C(20)	1.8148(18)
P(2)-C(14)	1.8229(19)
N(1)-C(26)	1.450(2)
N(1)-B(1)	1.585(3)
N(2)-C(35)	1.450(2)
N(2)-B(1)	1.596(3)
C(2)-C(7)	1.391(3)
C(2)-C(3)	1.394(3)
C(3)-C(4)	1.384(3)
C(4)-C(5)	1.382(4)
C(5)-C(6)	1.370(4)

C(6)-C(7)	1.396(3)
C(8)-C(13)	1.392(3)
C(8)-C(9)	1.394(3)
C(9)-C(10)	1.387(3)
C(10)-C(11)	1.374(4)
C(11)-C(12)	1.359(4)
C(12)-C(13)	1.384(3)
C(14)-C(19)	1.383(3)
C(14)-C(15)	1.392(3)
C(15)-C(16)	1.390(3)
C(16)-C(17)	1.373(3)
C(17)-C(18)	1.374(4)
C(18)-C(19)	1.391(3)
C(20)-C(21)	1.388(3)
C(20)-C(25)	1.402(3)
C(21)-C(22)	1.397(3)
C(22)-C(23)	1.381(3)
C(23)-C(24)	1.373(3)
C(24)-C(25)	1.389(3)
C(26)-C(27)	1.400(3)
C(26)-C(31)	1.408(3)
C(27)-C(28)	1.386(3)
C(27)-C(32)	1.500(3)
C(28)-C(29)	1.392(3)
C(29)-C(30)	1.376(4)
C(29)-C(33)	1.518(4)
C(30)-C(31)	1.398(3)
C(31)-C(34)	1.504(3)
C(35)-C(40)	1.399(3)
C(35)-C(36)	1.402(3)
C(36)-C(37)	1.391(3)
C(36)-C(41)	1.504(3)
C(37)-C(38)	1.385(3)
C(38)-C(39)	1.375(3)
C(38)-C(42)	1.516(3)
C(39)-C(40)	1.405(3)
C(40)-C(43)	1.506(3)

P(2)-C(1)-P(1)	126.75(11)
P(2)-C(1)-Cl(1)	115.24(11)
P(1)-C(1)-Cl(1)	113.65(10)
N(1)-P(1)-C(1)	108.77(8)
N(1)-P(1)-C(8)	108.55(8)
C(1)-P(1)-C(8)	111.87(9)
N(1)-P(1)-C(2)	116.37(8)
C(1)-P(1)-C(2)	105.29(9)
C(8)-P(1)-C(2)	106.01(9)
N(2)-P(2)-C(1)	106.83(9)
N(2)-P(2)-C(20)	111.52(8)
C(1)-P(2)-C(20)	111.86(9)
N(2)-P(2)-C(14)	114.68(9)
C(1)-P(2)-C(14)	109.60(9)
C(20)-P(2)-C(14)	102.44(9)
C(26)-N(1)-B(1)	117.66(15)
C(26)-N(1)-P(1)	120.40(12)
B(1)-N(1)-P(1)	121.25(13)
C(35)-N(2)-B(1)	118.32(15)
C(35)-N(2)-P(2)	123.22(12)
B(1)-N(2)-P(2)	118.40(12)
N(1)-B(1)-N(2)	110.59(15)
C(7)-C(2)-C(3)	119.00(19)
C(7)-C(2)-P(1)	124.97(17)
C(3)-C(2)-P(1)	115.88(16)
C(4)-C(3)-C(2)	120.2(2)
C(5)-C(4)-C(3)	120.2(3)
C(6)-C(5)-C(4)	120.3(2)
C(5)-C(6)-C(7)	120.0(3)
C(2)-C(7)-C(6)	120.2(2)
C(13)-C(8)-C(9)	119.00(19)
C(13)-C(8)-P(1)	118.23(16)
C(9)-C(8)-P(1)	122.63(15)
C(10)-C(9)-C(8)	119.6(2)
C(11)-C(10)-C(9)	120.3(2)
C(12)-C(11)-C(10)	120.8(2)
C(11)-C(12)-C(13)	119.9(2)
C(12)-C(13)-C(8)	120.4(2)

C(19)-C(14)-C(15)	118.46(19)
C(19)-C(14)-P(2)	119.91(15)
C(15)-C(14)-P(2)	121.49(16)
C(16)-C(15)-C(14)	120.4(2)
C(17)-C(16)-C(15)	120.4(2)
C(16)-C(17)-C(18)	119.8(2)
C(17)-C(18)-C(19)	120.1(2)
C(14)-C(19)-C(18)	120.8(2)
C(21)-C(20)-C(25)	119.05(17)
C(21)-C(20)-P(2)	121.18(15)
C(25)-C(20)-P(2)	119.77(15)
C(20)-C(21)-C(22)	120.5(2)
C(23)-C(22)-C(21)	119.6(2)
C(24)-C(23)-C(22)	120.50(19)
C(23)-C(24)-C(25)	120.4(2)
C(24)-C(25)-C(20)	119.9(2)
C(27)-C(26)-C(31)	119.86(19)
C(27)-C(26)-N(1)	119.24(16)
C(31)-C(26)-N(1)	120.78(17)
C(28)-C(27)-C(26)	119.3(2)
C(28)-C(27)-C(32)	119.74(19)
C(26)-C(27)-C(32)	120.92(18)
C(27)-C(28)-C(29)	122.0(2)
C(30)-C(29)-C(28)	117.9(2)
C(30)-C(29)-C(33)	121.4(3)
C(28)-C(29)-C(33)	120.7(3)
C(29)-C(30)-C(31)	122.5(2)
C(30)-C(31)-C(26)	118.4(2)
C(30)-C(31)-C(34)	119.0(2)
C(26)-C(31)-C(34)	122.55(19)
C(40)-C(35)-C(36)	119.96(17)
C(40)-C(35)-N(2)	121.61(17)
C(36)-C(35)-N(2)	118.39(16)
C(37)-C(36)-C(35)	119.15(19)
C(37)-C(36)-C(41)	119.09(19)
C(35)-C(36)-C(41)	121.74(17)
C(38)-C(37)-C(36)	122.3(2)
C(39)-C(38)-C(37)	117.34(19)

C(39)-C(38)-C(42)	121.4(2)
C(37)-C(38)-C(42)	121.2(2)
C(38)-C(39)-C(40)	123.1(2)
C(35)-C(40)-C(39)	118.09(19)
C(35)-C(40)-C(43)	124.34(17)
C(39)-C(40)-C(43)	117.56(18)

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	48(1)	29(1)	59(1)	2(1)	22(1)	8(1)
C(1)	32(1)	23(1)	36(1)	-1(1)	10(1)	4(1)
P(1)	22(1)	26(1)	26(1)	-3(1)	6(1)	-1(1)
P(2)	22(1)	24(1)	27(1)	-1(1)	6(1)	-3(1)
N(1)	28(1)	24(1)	27(1)	-1(1)	9(1)	-2(1)
N(2)	24(1)	24(1)	28(1)	-2(1)	8(1)	-1(1)
B(1)	33(1)	26(1)	28(1)	-4(1)	10(1)	-6(1)
C(2)	23(1)	32(1)	42(1)	1(1)	8(1)	0(1)
C(3)	33(1)	66(2)	46(1)	4(1)	2(1)	-1(1)
C(4)	40(1)	79(2)	68(2)	16(2)	-10(1)	-4(1)
C(5)	27(1)	68(2)	109(3)	19(2)	8(1)	9(1)
C(6)	35(1)	68(2)	94(2)	-4(2)	27(1)	7(1)
C(7)	32(1)	46(1)	58(2)	-7(1)	15(1)	1(1)
C(8)	32(1)	29(1)	29(1)	-4(1)	4(1)	4(1)
C(9)	49(1)	39(1)	34(1)	-1(1)	10(1)	0(1)
C(10)	78(2)	49(2)	32(1)	5(1)	8(1)	6(1)
C(11)	82(2)	43(1)	34(1)	-7(1)	-7(1)	8(1)
C(12)	52(1)	37(1)	49(1)	-11(1)	-10(1)	4(1)
C(13)	37(1)	34(1)	38(1)	-6(1)	2(1)	2(1)
C(14)	25(1)	33(1)	29(1)	2(1)	7(1)	-2(1)
C(15)	34(1)	41(1)	35(1)	0(1)	5(1)	-7(1)
C(16)	36(1)	62(2)	36(1)	-2(1)	0(1)	-8(1)
C(17)	36(1)	70(2)	36(1)	11(1)	2(1)	7(1)
C(18)	51(1)	49(2)	54(2)	21(1)	1(1)	3(1)

C(19)	41(1)	37(1)	47(1)	8(1)	2(1)	-4(1)
C(20)	24(1)	26(1)	33(1)	3(1)	5(1)	-2(1)
C(21)	36(1)	33(1)	40(1)	-4(1)	8(1)	-5(1)
C(22)	42(1)	36(1)	51(1)	-7(1)	0(1)	-11(1)
C(23)	29(1)	37(1)	63(2)	7(1)	4(1)	-8(1)
C(24)	32(1)	41(1)	51(1)	9(1)	16(1)	-2(1)
C(25)	30(1)	33(1)	38(1)	5(1)	8(1)	-1(1)
C(26)	36(1)	24(1)	32(1)	-2(1)	15(1)	0(1)
C(27)	40(1)	29(1)	35(1)	1(1)	14(1)	6(1)
C(28)	56(1)	37(1)	47(1)	9(1)	20(1)	15(1)
C(29)	74(2)	32(1)	56(2)	11(1)	34(1)	4(1)
C(30)	62(2)	38(1)	64(2)	0(1)	31(1)	-12(1)
C(31)	46(1)	33(1)	42(1)	-4(1)	19(1)	-9(1)
C(32)	35(1)	43(1)	52(1)	7(1)	4(1)	7(1)
C(33)	112(3)	49(2)	101(3)	32(2)	46(2)	6(2)
C(34)	43(1)	53(2)	62(2)	-3(1)	8(1)	-22(1)
C(35)	27(1)	26(1)	30(1)	4(1)	10(1)	2(1)
C(36)	39(1)	29(1)	32(1)	-1(1)	12(1)	3(1)
C(37)	50(1)	39(1)	36(1)	2(1)	20(1)	11(1)
C(38)	41(1)	46(1)	43(1)	14(1)	20(1)	14(1)
C(39)	28(1)	47(1)	40(1)	15(1)	8(1)	6(1)
C(40)	29(1)	32(1)	29(1)	7(1)	8(1)	1(1)
C(41)	50(1)	48(1)	36(1)	-16(1)	8(1)	1(1)
C(42)	50(1)	78(2)	69(2)	19(2)	30(1)	30(1)
C(43)	30(1)	46(1)	33(1)	1(1)	1(1)	-2(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	2258(16)	5896(12)	2791(13)	35(5)
H(1B)	3425(16)	5327(12)	3341(13)	36(6)
H(3)	4910	4383	3239	60
H(4)	6733	4102	3634	79
H(5)	7698	3748	2655	83

H(6)	6864	3700	1276	76
H(7)	5018	3939	871	53
H(9)	3804	4887	253	49
H(10)	3091	4635	-1133	64
H(11)	1704	3797	-1497	67
H(12)	1030	3186	-502	59
H(13)	1756	3397	886	45
H(15)	3729	4692	4426	44
H(16)	4907	4361	5645	55
H(17)	4947	3163	6122	58
H(18)	3843	2281	5365	63
H(19)	2655	2606	4148	51
H(21)	1193	2711	2161	43
H(22)	-289	1943	2153	53
H(23)	-1338	2108	3130	53
H(24)	-898	3002	4134	49
H(25)	611	3745	4181	40
H(28)	1496	6657	-78	55
H(30)	4565	7057	1021	62
H(32A)	484	5752	353	66
H(32B)	801	5594	1320	66
H(32C)	1138	5026	686	66
H(33A)	3341	8043	156	125
H(33B)	2315	7722	-470	125
H(33C)	3500	7507	-570	125
H(34A)	5386	5684	1946	79
H(34B)	4721	5827	2648	79
H(34C)	5320	6493	2306	79
H(37)	-152	6042	4518	48
H(39)	-1761	5131	2430	46
H(41A)	1648	5877	5013	67
H(41B)	2365	5772	4337	67
H(41C)	2052	5077	4825	67
H(42A)	-2333	6421	3230	94
H(42B)	-2049	6186	4178	94
H(42C)	-2734	5648	3508	94
H(43A)	464	4331	1800	56
H(43B)	-664	4710	1417	56

H(43C)	-627	3984	1963	56

3. Computational Details

Calculations were performed with the Gaussian09 suite of software,[5] using the B3LYP functional, the 6-31G* basis set for all atoms. All geometries have been computed and optimized in the gas phase. The stationary points were characterized as minima by full vibration frequencies calculations (no imaginary frequency). The NBO analysis was carried out on the optimized geometries.

Data for Compound **4**.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.001094	0.003221	0.003756
2	6	0	-0.000367	-0.000551	1.802086
3	15	0	1.580791	-0.000128	2.542383
4	15	0	-1.504980	-0.463690	2.539355
5	7	0	1.413943	-0.443554	4.132389
6	7	0	-1.215192	-0.624701	4.159558
7	5	0	0.157761	-1.316204	4.585039
8	1	0	0.186060	-1.374175	5.787902
9	1	0	0.238593	-2.423236	4.084409
10	6	0	2.637330	-1.107983	1.509035
11	6	0	2.123634	-2.379766	1.199033
12	1	0	1.125178	-2.650463	1.527239
13	6	0	2.879156	-3.289109	0.463708
14	1	0	2.467598	-4.267515	0.231419
15	6	0	4.157893	-2.941295	0.018496
16	1	0	4.746444	-3.650727	-0.557292
17	6	0	4.669387	-1.675644	0.303374
18	1	0	5.655844	-1.391529	-0.053221
19	6	0	3.911965	-0.761184	1.040255
20	1	0	4.317422	0.224956	1.233395
21	6	0	2.395793	1.646903	2.456920
22	6	0	3.676166	1.886746	2.989154
23	1	0	4.231919	1.088040	3.467803
24	6	0	4.236869	3.162808	2.924840
25	1	0	5.222562	3.336147	3.347844
26	6	0	3.535113	4.211904	2.326763
27	1	0	3.976325	5.203886	2.278087
28	6	0	2.266341	3.981969	1.793868
29	1	0	1.714391	4.793102	1.326748
30	6	0	1.699767	2.708035	1.860332
31	1	0	0.711172	2.529052	1.452329
32	6	0	-2.170812	-1.981667	1.712350
33	6	0	-1.798731	-3.260132	2.162117
34	1	0	-1.157815	-3.355782	3.030843
35	6	0	-2.250533	-4.402755	1.500788
36	1	0	-1.962933	-5.383984	1.869045
37	6	0	-3.067633	-4.287598	0.374097
38	1	0	-3.417383	-5.178732	-0.140495

39	6	0	-3.431968	-3.022847	-0.088601
40	1	0	-4.063884	-2.923096	-0.967085
41	6	0	-2.989218	-1.877535	0.575748
42	1	0	-3.285596	-0.902589	0.204014
43	6	0	-2.850342	0.740806	2.214724
44	6	0	-2.592646	1.911131	1.490199
45	1	0	-1.586212	2.110590	1.140146
46	6	0	-3.623409	2.812370	1.215832
47	1	0	-3.414163	3.713959	0.646571
48	6	0	-4.916506	2.556081	1.674213
49	1	0	-5.717792	3.260047	1.465637
50	6	0	-5.181511	1.390351	2.398126
51	1	0	-6.186013	1.187615	2.758842
52	6	0	-4.157566	0.480527	2.657888
53	1	0	-4.377166	-0.425693	3.213835
54	6	0	2.524646	-0.333725	5.056371
55	6	0	2.582136	0.781012	5.928077
56	6	0	3.657731	0.903803	6.812905
57	1	0	3.699187	1.767217	7.472620
58	6	0	4.660801	-0.061545	6.867033
59	6	0	4.567162	-1.183469	6.052207
60	1	0	5.320042	-1.966001	6.117938
61	6	0	3.502672	-1.350271	5.152618
62	6	0	1.490142	1.817212	5.945528
63	1	0	1.696976	2.581530	6.702079
64	1	0	0.525478	1.356646	6.179458
65	1	0	1.382948	2.318255	4.978908
66	6	0	3.442945	-2.636713	4.359321
67	1	0	4.069670	-2.594618	3.460835
68	1	0	2.425191	-2.871745	4.047103
69	1	0	3.812105	-3.466139	4.973013
70	6	0	-2.153964	-0.211690	5.178275
71	6	0	-2.845059	-1.212982	5.907436
72	6	0	-3.716514	-0.834711	6.932553
73	1	0	-4.239984	-1.609190	7.488135
74	6	0	-3.920411	0.506827	7.250632
75	6	0	-3.237969	1.482201	6.536676
76	1	0	-3.380975	2.532803	6.780899
77	6	0	-2.350206	1.150425	5.501029
78	6	0	-2.664523	-2.682191	5.608329
79	1	0	-3.266790	-3.287201	6.293810
80	1	0	-1.618649	-2.987067	5.711032
81	1	0	-2.970889	-2.929753	4.586307
82	6	0	-1.666383	2.293283	4.785560
83	1	0	-0.841093	1.957596	4.158352
84	1	0	-1.268851	3.012122	5.510987
85	1	0	-2.375430	2.835073	4.149372
86	1	0	5.492444	0.047897	7.558554
87	1	0	-4.599662	0.784782	8.052483

Harmonic Frequencies

	1	2	3
	A	A	A
Frequencies --	14.8200	21.5165	32.0346
Red. masses --	5.1467	5.8621	4.7129
Frc consts --	0.0007	0.0016	0.0028
IR Inten --	0.0046	0.1414	0.0458

Thermochemistry

Sum of electronic and zero-point Energies=	-2862.970057
Sum of electronic and thermal Energies=	-2862.926590
Sum of electronic and thermal Enthalpies=	-2862.925646
Sum of electronic and thermal Free Energies=	-2863.047017

Data for compound **IV**

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011108	-0.005769	0.050016
2	6	0	0.007361	-0.023738	1.428145
3	6	0	1.201273	0.013611	-0.707082
4	6	0	1.224016	-0.039470	2.141964
5	1	0	-0.918493	-0.026715	1.991433
6	6	0	2.436447	0.011552	0.038150
7	6	0	1.305213	0.043412	-2.132319
8	6	0	2.412702	-0.022135	1.456525
9	1	0	1.206048	-0.061951	3.226458
10	6	0	3.680117	0.048522	-0.643430
11	6	0	2.533324	0.095315	-2.757100
12	1	0	3.358383	-0.029863	1.990203
13	6	0	3.731946	0.096533	-2.014139
14	1	0	4.593234	0.042580	-0.055730
15	1	0	2.600201	0.130057	-3.838520
16	1	0	4.682819	0.131324	-2.535295
17	5	0	-1.197981	-0.531324	-2.157704
18	6	0	-2.345870	-0.859082	-0.022071
19	1	0	-2.669660	-0.454723	0.937330
20	1	0	-3.203411	-0.915187	-0.694026
21	1	0	-1.911451	-1.848761	0.107653
22	6	0	0.190552	-0.896368	-4.141240
23	1	0	0.885378	-0.497522	-4.880695
24	1	0	0.531155	-1.865677	-3.781643
25	1	0	-0.797547	-0.994371	-4.593499
26	6	0	-1.862439	1.457602	-0.585286
27	1	0	-2.769641	1.513599	-1.189155
28	1	0	-2.085652	1.704925	0.454594
29	1	0	-1.119511	2.161079	-0.955951
30	6	0	-0.149429	1.433846	-3.530304
31	1	0	-1.093255	1.439810	-4.077613
32	1	0	-0.180515	2.163970	-2.724238
33	1	0	0.674882	1.688653	-4.199283
34	1	0	-2.189343	-0.225814	-2.756638
35	1	0	-1.011583	-1.706731	-2.041336

36	7	0	-1.317812	0.052171	-0.657624
37	7	0	0.072551	0.051937	-2.965679

Harmonic Frequencies

	1	2	3
	A	A	A
Frequencies --	23.3454	127.7744	150.3857
Red. masses --	3.6032	3.4749	2.2391
Frc consts --	0.0012	0.0334	0.0298
IR Inten --	0.0276	0.2553	3.3853

Thermochemistry

Sum of electronic and zero-point Energies=	-679.374063
Sum of electronic and thermal Energies=	-679.359347
Sum of electronic and thermal Enthalpies=	-679.358403
Sum of electronic and thermal Free Energies=	-679.414249

Data for BH_4^-

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.079429	-0.056169	-0.137581
2	1	0	-0.079428	-0.056169	1.884883
3	1	0	1.672069	-0.056171	0.873651
4	1	0	0.504402	1.595170	0.873651
5	5	0	0.504401	0.356673	0.873651

Harmonic Frequencies

	1	2	3
	A	A	A
Frequencies --	1108.5359	1108.5932	1108.5952
Red. masses --	1.1946	1.1946	1.1946
Frc consts --	0.8649	0.8650	0.8650
IR Inten --	88.3790	88.3430	88.3602

Thermochemistry

Sum of electronic and zero-point Energies=	-27.233650
Sum of electronic and thermal Energies=	-27.230714
Sum of electronic and thermal Enthalpies=	-27.229770
Sum of electronic and thermal Free Energies=	-27.253596

5. References

1. O. J. Cooper, J. McMaster, W. Lewis, A. J. Blake and S. T. Liddle, *Dalton Trans.* 2010, **39**, 5074.
2. Sheldrick, G.M.; University of Göttingen, *Acta Crystallogr*., 2008, Sect. **A 64**, 112.
3. G. Povie, G. Villa, L. Ford, D. Pozzi, C. H. Schiesser and P. Renaud, *Chem. Commun.* 2010, **46**, 803.
4. M.-A. Courtemanche, M.-A. Légaré, L. Maron and F.-G. Fontaine, *J. Am. Chem. Soc.* 2013, **135**, 9326.
5. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01, 2009.