Bis(phosphino)borates: a new family of monoanionic chelating phosphine ligands

J. Christopher Thomas and Jonas C. Peters*

Division of Chemistry and Chemical Engineering,
Arnold and Mabel Beckman Laboratories of Chemical Synthesis
California Institute of Technology, Pasadena, CA 91125

Supporting Information

General X-ray diffraction experimental information

Crystals were mounted on a glass fiber with Paratone-N oil. Crystallographic data were collected on a Bruker P4 diffractometer (0.71073 Å MoKα) with a CCD area detector. Data were collected using the Bruker SMART program, collecting ω scans at 5 ϕ settings. Data reduction was performed using Bruker SAINT v6.2. Structure solution and structure refinement were performed using SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997).

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 150792 (**25**[Li]), 203701 (**25**[Tl]), 203703 (**36**[Li]), 203700 (**37**[Li]), 203702 (**38**[Tl]).

Figure 1. Fully-labeled displacement ellipsoid representation of $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (**25**[Li]) (hydrogens and disordered TMEDA positions omitted for clarity).

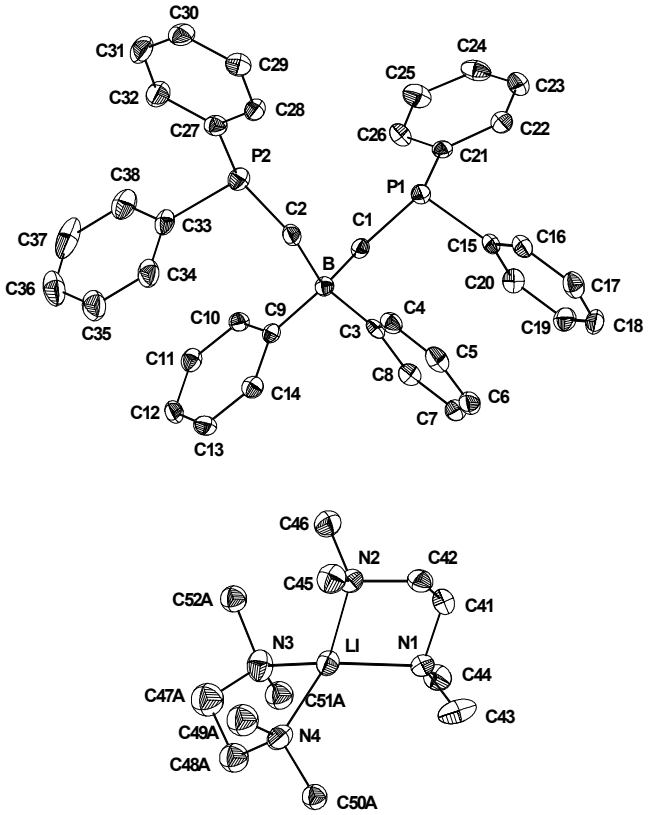

Table 1. Crystal data and structure refinement for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]).

Empirical formula	$C_{50}H_{65}BLiN_4P_2$
Formula weight	801.75
Crystallization Solvent	Toluene
Crystal Habit	Prisms
Crystal color	Colorless
Crystal size	0.41 x 0.34 x 0.16 mm^3
Data Collection	
Data Collection Temperature	98(2) K
Unit cell dimensions	a = 11.7922(6) Å
	b = 11.7081(6) Å β= 94.0620(10)°
	c = 33.1336(18) Å
Volume	4563.1(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.167 g/cm^3
F(000)	1724
θ range for data collection	1.73 to 28.39°
Completeness to θ = 28.39°	93.3%
Index ranges	$-15 \le h \le 15$, $-15 \le k \le 15$, $-44 \le l \le 43$
Reflections collected	65068
Independent reflections	10687 [R_{int}= 0.0648]
Absorption coefficient	0.133 mm^{-1}
Absorption correction	None
Structure solution and Refinement	
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10687 / 0 / 714
Goodness-of-fit on F^2	1.952
Final R indices [I>2σ(I), 7530 reflections]	R1 = 0.0608, *w*R2 = 0.0862
R indices (all data)	R1 = 0.0882, *w*R2 = 0.0879
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Largest diff. peak and hole	1.130 and -0.580 e.$Å^{-3}$

Special Refinement Details

There is disorder in one of the tetramethyl ethyldiamine ligands bound to lithium. The disorder is seen as alternate conformations of the ethyl bridge between the bound nitrogen atoms accompanied by alternate positions for the methyl groups. This disorder was successfully modeled and the hydrogen atoms associated with the disordered atoms were restrained to calculated geometries; all other hydrogen atoms were refined without restraint.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
P(1)	11110(1)	6033(1)	1606(1)	19(1)	1
P(2)	9278(1)	7541(1)	688(1)	23(1)	1
B	8947(2)	5458(2)	1165(1)	17(1)	1
C(1)	10337(2)	5271(2)	1191(1)	19(1)	1
C(2)	8661(2)	6842(2)	1114(1)	22(1)	1
C(3)	8455(2)	4973(2)	1581(1)	18(1)	1
C(4)	7890(2)	5610(2)	1862(1)	22(1)	1
C(5)	7531(2)	5144(2)	2217(1)	26(1)	1
C(6)	7727(2)	4012(2)	2308(1)	27(1)	1
C(7)	8281(2)	3345(2)	2037(1)	26(1)	1
C(8)	8622(2)	3820(2)	1687(1)	21(1)	1
C(9)	8348(2)	4741(2)	782(1)	17(1)	1
C(10)	8873(2)	4503(2)	425(1)	20(1)	1
C(11)	8327(2)	3958(2)	95(1)	23(1)	1
C(12)	7216(2)	3613(2)	107(1)	25(1)	1
C(13)	6661(2)	3818(2)	455(1)	25(1)	1
C(14)	7225(2)	4363(2)	781(1)	22(1)	1
C(15)	11059(2)	5044(2)	2038(1)	19(1)	1
C(16)	10612(2)	5422(2)	2389(1)	23(1)	1
C(17)	10512(2)	4700(2)	2716(1)	28(1)	1
C(18)	10860(2)	3584(2)	2696(1)	29(1)	1
C(19)	11325(2)	3191(2)	2351(1)	27(1)	1
C(20)	11421(2)	3913(2)	2026(1)	23(1)	1
C(21)	12617(2)	5878(2)	1506(1)	18(1)	1
C(22)	13449(2)	5947(2)	1827(1)	25(1)	1
C(23)	14593(2)	5932(2)	1764(1)	29(1)	1
C(24)	14949(2)	5867(2)	1378(1)	28(1)	1
C(25)	14147(2)	5812(2)	1056(1)	30(1)	1
C(26)	12996(2)	5817(2)	1120(1)	25(1)	1
C(27)	8910(2)	9065(2)	739(1)	23(1)	1
C(28)	8823(2)	9592(2)	1107(1)	23(1)	1
C(29)	8657(2)	10761(2)	1136(1)	26(1)	1
C(30)	8563(2)	11433(2)	795(1)	29(1)	1
C(31)	8640(2)	10926(2)	424(1)	37(1)	1
C(32)	8821(2)	9763(2)	393(1)	33(1)	1
C(33)	8301(2)	7182(2)	247(1)	24(1)	1
C(34)	7173(2)	6883(2)	276(1)	31(1)	1
C(35)	6493(2)	6575(2)	-59(1)	41(1)	1
C(36)	6909(3)	6550(2)	-431(1)	46(1)	1
C(37)	8021(3)	6839(2)	-476(1)	46(1)	1
C(38)	8729(2)	7165(2)	-131(1)	34(1)	1
Li	4435(3)	316(3)	1368(1)	28(1)	1
N(1)	5540(1)	-468(1)	1820(1)	23(1)	1
N(2)	4904(1)	1916(1)	1644(1)	25(1)	1
N(3)	4686(2)	-98(2)	767(1)	37(1)	1
N(4)	2685(2)	-76(2)	1245(1)	37(1)	1
C(41)	6222(2)	515(2)	1976(1)	28(1)	1
C(42)	5505(2)	1557(2)	2029(1)	30(1)	1
C(43)	4877(2)	-927(2)	2140(1)	43(1)	1

C(44)	6322(2)	-1372(2)	1707(1)	33(1)	1
C(45)	3979(2)	2696(2)	1730(1)	38(1)	1
C(46)	5692(2)	2560(2)	1405(1)	36(1)	1
C(47A)	3547(5)	-59(7)	559(2)	51(2)	0.445(6)
C(48A)	2787(5)	-741(6)	809(2)	40(2)	0.445(6)
C(49A)	1975(5)	842(5)	1180(2)	47(2)	0.445(6)
C(50A)	2113(5)	-936(5)	1511(2)	30(2)	0.445(6)
C(51A)	5197(6)	-1183(5)	711(2)	37(2)	0.445(6)
C(52A)	5387(6)	844(4)	554(2)	33(2)	0.445(6)
C(47B)	3576(4)	-616(5)	643(2)	42(1)	0.555(6)
C(48B)	2562(4)	-33(5)	821(1)	42(2)	0.555(6)
C(49B)	1850(4)	817(4)	1410(2)	44(1)	0.555(6)
C(50B)	2453(5)	-1161(4)	1412(2)	43(1)	0.555(6)
C(51B)	5624(4)	-936(4)	695(1)	36(1)	0.555(6)
C(52B)	4837(5)	924(4)	555(1)	45(1)	0.555(6)

Table 3. Selected bond lengths [Å] and angles [°] for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]).

P(1)-C(1)	1.829(2)	C(1)-P(1)-C(21)	104.59(9)
P(1)-C(21)	1.8401(19)	C(1)-P(1)-C(15)	103.67(9)
P(1)-C(15)	1.8438(19)	C(21)-P(1)-C(15)	99.35(8)
P(2)-C(2)	1.825(2)	C(2)-P(2)-C(33)	104.45(10)
P(2)-C(33)	1.844(2)	C(2)-P(2)-C(27)	104.73(9)
P(2)-C(27)	1.847(2)	C(33)-P(2)-C(27)	98.88(9)
B-C(3)	1.636(3)	C(3)-B-C(9)	108.43(15)
B-C(9)	1.639(3)	C(3)-B-C(1)	108.70(16)
B-C(1)	1.650(3)	C(9)-B-C(1)	110.14(15)
B-C(2)	1.662(3)	C(3)-B-C(2)	110.01(16)
		C(9)-B-C(2)	110.34(16)
		C(1)-B-C(2)	109.18(16)

Table 4. Bond lengths [Å] and angles [°] for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]).

P(1)-C(1)	1.829(2)	C(28)-H(28)	0.921(17)
P(1)-C(21)	1.8401(19)	C(29)-C(30)	1.374(3)
P(1)-C(15)	1.8438(19)	C(29)-H(29)	0.927(17)
P(2)-C(2)	1.825(2)	C(30)-C(31)	1.373(3)
P(2)-C(33)	1.844(2)	C(30)-H(30)	0.925(17)
P(2)-C(27)	1.847(2)	C(31)-C(32)	1.383(3)
B-C(3)	1.636(3)	C(31)-H(31)	0.986(19)
B-C(9)	1.639(3)	C(32)-H(32)	0.932(19)
B-C(1)	1.650(3)	C(33)-C(38)	1.384(3)
B-C(2)	1.662(3)	C(33)-C(34)	1.385(3)
C(1)-H(1A)	0.924(16)	C(34)-C(35)	1.369(3)
C(1)-H(1B)	0.999(17)	C(34)-H(34)	1.001(19)
C(2)-H(2A)	1.14(2)	C(35)-C(36)	1.360(3)
C(2)-H(2B)	0.947(17)	C(35)-H(35)	1.00(2)
C(3)-C(4)	1.397(3)	C(36)-C(37)	1.373(4)
C(3)-C(8)	1.405(3)	C(36)-H(36)	0.97(2)
C(4)-C(5)	1.389(3)	C(37)-C(38)	1.420(3)
C(4)-H(4)	0.925(15)	C(37)-H(37)	0.85(2)
C(5)-C(6)	1.375(3)	C(38)-H(38)	0.913(17)
C(5)-H(5)	0.964(17)	Li-N(3)	2.091(4)
C(6)-C(7)	1.385(3)	Li-N(1)	2.122(4)
C(6)-H(6)	0.960(18)	Li-N(4)	2.126(4)
C(7)-C(8)	1.375(3)	Li-N(2)	2.140(4)
C(7)-H(7)	0.981(18)	Li-C(47B)	2.766(6)
C(8)-H(8)	0.914(16)	Li-C(48B)	2.787(6)
C(9)-C(14)	1.396(3)	N(1)-C(43)	1.463(3)
C(9)-C(10)	1.400(3)	N(1)-C(44)	1.470(3)
C(10)-C(11)	1.384(3)	N(1)-C(41)	1.477(2)
C(10)-H(10)	0.894(15)	N(2)-C(45)	1.466(3)
C(11)-C(12)	1.374(3)	N(2)-C(46)	1.471(3)
C(11)-H(11)	0.922(16)	N(2)-C(42)	1.474(3)
C(12)-C(13)	1.385(3)	N(3)-C(52B)	1.404(5)
C(12)-H(12)	0.940(17)	N(3)-C(51A)	1.424(6)
C(13)-C(14)	1.384(3)	N(3)-C(47A)	1.467(6)
C(13)-H(13)	0.952(17)	N(3)-C(47B)	1.475(5)
C(14)-H(14)	0.962(15)	N(3)-C(51B)	1.510(5)
C(15)-C(16)	1.384(3)	N(3)-C(52A)	1.574(5)
C(15)-C(20)	1.393(3)	N(4)-C(49A)	1.370(5)
C(16)-C(17)	1.384(3)	N(4)-C(48B)	1.404(4)
C(16)-H(16)	0.942(16)	N(4)-C(50B)	1.420(5)
C(17)-C(18)	1.372(3)	N(4)-C(50A)	1.526(5)
C(17)-H(17)	0.951(16)	N(4)-C(49B)	1.561(5)
C(18)-C(19)	1.380(3)	N(4)-C(48A)	1.651(6)
C(18)-H(18)	0.908(17)	C(41)-C(42)	1.502(3)
C(19)-C(20)	1.381(3)	C(41)-H(41A)	0.993(18)
C(19)-H(19)	0.938(19)	C(41)-H(41B)	0.982(19)
C(20)-H(20)	0.924(16)	C(42)-H(42A)	1.026(18)
C(21)-C(26)	1.386(3)	C(42)-H(42B)	0.988(18)
C(21)-C(22)	1.396(3)	C(43)-H(43A)	0.834(18)
C(22)-C(23)	1.379(3)	C(43)-H(43B)	0.907(17)
C(22)-H(22)	0.941(17)	C(44)-H(44A)	1.01(2)
C(23)-C(24)	1.375(3)	C(44)-H(44B)	0.961(18)
C(23)-H(23)	0.956(18)	C(44)-H(44C)	1.00(2)
C(24)-C(25)	1.376(3)	C(45)-H(45A)	1.01(2)
C(24)-H(24)	0.941(18)	C(45)-H(45B)	1.02(2)
C(25)-C(26)	1.389(3)	C(45)-H(45C)	0.98(2)
C(25)-H(25)	0.907(18)	C(46)-H(46A)	0.981(19)
C(26)-H(26)	0.901(16)	C(46)-H(46B)	0.96(2)
C(27)-C(28)	1.379(3)	C(46)-H(46C)	1.05(2)
C(27)-C(32)	1.404(3)	C(47A)-C(48A)	1.496(9)
C(28)-C(29)	1.386(3)	C(47A)-H(47A)	0.9900

C(47A)-H(47B)	0.9900
C(48A)-H(48A)	0.9900
C(48A)-H(48B)	0.9900
C(49A)-H(49A)	0.9800
C(49A)-H(49B)	0.9800
C(49A)-H(49C)	0.9800
C(50A)-H(50A)	0.9800
C(50A)-H(50B)	0.9800
C(50A)-H(50C)	0.9800
C(51A)-H(51A)	0.9800
C(51A)-H(51B)	0.9800
C(51A)-H(51C)	0.9800
C(52A)-H(52A)	0.9800
C(52A)-H(52B)	0.9800
C(52A)-H(52C)	0.9800
C(47B)-C(48B)	1.532(7)
C(47B)-H(47C)	0.9900
C(47B)-H(47D)	0.9900
C(48B)-H(48C)	0.9900
C(48B)-H(48D)	0.9900
C(49B)-H(49D)	0.9800
C(49B)-H(49E)	0.9800
C(49B)-H(49F)	0.9800
C(50B)-H(50D)	0.9800
C(50B)-H(50E)	0.9800
C(50B)-H(50F)	0.9800
C(51B)-H(51D)	0.9800
C(51B)-H(51E)	0.9800
C(51B)-H(51F)	0.9800
C(52B)-H(52D)	0.9800
C(52B)-H(52E)	0.9800
C(52B)-H(52F)	0.9800

C(1)-P(1)-C(21)	104.59(9)
C(1)-P(1)-C(15)	103.67(9)
C(21)-P(1)-C(15)	99.35(8)
C(2)-P(2)-C(33)	104.45(10)
C(2)-P(2)-C(27)	104.73(9)
C(33)-P(2)-C(27)	98.88(9)
C(3)-B-C(9)	108.43(15)
C(3)-B-C(1)	108.70(16)
C(9)-B-C(1)	110.14(15)
C(3)-B-C(2)	110.01(16)
C(9)-B-C(2)	110.34(16)
C(1)-B-C(2)	109.18(16)
B-C(1)-P(1)	114.46(13)
B-C(1)-H(1A)	109.4(11)
P(1)-C(1)-H(1A)	104.4(11)
B-C(1)-H(1B)	111.8(10)
P(1)-C(1)-H(1B)	108.9(10)
H(1A)-C(1)-H(1B)	107.4(14)
B-C(2)-P(2)	115.25(14)
B-C(2)-H(2A)	123.9(10)
P(2)-C(2)-H(2A)	91.4(10)
B-C(2)-H(2B)	107.3(10)
P(2)-C(2)-H(2B)	101.8(10)
H(2A)-C(2)-H(2B)	114.4(15)
C(4)-C(3)-C(8)	114.38(18)
C(4)-C(3)-B	126.21(17)
C(8)-C(3)-B	119.38(17)
C(5)-C(4)-C(3)	122.8(2)
C(5)-C(4)-H(4)	118.6(10)
C(3)-C(4)-H(4)	118.6(10)
C(6)-C(5)-C(4)	120.5(2)
C(6)-C(5)-H(5)	120.1(10)
C(4)-C(5)-H(5)	119.4(11)
C(5)-C(6)-C(7)	118.7(2)
C(5)-C(6)-H(6)	120.6(11)
C(7)-C(6)-H(6)	120.6(11)
C(8)-C(7)-C(6)	119.9(2)
C(8)-C(7)-H(7)	121.0(11)
C(6)-C(7)-H(7)	119.1(11)
C(7)-C(8)-C(3)	123.7(2)
C(7)-C(8)-H(8)	119.8(10)
C(3)-C(8)-H(8)	116.6(10)
C(14)-C(9)-C(10)	114.32(18)
C(14)-C(9)-B	121.37(17)
C(10)-C(9)-B	124.24(17)
C(11)-C(10)-C(9)	123.2(2)
C(11)-C(10)-H(10)	118.1(10)
C(9)-C(10)-H(10)	118.6(10)
C(12)-C(11)-C(10)	120.3(2)
C(12)-C(11)-H(11)	119.7(10)
C(10)-C(11)-H(11)	120.0(11)
C(11)-C(12)-C(13)	118.7(2)
C(11)-C(12)-H(12)	119.8(11)
C(13)-C(12)-H(12)	121.4(11)
C(14)-C(13)-C(12)	119.9(2)
C(14)-C(13)-H(13)	120.7(10)
C(12)-C(13)-H(13)	119.3(10)
C(13)-C(14)-C(9)	123.47(19)
C(13)-C(14)-H(14)	117.9(10)
C(9)-C(14)-H(14)	118.6(10)
C(16)-C(15)-C(20)	117.60(18)
C(16)-C(15)-P(1)	119.14(15)
C(20)-C(15)-P(1)	123.23(15)
C(17)-C(16)-C(15)	121.4(2)
C(17)-C(16)-H(16)	120.5(10)
C(15)-C(16)-H(16)	118.2(10)
C(18)-C(17)-C(16)	120.2(2)
C(18)-C(17)-H(17)	118.5(10)
C(16)-C(17)-H(17)	121.3(10)
C(17)-C(18)-C(19)	119.6(2)
C(17)-C(18)-H(18)	122.4(12)
C(19)-C(18)-H(18)	118.0(12)
C(18)-C(19)-C(20)	120.1(2)
C(18)-C(19)-H(19)	121.0(12)
C(20)-C(19)-H(19)	118.9(12)
C(19)-C(20)-C(15)	121.2(2)
C(19)-C(20)-H(20)	118.9(11)
C(15)-C(20)-H(20)	119.9(11)
C(26)-C(21)-C(22)	116.73(19)
C(26)-C(21)-P(1)	123.35(15)
C(22)-C(21)-P(1)	119.55(15)
C(23)-C(22)-C(21)	121.8(2)
C(23)-C(22)-H(22)	120.8(11)
C(21)-C(22)-H(22)	117.3(11)
C(24)-C(23)-C(22)	120.5(2)
C(24)-C(23)-H(23)	118.4(11)
C(22)-C(23)-H(23)	121.1(11)
C(25)-C(24)-C(23)	119.0(2)
C(25)-C(24)-H(24)	122.0(11)
C(23)-C(24)-H(24)	118.8(11)
C(24)-C(25)-C(26)	120.4(2)
C(24)-C(25)-H(25)	118.5(13)
C(26)-C(25)-H(25)	121.1(13)

C(21)-C(26)-C(25)	121.6(2)	C(45)-N(2)-Li	117.09(17)
C(21)-C(26)-H(26)	121.5(11)	C(46)-N(2)-Li	111.83(17)
C(25)-C(26)-H(26)	116.9(11)	C(42)-N(2)-Li	102.33(15)
C(28)-C(27)-C(32)	117.11(19)	C(52B)-N(3)-C(51A)	128.7(3)
C(28)-C(27)-P(2)	123.04(16)	C(52B)-N(3)-C(47A)	83.3(3)
C(32)-C(27)-P(2)	119.54(16)	C(51A)-N(3)-C(47A)	110.4(4)
C(27)-C(28)-C(29)	121.4(2)	C(52B)-N(3)-C(47B)	110.7(3)
C(27)-C(28)-H(28)	120.2(11)	C(51A)-N(3)-C(47B)	88.3(3)
C(29)-C(28)-H(28)	118.4(11)	C(47A)-N(3)-C(47B)	27.9(3)
C(30)-C(29)-C(28)	120.9(2)	C(52B)-N(3)-C(51B)	110.8(3)
C(30)-C(29)-H(29)	120.5(11)	C(51A)-N(3)-C(51B)	22.8(3)
C(28)-C(29)-H(29)	118.6(11)	C(47A)-N(3)-C(51B)	127.1(3)
C(31)-C(30)-C(29)	118.7(2)	C(47B)-N(3)-C(51B)	109.5(3)
C(31)-C(30)-H(30)	120.9(11)	C(52B)-N(3)-C(52A)	24.6(3)
C(29)-C(30)-H(30)	120.4(11)	C(51A)-N(3)-C(52A)	109.0(3)
C(30)-C(31)-C(32)	120.8(2)	C(47A)-N(3)-C(52A)	105.1(3)
C(30)-C(31)-H(31)	121.9(11)	C(47B)-N(3)-C(52A)	130.4(3)
C(32)-C(31)-H(31)	117.3(11)	C(51B)-N(3)-C(52A)	88.3(3)
C(31)-C(32)-C(27)	121.0(2)	C(52B)-N(3)-Li	108.1(2)
C(31)-C(32)-H(32)	118.9(12)	C(51A)-N(3)-Li	114.9(3)
C(27)-C(32)-H(32)	120.0(12)	C(47A)-N(3)-Li	104.7(3)
C(38)-C(33)-C(34)	118.1(2)	C(47B)-N(3)-Li	100.3(2)
C(38)-C(33)-P(2)	118.29(18)	C(51B)-N(3)-Li	117.1(2)
C(34)-C(33)-P(2)	123.54(16)	C(52A)-N(3)-Li	112.2(2)
C(35)-C(34)-C(33)	121.4(2)	C(49A)-N(4)-C(48B)	78.2(3)
C(35)-C(34)-H(34)	118.2(12)	C(49A)-N(4)-C(50B)	129.1(3)
C(33)-C(34)-H(34)	120.4(12)	C(48B)-N(4)-C(50B)	114.5(3)
C(36)-C(35)-C(34)	120.8(3)	C(49A)-N(4)-C(50A)	108.6(3)
C(36)-C(35)-H(35)	123.8(14)	C(48B)-N(4)-C(50A)	125.7(3)
C(34)-C(35)-H(35)	115.4(14)	C(50B)-N(4)-C(50A)	23.0(3)
C(35)-C(36)-C(37)	120.2(3)	C(49A)-N(4)-C(49B)	30.3(3)
C(35)-C(36)-H(36)	120.9(14)	C(48B)-N(4)-C(49B)	107.7(3)
C(37)-C(36)-H(36)	118.8(14)	C(50B)-N(4)-C(49B)	108.6(3)
C(36)-C(37)-C(38)	119.3(3)	C(50A)-N(4)-C(49B)	85.7(3)
C(36)-C(37)-H(37)	125.4(16)	C(49A)-N(4)-C(48A)	108.3(3)
C(38)-C(37)-H(37)	115.3(16)	C(48B)-N(4)-C(48A)	31.9(2)
C(33)-C(38)-C(37)	120.2(3)	C(50B)-N(4)-C(48A)	87.0(3)
C(33)-C(38)-H(38)	117.5(12)	C(50A)-N(4)-C(48A)	104.8(3)
C(37)-C(38)-H(38)	122.3(12)	C(49B)-N(4)-C(48A)	135.1(3)
N(3)-Li-N(1)	116.79(17)	C(49A)-N(4)-Li	115.8(3)
N(3)-Li-N(4)	88.19(15)	C(48B)-N(4)-Li	102.4(2)
N(1)-Li-N(4)	125.50(17)	C(50B)-N(4)-Li	109.2(2)
N(3)-Li-N(2)	124.06(17)	C(50A)-N(4)-Li	119.7(2)
N(1)-Li-N(2)	87.14(14)	C(49B)-N(4)-Li	114.6(2)
N(4)-Li-N(2)	119.27(17)	C(48A)-N(4)-Li	98.0(2)
N(3)-Li-C(47B)	31.65(12)	N(1)-C(41)-C(42)	112.13(18)
N(1)-Li-C(47B)	127.66(19)	N(1)-C(41)-H(41A)	111.2(10)
N(4)-Li-C(47B)	57.13(14)	C(42)-C(41)-H(41A)	110.0(10)
N(2)-Li-C(47B)	141.7(2)	N(1)-C(41)-H(41B)	108.3(11)
N(3)-Li-C(48B)	60.36(13)	C(42)-C(41)-H(41B)	107.2(11)
N(1)-Li-C(48B)	144.50(19)	H(41A)-C(41)-H(41B)	107.7(15)
N(4)-Li-C(48B)	29.48(10)	N(2)-C(42)-C(41)	111.82(18)
N(2)-Li-C(48B)	125.11(19)	N(2)-C(42)-H(42A)	108.6(10)
C(47B)-Li-C(48B)	32.02(15)	C(41)-C(42)-H(42A)	108.4(10)
C(43)-N(1)-C(44)	107.32(18)	N(2)-C(42)-H(42B)	111.4(11)
C(43)-N(1)-C(41)	109.73(18)	C(41)-C(42)-H(42B)	107.8(10)
C(44)-N(1)-C(41)	108.29(17)	H(42A)-C(42)-H(42B)	108.7(15)
C(43)-N(1)-Li	109.75(17)	N(1)-C(43)-H(43A)	109.1(13)
C(44)-N(1)-Li	119.77(17)	N(1)-C(43)-H(43B)	106.8(11)
C(41)-N(1)-Li	101.65(15)	H(43A)-C(43)-H(43B)	110.7(18)
C(45)-N(2)-C(46)	107.02(19)	N(1)-C(44)-H(44A)	109.0(11)
C(45)-N(2)-C(42)	109.16(17)	N(1)-C(44)-H(44B)	109.7(11)
C(46)-N(2)-C(42)	109.18(18)	H(44A)-C(44)-H(44B)	106.4(16)

N(1)-C(44)-H(44C)	110.9(11)	N(3)-C(52A)-H(52C)	109.5
H(44A)-C(44)-H(44C)	113.3(16)	H(52A)-C(52A)-H(52C)	109.5
H(44B)-C(44)-H(44C)	107.4(16)	H(52B)-C(52A)-H(52C)	109.5
N(2)-C(45)-H(45A)	108.2(11)	N(3)-C(47B)-C(48B)	114.2(4)
N(2)-C(45)-H(45B)	110.1(11)	N(3)-C(47B)-Li	48.05(17)
H(45A)-C(45)-H(45B)	109.2(16)	C(48B)-C(47B)-Li	74.8(2)
N(2)-C(45)-H(45C)	111.2(12)	N(3)-C(47B)-H(47C)	108.7
H(45A)-C(45)-H(45C)	109.6(16)	C(48B)-C(47B)-H(47C)	108.7
H(45B)-C(45)-H(45C)	108.6(16)	Li-C(47B)-H(47C)	98.0
N(2)-C(46)-H(46A)	109.2(11)	N(3)-C(47B)-H(47D)	108.7
N(2)-C(46)-H(46B)	110.6(12)	C(48B)-C(47B)-H(47D)	108.7
H(46A)-C(46)-H(46B)	101.6(16)	Li-C(47B)-H(47D)	150.8
N(2)-C(46)-H(46C)	111.2(12)	H(47C)-C(47B)-H(47D)	107.6
H(46A)-C(46)-H(46C)	113.6(16)	N(4)-C(48B)-C(47B)	110.0(4)
H(46B)-C(46)-H(46C)	110.3(17)	N(4)-C(48B)-Li	48.16(17)
N(3)-C(47A)-C(48A)	106.7(5)	C(47B)-C(48B)-Li	73.2(2)
N(3)-C(47A)-H(47A)	110.4	N(4)-C(48B)-H(48C)	109.7
C(48A)-C(47A)-H(47A)	110.4	C(47B)-C(48B)-H(48C)	109.7
N(3)-C(47A)-H(47B)	110.4	Li-C(48B)-H(48C)	94.7
C(48A)-C(47A)-H(47B)	110.4	N(4)-C(48B)-H(48D)	109.7
H(47A)-C(47A)-H(47B)	108.6	C(47B)-C(48B)-H(48D)	109.7
C(47A)-C(48A)-N(4)	108.5(5)	Li-C(48B)-H(48D)	153.6
C(47A)-C(48A)-H(48A)	110.0	H(48C)-C(48B)-H(48D)	108.2
N(4)-C(48A)-H(48A)	110.0	N(4)-C(49B)-H(49D)	109.5
C(47A)-C(48A)-H(48B)	110.0	N(4)-C(49B)-H(49E)	109.5
N(4)-C(48A)-H(48B)	110.0	H(49D)-C(49B)-H(49E)	109.5
H(48A)-C(48A)-H(48B)	108.4	N(4)-C(49B)-H(49F)	109.5
N(4)-C(49A)-H(49A)	109.5	H(49D)-C(49B)-H(49F)	109.5
N(4)-C(49A)-H(49B)	109.5	H(49E)-C(49B)-H(49F)	109.5
H(49A)-C(49A)-H(49B)	109.5	N(4)-C(50B)-H(50D)	109.5
N(4)-C(49A)-H(49C)	109.5	N(4)-C(50B)-H(50E)	109.5
H(49A)-C(49A)-H(49C)	109.5	H(50D)-C(50B)-H(50E)	109.5
H(49B)-C(49A)-H(49C)	109.5	N(4)-C(50B)-H(50F)	109.5
N(4)-C(50A)-H(50A)	109.5	H(50D)-C(50B)-H(50F)	109.5
N(4)-C(50A)-H(50B)	109.5	H(50E)-C(50B)-H(50F)	109.5
H(50A)-C(50A)-H(50B)	109.5	N(3)-C(51B)-H(51D)	109.5
N(4)-C(50A)-H(50C)	109.5	N(3)-C(51B)-H(51E)	109.5
H(50A)-C(50A)-H(50C)	109.5	H(51D)-C(51B)-H(51E)	109.5
H(50B)-C(50A)-H(50C)	109.5	N(3)-C(51B)-H(51F)	109.5
N(3)-C(51A)-H(51A)	109.5	H(51D)-C(51B)-H(51F)	109.5
N(3)-C(51A)-H(51B)	109.5	H(51E)-C(51B)-H(51F)	109.5
H(51A)-C(51A)-H(51B)	109.5	N(3)-C(52B)-H(52D)	109.5
N(3)-C(51A)-H(51C)	109.5	N(3)-C(52B)-H(52E)	109.5
H(51A)-C(51A)-H(51C)	109.5	H(52D)-C(52B)-H(52E)	109.5
H(51B)-C(51A)-H(51C)	109.5	N(3)-C(52B)-H(52F)	109.5
N(3)-C(52A)-H(52A)	109.5	H(52D)-C(52B)-H(52F)	109.5
N(3)-C(52A)-H(52B)	109.5	H(52E)-C(52B)-H(52F)	109.5
H(52A)-C(52A)-H(52B)	109.5		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]). 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}
P(1)	200(3)	181(3)	194(3)	3(2)	-10(2)	-4(2)
P(2)	254(3)	209(3)	237(3)	17(2)	19(2)	19(3)
B	186(13)	148(12)	180(13)	-4(10)	10(10)	15(10)
C(1)	228(12)	186(12)	148(12)	21(9)	13(9)	-14(10)
C(2)	272(13)	183(11)	198(12)	-10(9)	-68(10)	-4(10)
C(3)	117(10)	221(11)	192(11)	-26(9)	-36(8)	-16(9)
C(4)	174(12)	208(12)	269(13)	-19(10)	-23(9)	13(10)
C(5)	179(12)	380(14)	213(13)	-71(11)	24(10)	-9(10)
C(6)	220(12)	389(14)	207(12)	32(11)	5(10)	-70(11)
C(7)	217(12)	257(13)	288(13)	58(11)	-43(10)	-33(10)
C(8)	188(12)	235(12)	217(12)	-39(10)	27(9)	1(10)
C(9)	176(11)	127(10)	201(11)	31(8)	-17(9)	30(8)
C(10)	181(12)	175(11)	249(12)	31(9)	-15(10)	-14(10)
C(11)	296(13)	197(11)	186(12)	0(10)	19(10)	30(10)
C(12)	322(14)	210(12)	211(13)	-10(10)	-93(11)	-22(10)
C(13)	203(13)	239(12)	308(13)	31(10)	-15(10)	-49(10)
C(14)	236(12)	193(11)	219(12)	-2(9)	25(10)	20(9)
C(15)	140(11)	228(12)	188(11)	13(9)	-33(9)	-13(9)
C(16)	200(12)	240(13)	225(12)	-26(10)	-40(9)	5(10)
C(17)	232(13)	402(15)	192(13)	-14(11)	11(10)	-5(11)
C(18)	230(13)	382(15)	237(13)	131(11)	-32(10)	-25(11)
C(19)	229(13)	240(13)	332(14)	64(11)	-24(10)	27(10)
C(20)	226(12)	254(12)	216(12)	-8(10)	27(10)	37(10)
C(21)	197(11)	123(10)	229(12)	6(9)	-13(9)	-14(8)
C(22)	253(13)	279(12)	218(13)	25(10)	12(10)	-46(10)
C(23)	226(13)	308(13)	313(14)	27(11)	-76(11)	-28(10)
C(24)	164(12)	228(12)	449(16)	-64(10)	46(11)	-11(10)
C(25)	281(14)	335(14)	291(14)	-93(11)	77(11)	-58(11)
C(26)	222(13)	282(13)	240(13)	-32(10)	-35(10)	-29(10)
C(27)	210(12)	187(11)	287(13)	2(10)	7(9)	0(9)
C(28)	248(12)	218(12)	223(13)	40(10)	13(10)	0(10)
C(29)	259(13)	236(13)	281(14)	-47(11)	41(10)	-1(10)
C(30)	317(14)	159(12)	390(15)	10(11)	-7(11)	6(10)
C(31)	582(17)	220(13)	286(14)	67(11)	-54(12)	-4(12)
C(32)	503(16)	233(13)	240(14)	-5(11)	-1(12)	-25(11)
C(33)	380(14)	142(11)	198(12)	-1(9)	-23(10)	73(10)
C(34)	389(15)	243(13)	294(14)	21(11)	-82(12)	76(11)
C(35)	519(19)	302(14)	394(17)	22(12)	-160(14)	50(13)
C(36)	680(20)	283(15)	385(18)	-61(12)	-254(16)	138(14)
C(37)	900(30)	298(15)	194(15)	13(12)	91(16)	292(15)
C(38)	423(17)	249(13)	335(15)	44(10)	35(13)	126(12)
Li	330(20)	260(20)	240(20)	8(16)	27(16)	19(17)
N(1)	235(10)	208(9)	247(10)	0(8)	44(8)	13(8)
N(2)	260(10)	233(10)	264(11)	12(8)	43(8)	22(8)
N(3)	470(13)	365(12)	287(11)	-40(9)	14(9)	78(10)
N(4)	351(11)	353(12)	413(13)	151(9)	-8(9)	-51(9)
C(41)	263(13)	319(14)	245(14)	-14(11)	-30(11)	5(11)
C(42)	339(15)	258(13)	292(14)	-39(11)	7(12)	-53(11)
C(43)	538(19)	255(15)	529(18)	-32(13)	292(15)	-51(15)
C(44)	305(15)	289(14)	389(17)	-44(12)	19(13)	27(12)
C(45)	414(17)	306(15)	416(17)	-23(13)	45(14)	61(13)
C(46)	348(16)	392(16)	354(16)	53(13)	38(13)	-37(13)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2PPh_2)_2][Li(TMEDA)_2]$ (25[Li]).

	x	y	z	U_{iso}
H(47A)	3558	-390	284	61
H(47B)	3275	740	534	61
H(48A)	3106	-1515	857	48
H(48B)	2025	-818	666	48
H(49A)	2334	1404	1011	71
H(49B)	1826	1191	1440	71
H(49C)	1256	587	1042	71
H(50A)	2599	-1610	1552	46
H(50B)	1378	-1164	1378	46
H(50C)	1992	-586	1773	46
H(51A)	5949	-1203	857	56
H(51B)	5275	-1310	422	56
H(51C)	4717	-1782	815	56
H(52A)	5034	1592	589	49
H(52B)	5396	669	265	49
H(52C)	6168	857	677	49
H(47C)	3591	-1429	725	51
H(47D)	3464	-593	344	51
H(48C)	2516	773	730	50
H(48D)	1849	-421	723	50
H(49D)	1925	813	1706	66
H(49E)	1068	619	1316	66
H(49F)	2033	1579	1311	66
H(50D)	2564	-1122	1708	65
H(50E)	2969	-1732	1311	65
H(50F)	1665	-1378	1334	65
H(51D)	5503	-1642	845	54
H(51E)	6359	-603	788	54
H(51F)	5620	-1106	405	54
H(52D)	5572	1263	646	67
H(52E)	4225	1458	608	67
H(52F)	4821	764	265	67
H(1A)	10627(14)	5563(14)	960(5)	13(5)
H(1B)	10546(14)	4444(15)	1207(5)	17(5)
H(2A)	7784(19)	7196(17)	1017(6)	60(7)
H(2B)	9037(14)	7222(14)	1337(5)	18(5)
H(4)	7748(13)	6374(13)	1809(5)	4(4)
H(5)	7133(14)	5619(14)	2397(5)	21(5)
H(6)	7493(15)	3692(15)	2555(6)	27(6)
H(7)	8426(15)	2538(16)	2101(5)	29(6)
H(8)	8998(13)	3382(13)	1511(5)	9(5)
H(10)	9592(14)	4729(13)	406(5)	6(5)
H(11)	8713(14)	3809(13)	-131(5)	11(5)
H(12)	6848(14)	3249(14)	-118(5)	17(5)
H(13)	5895(15)	3570(14)	468(5)	19(5)
H(14)	6811(13)	4509(13)	1015(5)	6(4)
H(16)	10383(14)	6191(14)	2403(5)	12(5)
H(17)	10166(14)	4948(13)	2951(5)	15(5)
H(18)	10793(15)	3084(15)	2903(5)	25(6)
H(19)	11565(16)	2431(16)	2331(5)	34(6)
H(20)	11706(14)	3627(14)	1794(5)	14(5)
H(22)	13201(15)	6040(14)	2088(5)	20(5)
H(23)	15156(16)	5968(15)	1986(5)	27(6)
H(24)	15732(16)	5819(14)	1344(5)	23(5)
H(25)	14389(16)	5767(16)	803(6)	32(6)
H(26)	12507(14)	5760(13)	900(5)	12(5)
H(28)	8865(14)	9168(14)	1342(5)	20(5)

H(29)	8597(15)	11079(14)	1389(5)	20(5)
H(30)	8459(14)	12212(15)	816(5)	17(5)
H(31)	8554(16)	11366(16)	170(6)	35(6)
H(32)	8880(16)	9444(16)	138(6)	38(7)
H(34)	6832(17)	6892(17)	544(6)	44(7)
H(35)	5700(20)	6360(20)	-6(7)	73(9)
H(36)	6445(19)	6278(18)	-666(7)	60(8)
H(37)	8339(18)	6843(18)	-699(7)	45(8)
H(38)	9473(15)	7365(15)	-147(5)	23(6)
H(41A)	6655(15)	324(14)	2235(6)	23(5)
H(41B)	6773(16)	707(15)	1778(6)	32(6)
H(42A)	4913(16)	1368(15)	2231(5)	27(6)
H(42B)	6007(15)	2168(15)	2143(5)	26(6)
H(43A)	4392(16)	-447(16)	2197(6)	22(6)
H(43B)	4538(15)	-1574(15)	2041(5)	16(5)
H(44A)	6805(17)	-1070(16)	1489(6)	37(6)
H(44B)	5895(15)	-2003(16)	1589(5)	25(6)
H(44C)	6782(17)	-1670(17)	1951(6)	42(7)
H(45A)	3579(16)	2938(16)	1463(6)	38(6)
H(45B)	3413(17)	2292(16)	1900(6)	37(6)
H(45C)	4271(17)	3375(18)	1878(6)	44(7)
H(46A)	5299(16)	2781(15)	1146(6)	32(6)
H(46B)	6280(18)	2067(17)	1317(6)	38(7)
H(46C)	6051(18)	3250(20)	1569(7)	60(8)

Figure 2. Fully-labeled displacement ellipsoid representation of $\{[Ph_2B(CH_2PPh_2)_2][Tl]\}_n$ (**25**[Tl]) (hydrogens omitted for clarity).

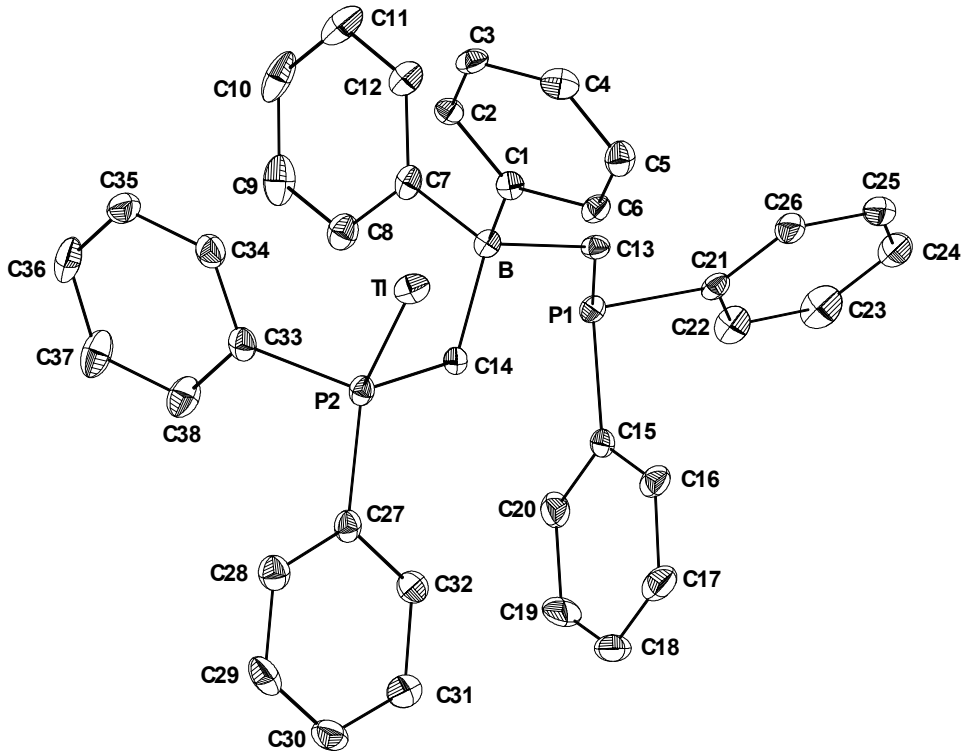

Figure 3. Fully-labeled displacement ellipsoid representation of the thallium coordination sphere of $\{[Ph_2B(CH_2PPh_2)_2][Tl]\}_n$ (**25**[Tl]).

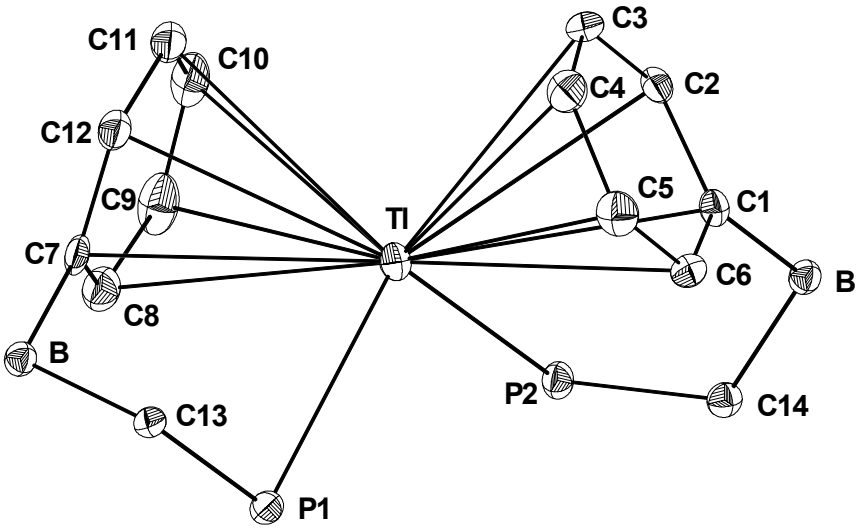

Table 7. Crystal data and structure refinement for $\{[Ph_2B(CH_2PPh_2)_2][Tl]\}_n$ (25[Tl]).

Empirical formula	$C_{34}H_{58}BP_2Tl$	
Formula weight	743.92	
Crystallization Solvent	Benzene	
Crystal Habit	triangular pyramid	
Crystal Color	yellow	
Crystal size	0.48 x 0.21 x 0.13 mm^3	
Data Collection		
Data collection temperature	98(2) K	
Unit cell dimensions	a = 11.7142(9) Å	α= 83.2880(10)°
	b = 16.4401(13) Å	β= 81.3910(10)°
	c = 19.1967(15) Å	γ = 72.0640(10)°
Volume	3467.8(5) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (#2)	
Density (calculated)	1.425 g/cm^3	
F(000)	1512	
Theta range for data collection	1.63 to 28.56°	
Completeness to θ = 28.56°	91.1%	
Index ranges	-15<=*h*<=15, -22<=*k*<=21, -24<=*l*<=25	
Reflections collected	52882	
Independent reflections	16102 [R(int) = 0.1000]	
Absorption coefficient	4.770 mm^{-1}	
Absorption correction	None	
Structure solution and Refinement		
Primary solution method	Patterson methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Calculated	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16102 / 0 / 717	
Goodness-of-fit on F^2	1.141	
Final R indices [I>2σ(I)]	R1 = 0.0370, wR2 = 0.0723	
R indices (all data)	R1 = 0.0566, wR2 = 0.0770	
Largest diff. peak and hole	2.317 and -1.572 e.$Å^{-3}$	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {[$Ph_2B(CH_2PPh_2)_2$][Tl]}$_n$ (25[Tl]). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tl(1)	8277(1)	1909(1)	115(1)	17(1)
P(1)	9741(1)	1805(1)	1291(1)	13(1)
P(2)	6365(1)	2470(1)	1290(1)	12(1)
B(1)	7742(4)	2094(3)	2619(3)	13(1)
C(1)	7175(4)	1432(2)	3168(2)	13(1)
C(2)	7747(3)	549(2)	3298(2)	12(1)
C(3)	7196(4)	-5(2)	3716(2)	15(1)
C(4)	6002(4)	325(2)	4020(2)	16(1)
C(5)	5403(4)	1199(3)	3931(2)	16(1)
C(6)	6010(4)	1726(2)	3536(2)	14(1)
C(7)	7862(4)	-945(2)	3827(3)	21(1)
C(8)	4070(4)	1541(3)	4206(3)	20(1)
C(9)	8131(3)	2693(2)	3127(2)	13(1)
C(10)	8999(4)	2304(3)	3594(2)	16(1)
C(11)	9509(4)	2759(3)	3957(2)	18(1)
C(12)	9111(4)	3657(3)	3876(3)	18(1)
C(13)	8205(4)	4074(3)	3461(2)	16(1)
C(14)	7748(4)	3587(2)	3090(2)	15(1)
C(15)	10530(4)	2301(3)	4388(3)	25(1)
C(16)	7738(4)	5044(2)	3371(3)	24(1)
C(17)	9013(3)	1520(2)	2150(2)	12(1)
C(18)	6707(3)	2715(2)	2124(2)	11(1)
C(19)	11049(4)	794(3)	1102(3)	18(1)
C(20)	10522(4)	28(3)	1240(3)	28(1)
C(21)	12063(4)	625(3)	1564(3)	27(1)
C(22)	11559(4)	819(3)	319(3)	24(1)
C(23)	10370(4)	2720(2)	1373(2)	15(1)
C(24)	11288(4)	2804(3)	724(3)	20(1)
C(25)	9285(4)	3531(2)	1346(3)	21(1)
C(26)	10934(4)	2670(3)	2047(3)	18(1)
C(27)	5638(4)	1575(2)	1444(3)	17(1)
C(28)	6682(4)	758(3)	1584(3)	26(1)
C(29)	4662(4)	1641(3)	2077(3)	26(1)
C(30)	5151(4)	1484(3)	775(3)	20(1)
C(31)	5231(4)	3501(2)	979(3)	17(1)
C(32)	3941(4)	3644(3)	1373(3)	34(1)
C(33)	5174(5)	3498(3)	187(3)	28(1)
C(34)	5672(4)	4250(3)	1078(3)	32(1)
Tl(2)	6974(1)	3275(1)	5126(1)	17(1)
P(3)	7485(1)	4078(1)	6312(1)	13(1)
P(4)	6927(1)	1951(1)	6292(1)	13(1)
B(2)	6995(4)	2842(3)	7645(3)	11(1)
C(35)	8067(4)	2758(2)	8146(2)	13(1)
C(36)	7887(4)	3402(2)	8615(2)	15(1)
C(37)	8809(4)	3487(3)	8953(3)	17(1)
C(38)	9943(4)	2879(3)	8874(2)	18(1)
C(39)	10147(4)	2196(2)	8450(2)	15(1)
C(40)	9205(4)	2156(2)	8108(2)	14(1)
C(41)	8603(4)	4258(3)	9377(3)	24(1)
C(42)	11385(4)	1547(3)	8351(3)	22(1)
C(43)	5770(4)	2816(2)	8184(2)	11(1)

C(44)	5709(4)	2038(2)	8550(2)	14(1)
C(45)	4674(4)	1918(3)	8941(2)	16(1)
C(46)	3643(4)	2631(2)	9021(2)	15(1)
C(47)	3665(4)	3435(2)	8710(2)	16(1)
C(48)	4723(4)	3509(2)	8293(2)	15(1)
C(49)	4617(4)	1030(2)	9231(3)	20(1)
C(50)	2563(4)	4205(3)	8814(3)	23(1)
C(51)	6732(4)	3797(2)	7171(2)	13(1)
C(52)	7414(4)	1994(2)	7145(2)	12(1)
C(53)	9132(4)	3927(2)	6384(2)	15(1)
C(54)	9755(4)	2960(2)	6361(3)	19(1)
C(55)	9384(4)	4221(3)	7066(3)	22(1)
C(56)	9673(4)	4378(3)	5734(3)	21(1)
C(57)	6693(4)	5269(2)	6137(3)	21(1)
C(58)	7013(4)	5853(3)	6596(3)	27(1)
C(59)	6935(4)	5554(3)	5352(3)	25(1)
C(60)	5315(4)	5392(3)	6299(3)	30(1)
C(61)	5275(4)	2019(3)	6415(2)	15(1)
C(62)	4579(4)	2963(3)	6548(3)	25(1)
C(63)	4926(4)	1840(3)	5722(3)	20(1)
C(64)	4866(4)	1453(3)	7028(3)	26(1)
C(65)	7859(4)	856(2)	5992(3)	18(1)
C(66)	7893(4)	860(3)	5194(3)	29(1)
C(67)	7417(5)	105(3)	6361(3)	34(1)
C(68)	9162(4)	701(3)	6141(3)	28(1)

Table 9. Selected bond lengths [Å] and angles [°] for {[$Ph_2B(CH_2PPh_2)_2$][Tl]}$_n$ (25[Tl]).

Tl(1)-P(2)	2.9426(11)	P(2)-Tl(1)-P(1)	78.75(3)
Tl(1)-P(1)	2.9919(12)	P(4)-Tl(2)-P(3)	78.73(3)
Tl(1)-B(1)	4.786(5)	P(4)-Tl(2)-C(12)	134.67(8)
		P(3)-Tl(2)-C(12)	99.05(8)
C(9)-Tl(2)	3.998(4)	P(4)-Tl(2)-C(11)	113.39(8)
C(10)-Tl(2)	3.675(4)	P(3)-Tl(2)-C(11)	108.27(8)
C(11)-Tl(2)	3.388(4)	P(4)-Tl(2)-C(13)	153.37(7)
C(12)-Tl(2)	3.353(4)	P(3)-Tl(2)-C(13)	110.81(7)
C(13)-Tl(2)	3.581(4)	P(4)-Tl(2)-C(10)	109.76(7)
C(14)-Tl(2)	3.889(5)	P(3)-Tl(2)-C(10)	130.08(7)
		P(4)-Tl(2)-C(14)	142.45(6)
Tl(2)-P(4)	2.9406(11)	P(3)-Tl(2)-C(14)	131.82(6)
Tl(2)-P(3)	2.9788(12)	P(4)-Tl(2)-C(9)	122.17(6)
Tl(2)-B(2)	4.807(5)	P(3)-Tl(2)-C(9)	143.24(6)

Table 10. Bond lengths [Å] and angles [°] for $\{[Ph_2B(CH_2PPh_2)_2][Tl]\}_n$ (25[Tl]).

Tl(1)-P(2)	2.9426(11)	C(20)-H(20B)	0.9800
Tl(1)-P(1)	2.9919(12)	C(20)-H(20C)	0.9800
Tl(1)-B(1)	4.786(5)	C(21)-H(21A)	0.9800
P(1)-C(17)	1.820(4)	C(21)-H(21B)	0.9800
P(1)-C(23)	1.898(4)	C(21)-H(21C)	0.9800
P(1)-C(19)	1.910(4)	C(22)-H(22A)	0.9800
P(2)-C(18)	1.825(4)	C(22)-H(22B)	0.9800
P(2)-C(27)	1.890(4)	C(22)-H(22C)	0.9800
P(2)-C(31)	1.899(4)	C(23)-C(26)	1.521(6)
B(1)-C(1)	1.645(6)	C(23)-C(25)	1.535(6)
B(1)-C(9)	1.662(6)	C(23)-C(24)	1.542(6)
B(1)-C(18)	1.664(6)	C(24)-H(24A)	0.9800
B(1)-C(17)	1.688(6)	C(24)-H(24B)	0.9800
C(1)-C(6)	1.407(5)	C(24)-H(24C)	0.9800
C(1)-C(2)	1.409(5)	C(25)-H(25A)	0.9800
C(2)-C(3)	1.388(6)	C(25)-H(25B)	0.9800
C(2)-H(2)	0.9500	C(25)-H(25C)	0.9800
C(3)-C(4)	1.398(6)	C(26)-H(26A)	0.9800
C(3)-C(7)	1.507(5)	C(26)-H(26B)	0.9800
C(4)-C(5)	1.394(6)	C(26)-H(26C)	0.9800
C(4)-H(4)	0.9500	C(27)-C(30)	1.522(6)
C(5)-C(6)	1.377(6)	C(27)-C(29)	1.528(6)
C(5)-C(8)	1.521(5)	C(27)-C(28)	1.541(6)
C(6)-H(6)	0.9500	C(28)-H(28A)	0.9800
C(7)-H(7A)	0.9800	C(28)-H(28B)	0.9800
C(7)-H(7B)	0.9800	C(28)-H(28C)	0.9800
C(7)-H(7C)	0.9800	C(29)-H(29A)	0.9800
C(8)-H(8A)	0.9800	C(29)-H(29B)	0.9800
C(8)-H(8B)	0.9800	C(29)-H(29C)	0.9800
C(8)-H(8C)	0.9800	C(30)-H(30A)	0.9800
C(9)-C(14)	1.395(5)	C(30)-H(30B)	0.9800
C(9)-C(10)	1.407(6)	C(30)-H(30C)	0.9800
C(9)-Tl(2)	3.998(4)	C(31)-C(34)	1.515(6)
C(10)-C(11)	1.388(6)	C(31)-C(33)	1.533(7)
C(10)-Tl(2)	3.675(4)	C(31)-C(32)	1.546(6)
C(10)-H(10)	0.9500	C(32)-H(32A)	0.9800
C(11)-C(12)	1.401(6)	C(32)-H(32B)	0.9800
C(11)-C(15)	1.509(6)	C(32)-H(32C)	0.9800
C(11)-Tl(2)	3.388(4)	C(33)-H(33A)	0.9800
C(12)-C(13)	1.382(6)	C(33)-H(33B)	0.9800
C(12)-Tl(2)	3.353(4)	C(33)-H(33C)	0.9800
C(12)-H(12)	0.9500	C(34)-H(34A)	0.9800
C(13)-C(14)	1.396(6)	C(34)-H(34B)	0.9800
C(13)-C(16)	1.516(5)	C(34)-H(34C)	0.9800
C(13)-Tl(2)	3.581(4)	Tl(2)-P(4)	2.9406(11)
C(14)-Tl(2)	3.889(5)	Tl(2)-P(3)	2.9788(12)
C(14)-H(14)	0.9500	Tl(2)-B(2)	4.807(5)
C(15)-H(15A)	0.9800	P(3)-C(51)	1.831(4)
C(15)-H(15B)	0.9800	P(3)-C(53)	1.893(4)
C(15)-H(15C)	0.9800	P(3)-C(57)	1.905(4)
C(16)-H(16A)	0.9800	P(4)-C(52)	1.828(4)
C(16)-H(16B)	0.9800	P(4)-C(61)	1.885(4)
C(16)-H(16C)	0.9800	P(4)-C(65)	1.899(4)
C(17)-H(17A)	0.9900	B(2)-C(43)	1.647(6)
C(17)-H(17B)	0.9900	B(2)-C(35)	1.656(6)
C(18)-H(18A)	0.9900	B(2)-C(51)	1.684(6)
C(18)-H(18B)	0.9900	B(2)-C(52)	1.690(6)
C(19)-C(21)	1.526(7)	C(35)-C(40)	1.392(5)
C(19)-C(22)	1.534(6)	C(35)-C(36)	1.415(6)
C(19)-C(20)	1.545(6)	C(36)-C(37)	1.390(6)
C(20)-H(20A)	0.9800	C(36)-H(36)	0.9500

C(37)-C(38)	1.395(6)	C(62)-H(62C)	0.9800
C(37)-C(41)	1.522(6)	C(63)-H(63A)	0.9800
C(38)-C(39)	1.404(6)	C(63)-H(63B)	0.9800
C(38)-H(38)	0.9500	C(63)-H(63C)	0.9800
C(39)-C(40)	1.387(6)	C(64)-H(64A)	0.9800
C(39)-C(42)	1.513(5)	C(64)-H(64B)	0.9800
C(40)-H(40)	0.9500	C(64)-H(64C)	0.9800
C(41)-H(41A)	0.9800	C(65)-C(66)	1.526(7)
C(41)-H(41B)	0.9800	C(65)-C(68)	1.533(6)
C(41)-H(41C)	0.9800	C(65)-C(67)	1.542(6)
C(42)-H(42A)	0.9800	C(66)-H(66A)	0.9800
C(42)-H(42B)	0.9800	C(66)-H(66B)	0.9800
C(42)-H(42C)	0.9800	C(66)-H(66C)	0.9800
C(43)-C(48)	1.402(5)	C(67)-H(67A)	0.9800
C(43)-C(44)	1.403(5)	C(67)-H(67B)	0.9800
C(44)-C(45)	1.383(6)	C(67)-H(67C)	0.9800
C(44)-H(44)	0.9500	C(68)-H(68A)	0.9800
C(45)-C(46)	1.403(5)	C(68)-H(68B)	0.9800
C(45)-C(49)	1.518(6)	C(68)-H(68C)	0.9800
C(46)-C(47)	1.391(6)		
C(46)-H(46)	0.9500	P(2)-Tl(1)-P(1)	78.75(3)
C(47)-C(48)	1.402(6)	P(2)-Tl(1)-B(1)	39.21(6)
C(47)-C(50)	1.512(5)	P(1)-Tl(1)-B(1)	40.31(6)
C(48)-H(48)	0.9500	C(17)-P(1)-C(23)	109.10(19)
C(49)-H(49A)	0.9800	C(17)-P(1)-C(19)	103.05(19)
C(49)-H(49B)	0.9800	C(23)-P(1)-C(19)	109.23(18)
C(49)-H(49C)	0.9800	C(17)-P(1)-Tl(1)	112.88(14)
C(50)-H(50A)	0.9800	C(23)-P(1)-Tl(1)	119.57(15)
C(50)-H(50B)	0.9800	C(19)-P(1)-Tl(1)	101.40(15)
C(50)-H(50C)	0.9800	C(18)-P(2)-C(27)	110.3(2)
C(51)-H(51A)	0.9900	C(18)-P(2)-C(31)	103.84(18)
C(51)-H(51B)	0.9900	C(27)-P(2)-C(31)	109.58(19)
C(52)-H(52A)	0.9900	C(18)-P(2)-Tl(1)	121.40(13)
C(52)-H(52B)	0.9900	C(27)-P(2)-Tl(1)	102.94(14)
C(53)-C(56)	1.531(6)	C(31)-P(2)-Tl(1)	108.55(15)
C(53)-C(54)	1.535(5)	C(1)-B(1)-C(9)	105.4(3)
C(53)-C(55)	1.543(6)	C(1)-B(1)-C(18)	110.5(3)
C(54)-H(54A)	0.9800	C(9)-B(1)-C(18)	109.7(3)
C(54)-H(54B)	0.9800	C(1)-B(1)-C(17)	108.8(3)
C(54)-H(54C)	0.9800	C(9)-B(1)-C(17)	108.0(3)
C(55)-H(55A)	0.9800	C(18)-B(1)-C(17)	114.1(4)
C(55)-H(55B)	0.9800	C(1)-B(1)-Tl(1)	121.8(3)
C(55)-H(55C)	0.9800	C(9)-B(1)-Tl(1)	132.6(2)
C(56)-H(56A)	0.9800	C(18)-B(1)-Tl(1)	59.5(2)
C(56)-H(56B)	0.9800	C(17)-B(1)-Tl(1)	55.0(2)
C(56)-H(56C)	0.9800	C(6)-C(1)-C(2)	114.3(4)
C(57)-C(59)	1.535(7)	C(6)-C(1)-B(1)	120.3(3)
C(57)-C(58)	1.536(6)	C(2)-C(1)-B(1)	125.3(4)
C(57)-C(60)	1.551(6)	C(3)-C(2)-C(1)	123.7(4)
C(58)-H(58A)	0.9800	C(3)-C(2)-H(2)	118.2
C(58)-H(58B)	0.9800	C(1)-C(2)-H(2)	118.2
C(58)-H(58C)	0.9800	C(2)-C(3)-C(4)	118.5(4)
C(59)-H(59A)	0.9800	C(2)-C(3)-C(7)	120.7(4)
C(59)-H(59B)	0.9800	C(4)-C(3)-C(7)	120.8(4)
C(59)-H(59C)	0.9800	C(5)-C(4)-C(3)	120.4(4)
C(60)-H(60A)	0.9800	C(5)-C(4)-H(4)	119.8
C(60)-H(60B)	0.9800	C(3)-C(4)-H(4)	119.8
C(60)-H(60C)	0.9800	C(6)-C(5)-C(4)	118.6(4)
C(61)-C(64)	1.526(6)	C(6)-C(5)-C(8)	121.0(4)
C(61)-C(63)	1.533(6)	C(4)-C(5)-C(8)	120.0(4)
C(61)-C(62)	1.545(6)	C(5)-C(6)-C(1)	124.2(4)
C(62)-H(62A)	0.9800	C(5)-C(6)-H(6)	117.9
C(62)-H(62B)	0.9800	C(1)-C(6)-H(6)	117.9

C(3)-C(7)-H(7A)	109.5	B(1)-C(17)-H(17B)	105.1
C(3)-C(7)-H(7B)	109.5	P(1)-C(17)-H(17B)	105.1
H(7A)-C(7)-H(7B)	109.5	H(17A)-C(17)-H(17B)	105.9
C(3)-C(7)-H(7C)	109.5	B(1)-C(18)-P(2)	126.9(3)
H(7A)-C(7)-H(7C)	109.5	B(1)-C(18)-H(18A)	105.6
H(7B)-C(7)-H(7C)	109.5	P(2)-C(18)-H(18A)	105.6
C(5)-C(8)-H(8A)	109.5	B(1)-C(18)-H(18B)	105.6
C(5)-C(8)-H(8B)	109.5	P(2)-C(18)-H(18B)	105.6
H(8A)-C(8)-H(8B)	109.5	H(18A)-C(18)-H(18B)	106.1
C(5)-C(8)-H(8C)	109.5	C(21)-C(19)-C(22)	110.2(4)
H(8A)-C(8)-H(8C)	109.5	C(21)-C(19)-C(20)	108.1(4)
H(8B)-C(8)-H(8C)	109.5	C(22)-C(19)-C(20)	106.5(4)
C(14)-C(9)-C(10)	114.8(4)	C(21)-C(19)-P(1)	114.3(3)
C(14)-C(9)-B(1)	125.0(4)	C(22)-C(19)-P(1)	110.3(3)
C(10)-C(9)-B(1)	119.9(3)	C(20)-C(19)-P(1)	107.2(3)
C(14)-C(9)-Tl(2)	75.4(2)	C(19)-C(20)-H(20A)	109.5
C(10)-C(9)-Tl(2)	66.7(2)	C(19)-C(20)-H(20B)	109.5
B(1)-C(9)-Tl(2)	131.6(2)	H(20A)-C(20)-H(20B)	109.5
C(11)-C(10)-C(9)	123.7(4)	C(19)-C(20)-H(20C)	109.5
C(11)-C(10)-Tl(2)	67.2(2)	H(20A)-C(20)-H(20C)	109.5
C(9)-C(10)-Tl(2)	92.7(2)	H(20B)-C(20)-H(20C)	109.5
C(11)-C(10)-H(10)	118.2	C(19)-C(21)-H(21A)	109.5
C(9)-C(10)-H(10)	118.2	C(19)-C(21)-H(21B)	109.5
Tl(2)-C(10)-H(10)	111.1	H(21A)-C(21)-H(21B)	109.5
C(10)-C(11)-C(12)	118.4(4)	C(19)-C(21)-H(21C)	109.5
C(10)-C(11)-C(15)	120.9(4)	H(21A)-C(21)-H(21C)	109.5
C(12)-C(11)-C(15)	120.6(4)	H(21B)-C(21)-H(21C)	109.5
C(10)-C(11)-Tl(2)	90.6(2)	C(19)-C(22)-H(22A)	109.5
C(12)-C(11)-Tl(2)	76.6(2)	C(19)-C(22)-H(22B)	109.5
C(15)-C(11)-Tl(2)	106.1(3)	H(22A)-C(22)-H(22B)	109.5
C(13)-C(12)-C(11)	120.4(4)	C(19)-C(22)-H(22C)	109.5
C(13)-C(12)-Tl(2)	88.0(3)	H(22A)-C(22)-H(22C)	109.5
C(11)-C(12)-Tl(2)	79.4(2)	H(22B)-C(22)-H(22C)	109.5
C(13)-C(12)-H(12)	119.8	C(26)-C(23)-C(25)	109.0(3)
C(11)-C(12)-H(12)	119.8	C(26)-C(23)-C(24)	109.8(3)
Tl(2)-C(12)-H(12)	102.7	C(25)-C(23)-C(24)	107.1(3)
C(12)-C(13)-C(14)	118.8(4)	C(26)-C(23)-P(1)	115.4(3)
C(12)-C(13)-C(16)	121.9(4)	C(25)-C(23)-P(1)	105.0(3)
C(14)-C(13)-C(16)	119.2(4)	C(24)-C(23)-P(1)	110.0(3)
C(12)-C(13)-Tl(2)	69.3(3)	C(23)-C(24)-H(24A)	109.5
C(14)-C(13)-Tl(2)	92.0(3)	C(23)-C(24)-H(24B)	109.5
C(16)-C(13)-Tl(2)	111.0(3)	H(24A)-C(24)-H(24B)	109.5
C(9)-C(14)-C(13)	123.7(4)	C(23)-C(24)-H(24C)	109.5
C(9)-C(14)-Tl(2)	84.2(3)	H(24A)-C(24)-H(24C)	109.5
C(13)-C(14)-Tl(2)	67.0(2)	H(24B)-C(24)-H(24C)	109.5
C(9)-C(14)-H(14)	118.2	C(23)-C(25)-H(25A)	109.5
C(13)-C(14)-H(14)	118.2	C(23)-C(25)-H(25B)	109.5
Tl(2)-C(14)-H(14)	121.4	H(25A)-C(25)-H(25B)	109.5
C(11)-C(15)-H(15A)	109.5	C(23)-C(25)-H(25C)	109.5
C(11)-C(15)-H(15B)	109.5	H(25A)-C(25)-H(25C)	109.5
H(15A)-C(15)-H(15B)	109.5	H(25B)-C(25)-H(25C)	109.5
C(11)-C(15)-H(15C)	109.5	C(23)-C(26)-H(26A)	109.5
H(15A)-C(15)-H(15C)	109.5	C(23)-C(26)-H(26B)	109.5
H(15B)-C(15)-H(15C)	109.5	H(26A)-C(26)-H(26B)	109.5
C(13)-C(16)-H(16A)	109.5	C(23)-C(26)-H(26C)	109.5
C(13)-C(16)-H(16B)	109.5	H(26A)-C(26)-H(26C)	109.5
H(16A)-C(16)-H(16B)	109.5	H(26B)-C(26)-H(26C)	109.5
C(13)-C(16)-H(16C)	109.5	C(30)-C(27)-C(29)	110.5(4)
H(16A)-C(16)-H(16C)	109.5	C(30)-C(27)-C(28)	107.9(3)
H(16B)-C(16)-H(16C)	109.5	C(29)-C(27)-C(28)	107.6(4)
B(1)-C(17)-P(1)	128.9(3)	C(30)-C(27)-P(2)	109.9(3)
B(1)-C(17)-H(17A)	105.1	C(29)-C(27)-P(2)	115.7(3)
P(1)-C(17)-H(17A)	105.1	C(28)-C(27)-P(2)	104.8(3)

C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(34)-C(31)-C(33)	107.3(4)
C(34)-C(31)-C(32)	108.8(4)
C(33)-C(31)-C(32)	108.7(4)
C(34)-C(31)-P(2)	108.7(3)
C(33)-C(31)-P(2)	109.4(3)
C(32)-C(31)-P(2)	113.9(3)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
P(4)-Tl(2)-P(3)	78.73(3)
P(4)-Tl(2)-C(12)	134.67(8)
P(3)-Tl(2)-C(12)	99.05(8)
P(4)-Tl(2)-C(11)	113.39(8)
P(3)-Tl(2)-C(11)	108.27(8)
C(12)-Tl(2)-C(11)	23.99(10)
P(4)-Tl(2)-C(13)	153.37(7)
P(3)-Tl(2)-C(13)	110.81(7)
C(12)-Tl(2)-C(13)	22.68(10)
C(11)-Tl(2)-C(13)	40.44(10)
P(4)-Tl(2)-C(10)	109.76(7)
P(3)-Tl(2)-C(10)	130.08(7)
C(12)-Tl(2)-C(10)	39.53(9)
C(11)-Tl(2)-C(10)	22.18(9)
C(13)-Tl(2)-C(10)	44.72(9)
P(4)-Tl(2)-C(14)	142.45(6)
P(3)-Tl(2)-C(14)	131.82(6)
C(12)-Tl(2)-C(14)	37.64(10)
C(11)-Tl(2)-C(14)	44.01(10)
C(13)-Tl(2)-C(14)	21.02(8)
C(10)-Tl(2)-C(14)	36.23(9)
P(4)-Tl(2)-C(9)	122.17(6)
P(3)-Tl(2)-C(9)	143.24(6)
C(12)-Tl(2)-C(9)	44.31(9)
C(11)-Tl(2)-C(9)	37.85(10)
C(13)-Tl(2)-C(9)	37.37(8)
C(10)-Tl(2)-C(9)	20.58(9)
C(14)-Tl(2)-C(9)	20.32(8)
P(4)-Tl(2)-B(2)	39.43(5)
P(3)-Tl(2)-B(2)	40.09(6)
C(12)-Tl(2)-B(2)	129.18(10)
C(11)-Tl(2)-B(2)	123.50(9)
C(13)-Tl(2)-B(2)	148.15(9)
C(10)-Tl(2)-B(2)	135.11(9)
C(14)-Tl(2)-B(2)	166.58(8)
C(9)-Tl(2)-B(2)	154.88(8)
C(51)-P(3)-C(53)	109.6(2)
C(51)-P(3)-C(57)	103.81(19)
C(53)-P(3)-C(57)	108.81(19)
C(51)-P(3)-Tl(2)	113.24(14)
C(53)-P(3)-Tl(2)	116.40(14)
C(57)-P(3)-Tl(2)	103.97(16)
C(52)-P(4)-C(61)	109.8(2)
C(52)-P(4)-C(65)	104.52(19)
C(61)-P(4)-C(65)	109.40(18)
C(52)-P(4)-Tl(2)	122.33(13)
C(61)-P(4)-Tl(2)	100.46(15)
C(65)-P(4)-Tl(2)	110.05(15)
C(43)-B(2)-C(35)	106.8(3)
C(43)-B(2)-C(51)	109.2(3)
C(35)-B(2)-C(51)	108.5(3)
C(43)-B(2)-C(52)	109.1(3)
C(35)-B(2)-C(52)	109.3(3)
C(51)-B(2)-C(52)	113.7(4)
C(43)-B(2)-Tl(2)	121.7(3)
C(35)-B(2)-Tl(2)	131.3(2)
C(51)-B(2)-Tl(2)	54.4(2)
C(52)-B(2)-Tl(2)	59.6(2)
C(40)-C(35)-C(36)	114.8(4)
C(40)-C(35)-B(2)	126.4(4)
C(36)-C(35)-B(2)	118.4(3)
C(37)-C(36)-C(35)	122.9(4)
C(37)-C(36)-H(36)	118.6
C(35)-C(36)-H(36)	118.6
C(36)-C(37)-C(38)	119.3(4)
C(36)-C(37)-C(41)	120.5(4)
C(38)-C(37)-C(41)	120.2(4)
C(37)-C(38)-C(39)	120.0(4)
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	118.4(4)
C(40)-C(39)-C(42)	121.6(4)
C(38)-C(39)-C(42)	120.0(4)
C(39)-C(40)-C(35)	124.4(4)
C(39)-C(40)-H(40)	117.8
C(35)-C(40)-H(40)	117.8
C(37)-C(41)-H(41A)	109.5
C(37)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(37)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5

H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(48)-C(43)-C(44)	115.1(4)
C(48)-C(43)-B(2)	125.5(3)
C(44)-C(43)-B(2)	119.3(3)
C(45)-C(44)-C(43)	123.9(4)
C(45)-C(44)-H(44)	118.0
C(43)-C(44)-H(44)	118.0
C(44)-C(45)-C(46)	118.3(4)
C(44)-C(45)-C(49)	121.1(4)
C(46)-C(45)-C(49)	120.4(4)
C(47)-C(46)-C(45)	120.6(4)
C(47)-C(46)-H(46)	119.7
C(45)-C(46)-H(46)	119.7
C(46)-C(47)-C(48)	118.5(4)
C(46)-C(47)-C(50)	120.4(4)
C(48)-C(47)-C(50)	121.1(4)
C(43)-C(48)-C(47)	123.2(4)
C(43)-C(48)-H(48)	118.4
C(47)-C(48)-H(48)	118.4
C(45)-C(49)-H(49A)	109.5
C(45)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(45)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(47)-C(50)-H(50A)	109.5
C(47)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(47)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
B(2)-C(51)-P(3)	129.0(3)
B(2)-C(51)-H(51A)	105.0
P(3)-C(51)-H(51A)	105.0
B(2)-C(51)-H(51B)	105.0
P(3)-C(51)-H(51B)	105.0
H(51A)-C(51)-H(51B)	105.9
B(2)-C(52)-P(4)	127.0(3)
B(2)-C(52)-H(52A)	105.6
P(4)-C(52)-H(52A)	105.6
B(2)-C(52)-H(52B)	105.6
P(4)-C(52)-H(52B)	105.6
H(52A)-C(52)-H(52B)	106.1
C(56)-C(53)-C(54)	107.7(3)
C(56)-C(53)-C(55)	110.1(3)
C(54)-C(53)-C(55)	108.6(4)
C(56)-C(53)-P(3)	109.3(3)
C(54)-C(53)-P(3)	105.4(3)
C(55)-C(53)-P(3)	115.3(3)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(53)-C(56)-H(56A)	109.5
C(53)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(53)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(59)-C(57)-C(58)	109.9(4)
C(59)-C(57)-C(60)	106.8(4)
C(58)-C(57)-C(60)	107.8(4)
C(59)-C(57)-P(3)	110.6(3)
C(58)-C(57)-P(3)	114.4(3)
C(60)-C(57)-P(3)	106.9(3)
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(57)-C(60)-H(60A)	109.5
C(57)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(57)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(64)-C(61)-C(63)	110.2(4)
C(64)-C(61)-C(62)	107.9(4)
C(63)-C(61)-C(62)	106.9(4)
C(64)-C(61)-P(4)	116.2(3)
C(63)-C(61)-P(4)	109.3(3)
C(62)-C(61)-P(4)	105.9(3)
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(61)-C(63)-H(63A)	109.5
C(61)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(61)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(61)-C(64)-H(64A)	109.5
C(61)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(61)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(66)-C(65)-C(68)	106.9(4)
C(66)-C(65)-C(67)	109.5(4)
C(68)-C(65)-C(67)	108.1(4)
C(66)-C(65)-P(4)	109.4(3)
C(68)-C(65)-P(4)	108.0(3)
C(67)-C(65)-P(4)	114.6(3)
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5

H(66A)-C(66)-H(66B)	109.5	H(67A)-C(67)-H(67C)	109.5
C(65)-C(66)-H(66C)	109.5	H(67B)-C(67)-H(67C)	109.5
H(66A)-C(66)-H(66C)	109.5	C(65)-C(68)-H(68A)	109.5
H(66B)-C(66)-H(66C)	109.5	C(65)-C(68)-H(68B)	109.5
C(65)-C(67)-H(67A)	109.5	H(68A)-C(68)-H(68B)	109.5
C(65)-C(67)-H(67B)	109.5	C(65)-C(68)-H(68C)	109.5
H(67A)-C(67)-H(67B)	109.5	H(68A)-C(68)-H(68C)	109.5
C(65)-C(67)-H(67C)	109.5	H(68B)-C(68)-H(68C)	109.5

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $\{[Ph_2B(CH_2PPh_2)_2][Tl]\}_n$ (25[Tl]). 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}
Tl(1)	19(1)	17(1)	14(1)	-4(1)	0(1)	-5(1)
P(1)	12(1)	13(1)	11(1)	-1(1)	1(1)	-2(1)
P(2)	12(1)	10(1)	12(1)	-1(1)	-2(1)	-2(1)
B(1)	14(2)	15(2)	10(3)	1(2)	0(2)	-7(2)
C(1)	15(2)	15(2)	11(2)	0(2)	-6(2)	-5(2)
C(2)	7(2)	18(2)	10(2)	-3(2)	-3(2)	-1(2)
C(3)	16(2)	14(2)	16(3)	1(2)	-6(2)	-5(2)
C(4)	16(2)	19(2)	16(3)	5(2)	-4(2)	-11(2)
C(5)	15(2)	23(2)	10(2)	-3(2)	-1(2)	-5(2)
C(6)	15(2)	11(2)	12(3)	-3(2)	0(2)	0(2)
C(7)	20(2)	15(2)	25(3)	3(2)	1(2)	-4(2)
C(8)	15(2)	21(2)	21(3)	2(2)	-2(2)	-4(2)
C(9)	11(2)	13(2)	11(2)	-1(2)	3(2)	-2(2)
C(10)	14(2)	15(2)	15(3)	2(2)	3(2)	-3(2)
C(11)	15(2)	27(2)	9(3)	-5(2)	0(2)	-2(2)
C(12)	19(2)	22(2)	16(3)	-7(2)	2(2)	-11(2)
C(13)	14(2)	20(2)	12(3)	-6(2)	5(2)	-5(2)
C(14)	11(2)	16(2)	14(3)	0(2)	1(2)	0(2)
C(15)	22(2)	34(3)	19(3)	-10(2)	-9(2)	-4(2)
C(16)	30(3)	16(2)	27(3)	-1(2)	-5(2)	-7(2)
C(17)	11(2)	14(2)	11(2)	-3(2)	1(2)	-4(2)
C(18)	12(2)	12(2)	11(2)	0(2)	-4(2)	-3(2)
C(19)	17(2)	19(2)	15(3)	-5(2)	4(2)	-1(2)
C(20)	31(3)	15(2)	34(3)	-7(2)	8(2)	-2(2)
C(21)	19(2)	23(2)	30(3)	3(2)	-5(2)	8(2)
C(22)	21(2)	25(2)	21(3)	-5(2)	4(2)	-2(2)
C(23)	16(2)	15(2)	15(3)	-2(2)	-2(2)	-7(2)
C(24)	20(2)	21(2)	17(3)	1(2)	0(2)	-7(2)
C(25)	23(2)	17(2)	21(3)	3(2)	0(2)	-7(2)
C(26)	20(2)	20(2)	18(3)	-2(2)	-3(2)	-10(2)
C(27)	23(2)	14(2)	17(3)	1(2)	-7(2)	-11(2)
C(28)	36(3)	14(2)	32(3)	1(2)	-15(2)	-10(2)
C(29)	31(3)	38(3)	18(3)	1(2)	-2(2)	-23(2)
C(30)	26(2)	19(2)	19(3)	-1(2)	-10(2)	-10(2)
C(31)	19(2)	13(2)	19(3)	3(2)	-10(2)	-1(2)
C(32)	25(3)	33(3)	32(4)	4(2)	-2(2)	4(2)
C(33)	39(3)	20(2)	24(3)	1(2)	-13(2)	-4(2)
C(34)	37(3)	19(2)	39(4)	8(2)	-21(3)	-4(2)
Tl(2)	19(1)	21(1)	13(1)	3(1)	-4(1)	-7(1)
P(3)	15(1)	13(1)	11(1)	1(1)	0(1)	-4(1)
P(4)	13(1)	12(1)	12(1)	-1(1)	-1(1)	-3(1)
B(2)	10(2)	9(2)	11(3)	-4(2)	2(2)	2(2)
C(35)	15(2)	13(2)	11(2)	2(2)	-1(2)	-6(2)
C(36)	14(2)	14(2)	13(3)	1(2)	-1(2)	-2(2)
C(37)	22(2)	15(2)	14(3)	0(2)	-3(2)	-5(2)
C(38)	18(2)	23(2)	14(3)	1(2)	-7(2)	-7(2)
C(39)	17(2)	15(2)	12(3)	1(2)	2(2)	-5(2)
C(40)	18(2)	11(2)	13(3)	1(2)	1(2)	-7(2)
C(41)	30(3)	25(2)	17(3)	-3(2)	-12(2)	-5(2)
C(42)	16(2)	26(2)	19(3)	-4(2)	-3(2)	-1(2)
C(43)	15(2)	13(2)	8(2)	-1(2)	-1(2)	-8(2)

C(44)	14(2)	13(2)	14(3)	-2(2)	-3(2)	0(2)
C(45)	21(2)	17(2)	12(3)	-3(2)	-4(2)	-6(2)
C(46)	13(2)	21(2)	13(3)	-1(2)	3(2)	-9(2)
C(47)	18(2)	16(2)	14(3)	-3(2)	-3(2)	-4(2)
C(48)	17(2)	13(2)	14(3)	1(2)	0(2)	-6(2)
C(49)	29(3)	14(2)	17(3)	1(2)	2(2)	-11(2)
C(50)	17(2)	19(2)	28(3)	-3(2)	9(2)	-2(2)
C(51)	12(2)	18(2)	8(2)	-1(2)	4(2)	-5(2)
C(52)	12(2)	13(2)	11(2)	1(2)	-3(2)	-2(2)
C(53)	14(2)	17(2)	16(3)	1(2)	-3(2)	-6(2)
C(54)	12(2)	18(2)	23(3)	-1(2)	1(2)	-2(2)
C(55)	23(2)	31(2)	18(3)	3(2)	-4(2)	-16(2)
C(56)	22(2)	27(2)	16(3)	0(2)	6(2)	-13(2)
C(57)	25(2)	12(2)	21(3)	5(2)	0(2)	-2(2)
C(58)	37(3)	10(2)	27(3)	2(2)	1(2)	-1(2)
C(59)	27(3)	22(2)	21(3)	8(2)	-1(2)	-4(2)
C(60)	25(3)	20(2)	34(3)	11(2)	-4(2)	5(2)
C(61)	11(2)	21(2)	15(3)	-4(2)	-2(2)	-6(2)
C(62)	15(2)	31(3)	28(3)	-11(2)	-5(2)	-1(2)
C(63)	17(2)	23(2)	23(3)	-2(2)	-4(2)	-8(2)
C(64)	23(2)	37(3)	23(3)	-2(2)	-5(2)	-16(2)
C(65)	19(2)	14(2)	19(3)	-7(2)	-3(2)	0(2)
C(66)	26(3)	31(3)	27(3)	-15(2)	-1(2)	1(2)
C(67)	41(3)	18(2)	39(4)	-3(2)	-4(3)	-4(2)
C(68)	24(3)	30(3)	29(3)	-13(2)	-3(2)	-3(2)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for {[$Ph_2B(CH_2PPh_2)_2$][Tl]}$_n$ (25[Tl]).

	x	y	z	U(eq)
H(2)	8555	320	3088	15
H(4)	5596	-48	4290	19
H(6)	5617	2325	3509	17
H(7A)	8618	-1081	3506	32
H(7B)	7358	-1286	3729	32
H(7C)	8042	-1079	4317	32
H(8A)	3916	2100	4392	30
H(8B)	3855	1140	4584	30
H(8C)	3582	1603	3820	30
H(10)	9249	1696	3664	19
H(12)	9467	3980	4107	22
H(14)	7142	3881	2795	18
H(15A)	11284	2111	4071	37
H(15B)	10354	1803	4661	37
H(15C)	10615	2693	4711	37
H(16A)	7958	5290	3754	35
H(16B)	6856	5223	3385	35
H(16C)	8097	5247	2916	35
H(17A)	8869	969	2099	14
H(17B)	9645	1385	2471	14
H(18A)	6904	3264	2022	14
H(18B)	5933	2841	2439	14
H(20A)	11104	-475	1029	43
H(20B)	9767	173	1028	43
H(20C)	10363	-101	1750	43
H(21A)	12611	45	1508	41
H(21B)	11716	679	2060	41
H(21C)	12512	1044	1421	41
H(22A)	11915	1292	207	36
H(22B)	10907	904	27	36
H(22C)	12182	276	221	36
H(24A)	10946	2787	292	29
H(24B)	12034	2328	752	29
H(24C)	11469	3349	715	29
H(25A)	8705	3519	1769	31
H(25B)	8895	3553	924	31
H(25C)	9563	4038	1328	31
H(26A)	11216	3173	2046	27
H(26B)	11618	2148	2072	27
H(26C)	10329	2658	2457	27
H(28A)	6371	261	1668	39
H(28B)	7038	814	2000	39
H(28C)	7300	679	1172	39
H(29A)	4412	1117	2146	39
H(29B)	3964	2137	1990	39
H(29C)	4984	1710	2502	39
H(30A)	5782	1454	372	30
H(30B)	4451	1980	691	30
H(30C)	4906	959	829	30
H(32A)	3976	3587	1884	51
H(32B)	3594	3217	1249	51
H(32C)	3435	4221	1236	51
H(33A)	4563	4018	30	42
H(33B)	4959	2992	99	42
H(33C)	5965	3484	-75	42
H(34A)	6518	4138	872	47
H(34B)	5604	4323	1583	47

H(34C)	5178	4773	841	47
H(36)	7102	3794	8702	18
H(38)	10577	2926	9108	21
H(40)	9346	1686	7829	17
H(41A)	8682	4751	9055	36
H(41B)	9204	4123	9710	36
H(41C)	7790	4395	9638	36
H(42A)	11458	1241	7930	32
H(42B)	11493	1136	8767	32
H(42C)	12007	1843	8292	32
H(44)	6422	1564	8528	17
H(46)	2924	2564	9290	18
H(48)	4731	4057	8074	18
H(49A)	4393	753	8870	30
H(49B)	4011	1079	9648	30
H(49C)	5409	686	9364	30
H(50A)	1850	4066	8715	35
H(50B)	2680	4689	8491	35
H(50C)	2444	4360	9303	35
H(51A)	6814	4199	7493	16
H(51B)	5863	3967	7111	16
H(52A)	7207	1522	7454	15
H(52B)	8308	1828	7063	15
H(54A)	9590	2761	5935	28
H(54B)	9445	2656	6780	28
H(54C)	10629	2844	6352	28
H(55A)	10253	4016	7102	34
H(55B)	8949	3986	7476	34
H(55C)	9108	4849	7051	34
H(56A)	10552	4219	5729	32
H(56B)	9331	5000	5753	32
H(56C)	9483	4204	5305	32
H(58A)	7842	5869	6443	40
H(58B)	6944	5630	7092	40
H(58C)	6455	6434	6547	40
H(59A)	6720	5184	5062	38
H(59B)	7793	5512	5232	38
H(59C)	6446	6149	5261	38
H(60A)	4871	5962	6108	44
H(60B)	5093	5338	6812	44
H(60C)	5112	4953	6080	44
H(62A)	3710	3051	6560	37
H(62B)	4843	3341	6167	37
H(62C)	4744	3094	7001	37
H(63A)	4043	2002	5747	30
H(63B)	5267	1228	5649	30
H(63C)	5244	2176	5328	30
H(64A)	5160	1533	7459	39
H(64B)	5193	851	6920	39
H(64C)	3981	1613	7098	39
H(66A)	8319	1263	4956	44
H(66B)	7065	1037	5070	44
H(66C)	8316	283	5044	44
H(67A)	6612	164	6238	51
H(67B)	7379	110	6874	51
H(67C)	7980	-438	6206	51
H(68A)	9676	165	5948	42
H(68B)	9186	662	6652	42
H(68C)	9456	1178	5918	42

Figure 4. Fully-labeled displacement ellipsoid representation of $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (**36**[Li]) (hydrogens omitted for clarity).

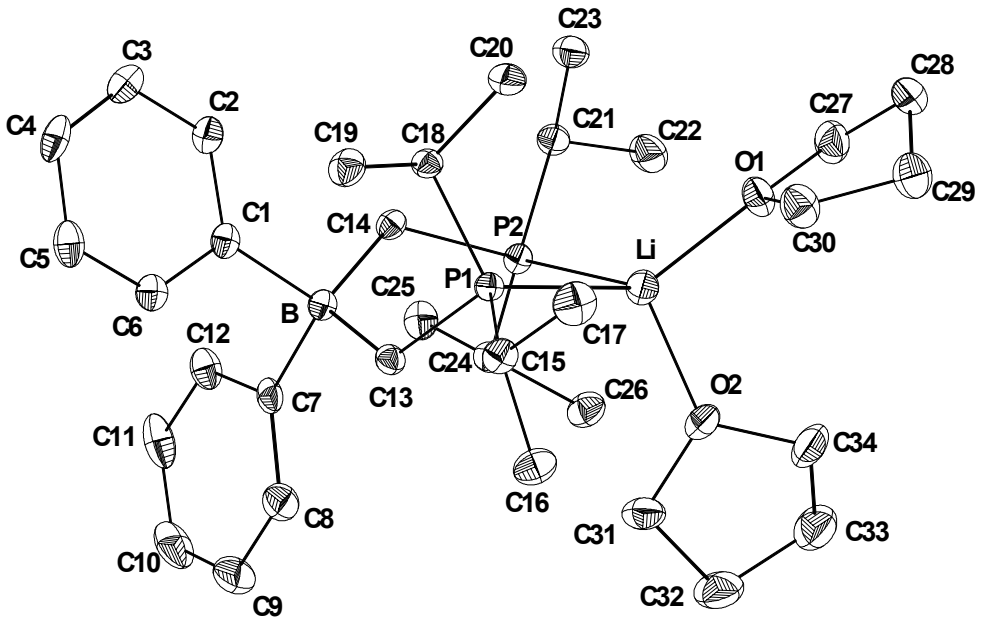

Table 13. Crystal data and structure refinement for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]).

Empirical formula	$C_{34}H_{58}BLiO_2P_2$
Formula weight	578.49
Crystallization solvent	Diethyl ether / THF
Crystal Habit	Block
Crystal Color	Colorless
Crystal size	0.33 x 0.33 x 0.27 mm^3
Data Collection	
Data collection temperature	98(2) K
Unit cell dimensions	a = 11.3226(9) Å
	b = 15.4574(12) Å β= 94.7040(10)°
	c = 20.5142(16) Å
Volume	3578.3(5) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.074 g/cm^3
F(000)	1264
θ range for data collection	1.65 to 28.61°
Completeness to θ= 28.61°	90.0%
Index ranges	-13<=*h*<=15, -20<=*k*<=14, -23<=*l*<=26
Reflections collected	22237
Independent reflections	8249 [R(int) = 0.0549]
Absorption coefficient	0.148 mm^{-1}
Absorption correction	None
Structure solution and refinement	
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8249 / 0 / 369
Goodness-of-fit on F^2	1.361
Final R indices [I>2σ(I)]	R1 = 0.0465, wR2 = 0.0868
R indices (all data)	R1 = 0.0776, wR2 = 0.0940
Largest diff. peak and hole	0.498 and -0.357 $e.Å^{-3}$

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Li	9444(2)	3276(2)	2214(1)	21(1)
P(1)	7203(1)	2968(1)	1905(1)	15(1)
P(2)	9861(1)	3304(1)	988(1)	15(1)
B	7476(2)	2528(1)	483(1)	16(1)
C(1)	6215(1)	2860(1)	101(1)	16(1)
C(2)	5994(2)	3695(1)	-146(1)	20(1)
C(3)	4902(2)	3947(1)	-453(1)	24(1)
C(4)	3986(2)	3357(1)	-535(1)	25(1)
C(5)	4169(2)	2518(1)	-306(1)	24(1)
C(6)	5258(1)	2283(1)	2(1)	20(1)
C(7)	7903(1)	1695(1)	53(1)	18(1)
C(8)	8039(2)	843(1)	282(1)	26(1)
C(9)	8401(2)	168(1)	-104(1)	34(1)
C(10)	8635(2)	313(1)	-742(1)	34(1)
C(11)	8494(2)	1140(1)	-995(1)	31(1)
C(12)	8127(1)	1809(1)	-603(1)	22(1)
C(13)	7232(1)	2192(1)	1230(1)	16(1)
C(14)	8454(1)	3331(1)	482(1)	15(1)
C(15)	6306(2)	2396(1)	2494(1)	20(1)
C(16)	6926(2)	1561(1)	2724(1)	27(1)
C(17)	6078(2)	2956(1)	3088(1)	30(1)
C(18)	6212(1)	3852(1)	1582(1)	17(1)
C(19)	4886(1)	3650(1)	1492(1)	25(1)
C(20)	6472(2)	4691(1)	1964(1)	26(1)
C(21)	10532(1)	4358(1)	773(1)	18(1)
C(22)	11837(2)	4439(1)	1026(1)	27(1)
C(23)	9811(2)	5096(1)	1047(1)	23(1)
C(24)	10725(1)	2458(1)	589(1)	18(1)
C(25)	10934(2)	2642(1)	-123(1)	22(1)
C(26)	11895(1)	2221(1)	979(1)	24(1)
O(1)	9824(1)	4236(1)	2821(1)	24(1)
C(27)	10811(2)	4834(1)	2902(1)	30(1)
C(28)	10630(2)	5346(1)	3514(1)	33(1)
C(29)	10043(2)	4685(1)	3929(1)	34(1)
C(30)	9224(2)	4219(1)	3419(1)	30(1)
O(2)	10265(1)	2291(1)	2608(1)	27(1)
C(31)	10219(2)	1433(1)	2327(1)	27(1)
C(32)	11324(2)	959(1)	2618(1)	39(1)
C(33)	12075(2)	1658(1)	2968(1)	37(1)
C(34)	11158(2)	2302(1)	3150(1)	34(1)

Table 15. Selected bond lengths [Å] and angles [°] for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]).

Li-O(2)	1.928(3)	O(2)-Li-O(1)	104.93(14)
Li-O(1)	1.962(3)	O(2)-Li-P(2)	107.46(13)
Li-P(2)	2.596(3)	O(1)-Li-P(2)	123.68(13)
Li-P(1)	2.608(3)	O(2)-Li-P(1)	112.56(13)
Li-B	4.197(3)	O(1)-Li-P(1)	116.77(13)
		P(2)-Li-P(1)	91.07(9)

Table 16. Bond lengths [Å] and angles [°] for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]).

Li-O(2)	1.928(3)	C(21)-H(21)	1.0000
Li-O(1)	1.962(3)	C(22)-H(22A)	0.9800
Li-P(2)	2.596(3)	C(22)-H(22B)	0.9800
Li-P(1)	2.608(3)	C(22)-H(22C)	0.9800
Li-B	4.197(3)	C(23)-H(23A)	0.9800
P(1)-C(13)	1.8349(16)	C(23)-H(23B)	0.9800
P(1)-C(18)	1.8566(16)	C(23)-H(23C)	0.9800
P(1)-C(15)	1.8629(16)	C(24)-C(25)	1.524(2)
P(2)-C(14)	1.8289(16)	C(24)-C(26)	1.534(2)
P(2)-C(24)	1.8625(16)	C(24)-H(24)	1.0000
P(2)-C(21)	1.8662(16)	C(25)-H(25A)	0.9800
B-C(1)	1.653(2)	C(25)-H(25B)	0.9800
B-C(7)	1.654(2)	C(25)-H(25C)	0.9800
B-C(13)	1.664(2)	C(26)-H(26A)	0.9800
B-C(14)	1.664(2)	C(26)-H(26B)	0.9800
C(1)-C(2)	1.401(2)	C(26)-H(26C)	0.9800
C(1)-C(6)	1.406(2)	O(1)-C(27)	1.449(2)
C(2)-C(3)	1.397(2)	O(1)-C(30)	1.452(2)
C(2)-H(2)	0.9500	C(27)-C(28)	1.512(3)
C(3)-C(4)	1.381(2)	C(27)-H(27A)	0.9900
C(3)-H(3)	0.9500	C(27)-H(27B)	0.9900
C(4)-C(5)	1.389(2)	C(28)-C(29)	1.517(3)
C(4)-H(4)	0.9500	C(28)-H(28A)	0.9900
C(5)-C(6)	1.386(2)	C(28)-H(28B)	0.9900
C(5)-H(5)	0.9500	C(29)-C(30)	1.521(3)
C(6)-H(6)	0.9500	C(29)-H(29A)	0.9900
C(7)-C(12)	1.402(2)	C(29)-H(29B)	0.9900
C(7)-C(8)	1.402(2)	C(30)-H(30A)	0.9900
C(8)-C(9)	1.393(2)	C(30)-H(30B)	0.9900
C(8)-H(8)	0.9500	O(2)-C(34)	1.440(2)
C(9)-C(10)	1.375(3)	O(2)-C(31)	1.446(2)
C(9)-H(9)	0.9500	C(31)-C(32)	1.527(2)
C(10)-C(11)	1.383(3)	C(31)-H(31A)	0.9900
C(10)-H(10)	0.9500	C(31)-H(31B)	0.9900
C(11)-C(12)	1.393(2)	C(32)-C(33)	1.518(3)
C(11)-H(11)	0.9500	C(32)-H(32A)	0.9900
C(12)-H(12)	0.9500	C(32)-H(32B)	0.9900
C(13)-H(13A)	0.9900	C(33)-C(34)	1.509(3)
C(13)-H(13B)	0.9900	C(33)-H(33A)	0.9900
C(14)-H(14A)	0.9900	C(33)-H(33B)	0.9900
C(14)-H(14B)	0.9900	C(34)-H(34A)	0.9900
C(15)-C(16)	1.526(2)	C(34)-H(34B)	0.9900
C(15)-C(17)	1.535(2)		
C(15)-H(15)	1.0000	O(2)-Li-O(1)	104.93(14)
C(16)-H(16A)	0.9800	O(2)-Li-P(2)	107.46(13)
C(16)-H(16B)	0.9800	O(1)-Li-P(2)	123.68(13)
C(16)-H(16C)	0.9800	O(2)-Li-P(1)	112.56(13)
C(17)-H(17A)	0.9800	O(1)-Li-P(1)	116.77(13)
C(17)-H(17B)	0.9800	P(2)-Li-P(1)	91.07(9)
C(17)-H(17C)	0.9800	O(2)-Li-B	109.99(11)
C(18)-C(19)	1.530(2)	O(1)-Li-B	144.99(13)
C(18)-C(20)	1.531(2)	P(2)-Li-B	46.47(5)
C(18)-H(18)	1.0000	P(1)-Li-B	46.05(5)
C(19)-H(19A)	0.9800	C(13)-P(1)-C(18)	105.04(7)
C(19)-H(19B)	0.9800	C(13)-P(1)-C(15)	102.86(8)
C(19)-H(19C)	0.9800	C(18)-P(1)-C(15)	103.61(7)
C(20)-H(20A)	0.9800	C(13)-P(1)-Li	103.02(8)
C(20)-H(20B)	0.9800	C(18)-P(1)-Li	119.99(8)
C(20)-H(20C)	0.9800	C(15)-P(1)-Li	120.06(9)
C(21)-C(22)	1.530(2)	C(14)-P(2)-C(24)	103.39(8)
C(21)-C(23)	1.535(2)	C(14)-P(2)-C(21)	101.43(7)

C(24)-P(2)-C(21)	105.70(7)	C(16)-C(15)-P(1)	109.94(11)
C(14)-P(2)-Li	109.33(8)	C(17)-C(15)-P(1)	112.55(12)
C(24)-P(2)-Li	123.93(8)	C(16)-C(15)-H(15)	108.2
C(21)-P(2)-Li	110.63(8)	C(17)-C(15)-H(15)	108.2
C(1)-B-C(7)	105.53(13)	P(1)-C(15)-H(15)	108.2
C(1)-B-C(13)	109.39(13)	C(15)-C(16)-H(16A)	109.5
C(7)-B-C(13)	109.01(13)	C(15)-C(16)-H(16B)	109.5
C(1)-B-C(14)	108.46(13)	H(16A)-C(16)-H(16B)	109.5
C(7)-B-C(14)	110.90(13)	C(15)-C(16)-H(16C)	109.5
C(13)-B-C(14)	113.25(13)	H(16A)-C(16)-H(16C)	109.5
C(1)-B-Li	133.90(11)	H(16B)-C(16)-H(16C)	109.5
C(7)-B-Li	120.47(10)	C(15)-C(17)-H(17A)	109.5
C(13)-B-Li	54.76(9)	C(15)-C(17)-H(17B)	109.5
C(14)-B-Li	59.18(9)	H(17A)-C(17)-H(17B)	109.5
C(2)-C(1)-C(6)	114.77(15)	C(15)-C(17)-H(17C)	109.5
C(2)-C(1)-B	125.40(15)	H(17A)-C(17)-H(17C)	109.5
C(6)-C(1)-B	119.83(15)	H(17B)-C(17)-H(17C)	109.5
C(3)-C(2)-C(1)	123.06(16)	C(19)-C(18)-C(20)	112.40(14)
C(3)-C(2)-H(2)	118.5	C(19)-C(18)-P(1)	116.81(12)
C(1)-C(2)-H(2)	118.5	C(20)-C(18)-P(1)	110.76(12)
C(4)-C(3)-C(2)	119.93(17)	C(19)-C(18)-H(18)	105.3
C(4)-C(3)-H(3)	120.0	C(20)-C(18)-H(18)	105.3
C(2)-C(3)-H(3)	120.0	P(1)-C(18)-H(18)	105.3
C(3)-C(4)-C(5)	119.05(16)	C(18)-C(19)-H(19A)	109.5
C(3)-C(4)-H(4)	120.5	C(18)-C(19)-H(19B)	109.5
C(5)-C(4)-H(4)	120.5	H(19A)-C(19)-H(19B)	109.5
C(6)-C(5)-C(4)	120.04(17)	C(18)-C(19)-H(19C)	109.5
C(6)-C(5)-H(5)	120.0	H(19A)-C(19)-H(19C)	109.5
C(4)-C(5)-H(5)	120.0	H(19B)-C(19)-H(19C)	109.5
C(5)-C(6)-C(1)	123.13(17)	C(18)-C(20)-H(20A)	109.5
C(5)-C(6)-H(6)	118.4	C(18)-C(20)-H(20B)	109.5
C(1)-C(6)-H(6)	118.4	H(20A)-C(20)-H(20B)	109.5
C(12)-C(7)-C(8)	114.59(16)	C(18)-C(20)-H(20C)	109.5
C(12)-C(7)-B	119.85(15)	H(20A)-C(20)-H(20C)	109.5
C(8)-C(7)-B	125.54(15)	H(20B)-C(20)-H(20C)	109.5
C(9)-C(8)-C(7)	122.87(18)	C(22)-C(21)-C(23)	110.10(14)
C(9)-C(8)-H(8)	118.6	C(22)-C(21)-P(2)	113.07(12)
C(7)-C(8)-H(8)	118.6	C(23)-C(21)-P(2)	108.90(11)
C(10)-C(9)-C(8)	120.53(19)	C(22)-C(21)-H(21)	108.2
C(10)-C(9)-H(9)	119.7	C(23)-C(21)-H(21)	108.2
C(8)-C(9)-H(9)	119.7	P(2)-C(21)-H(21)	108.2
C(9)-C(10)-C(11)	118.81(18)	C(21)-C(22)-H(22A)	109.5
C(9)-C(10)-H(10)	120.6	C(21)-C(22)-H(22B)	109.5
C(11)-C(10)-H(10)	120.6	H(22A)-C(22)-H(22B)	109.5
C(10)-C(11)-C(12)	120.06(18)	C(21)-C(22)-H(22C)	109.5
C(10)-C(11)-H(11)	120.0	H(22A)-C(22)-H(22C)	109.5
C(12)-C(11)-H(11)	120.0	H(22B)-C(22)-H(22C)	109.5
C(11)-C(12)-C(7)	123.11(18)	C(21)-C(23)-H(23A)	109.5
C(11)-C(12)-H(12)	118.4	C(21)-C(23)-H(23B)	109.5
C(7)-C(12)-H(12)	118.4	H(23A)-C(23)-H(23B)	109.5
B-C(13)-P(1)	120.38(11)	C(21)-C(23)-H(23C)	109.5
B-C(13)-H(13A)	107.2	H(23A)-C(23)-H(23C)	109.5
P(1)-C(13)-H(13A)	107.2	H(23B)-C(23)-H(23C)	109.5
B-C(13)-H(13B)	107.2	C(25)-C(24)-C(26)	110.44(13)
P(1)-C(13)-H(13B)	107.2	C(25)-C(24)-P(2)	114.72(12)
H(13A)-C(13)-H(13B)	106.9	C(26)-C(24)-P(2)	113.63(12)
B-C(14)-P(2)	122.06(11)	C(25)-C(24)-H(24)	105.7
B-C(14)-H(14A)	106.8	C(26)-C(24)-H(24)	105.7
P(2)-C(14)-H(14A)	106.8	P(2)-C(24)-H(24)	105.7
B-C(14)-H(14B)	106.8	C(24)-C(25)-H(25A)	109.5
P(2)-C(14)-H(14B)	106.8	C(24)-C(25)-H(25B)	109.5
H(14A)-C(14)-H(14B)	106.7	H(25A)-C(25)-H(25B)	109.5
C(16)-C(15)-C(17)	109.53(15)	C(24)-C(25)-H(25C)	109.5

H(25A)-C(25)-H(25C)	109.5	C(29)-C(30)-H(30A)	110.6
H(25B)-C(25)-H(25C)	109.5	O(1)-C(30)-H(30B)	110.6
C(24)-C(26)-H(26A)	109.5	C(29)-C(30)-H(30B)	110.6
C(24)-C(26)-H(26B)	109.5	H(30A)-C(30)-H(30B)	108.7
H(26A)-C(26)-H(26B)	109.5	C(34)-O(2)-C(31)	108.61(14)
C(24)-C(26)-H(26C)	109.5	C(34)-O(2)-Li	126.78(14)
H(26A)-C(26)-H(26C)	109.5	C(31)-O(2)-Li	123.83(14)
H(26B)-C(26)-H(26C)	109.5	O(2)-C(31)-C(32)	106.40(15)
C(27)-O(1)-C(30)	108.94(13)	O(2)-C(31)-H(31A)	110.4
C(27)-O(1)-Li	133.01(13)	C(32)-C(31)-H(31A)	110.4
C(30)-O(1)-Li	115.42(13)	O(2)-C(31)-H(31B)	110.4
O(1)-C(27)-C(28)	105.87(15)	C(32)-C(31)-H(31B)	110.4
O(1)-C(27)-H(27A)	110.6	H(31A)-C(31)-H(31B)	108.6
C(28)-C(27)-H(27A)	110.6	C(33)-C(32)-C(31)	104.67(15)
O(1)-C(27)-H(27B)	110.6	C(33)-C(32)-H(32A)	110.8
C(28)-C(27)-H(27B)	110.6	C(31)-C(32)-H(32A)	110.8
H(27A)-C(27)-H(27B)	108.7	C(33)-C(32)-H(32B)	110.8
C(27)-C(28)-C(29)	102.06(15)	C(31)-C(32)-H(32B)	110.8
C(27)-C(28)-H(28A)	111.4	H(32A)-C(32)-H(32B)	108.9
C(29)-C(28)-H(28A)	111.4	C(34)-C(33)-C(32)	102.49(16)
C(27)-C(28)-H(28B)	111.4	C(34)-C(33)-H(33A)	111.3
C(29)-C(28)-H(28B)	111.4	C(32)-C(33)-H(33A)	111.3
H(28A)-C(28)-H(28B)	109.2	C(34)-C(33)-H(33B)	111.3
C(28)-C(29)-C(30)	101.80(16)	C(32)-C(33)-H(33B)	111.3
C(28)-C(29)-H(29A)	111.4	H(33A)-C(33)-H(33B)	109.2
C(30)-C(29)-H(29A)	111.4	O(2)-C(34)-C(33)	104.72(15)
C(28)-C(29)-H(29B)	111.4	O(2)-C(34)-H(34A)	110.8
C(30)-C(29)-H(29B)	111.4	C(33)-C(34)-H(34A)	110.8
H(29A)-C(29)-H(29B)	109.3	O(2)-C(34)-H(34B)	110.8
O(1)-C(30)-C(29)	105.71(14)	C(33)-C(34)-H(34B)	110.8
O(1)-C(30)-H(30A)	110.6	H(34A)-C(34)-H(34B)	108.9

Table 17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]). 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}
Li	20(2)	22(2)	20(2)	1(1)	0(1)	-1(1)
P(1)	16(1)	15(1)	14(1)	0(1)	2(1)	0(1)
P(2)	14(1)	17(1)	14(1)	1(1)	1(1)	0(1)
B	15(1)	17(1)	15(1)	0(1)	1(1)	0(1)
C(1)	16(1)	22(1)	11(1)	-2(1)	3(1)	2(1)
C(2)	18(1)	25(1)	17(1)	1(1)	0(1)	-1(1)
C(3)	23(1)	29(1)	20(1)	5(1)	0(1)	5(1)
C(4)	15(1)	42(1)	18(1)	1(1)	-3(1)	5(1)
C(5)	17(1)	37(1)	19(1)	-5(1)	2(1)	-5(1)
C(6)	18(1)	24(1)	17(1)	-2(1)	3(1)	0(1)
C(7)	12(1)	21(1)	20(1)	-4(1)	-3(1)	-1(1)
C(8)	28(1)	24(1)	24(1)	-5(1)	1(1)	3(1)
C(9)	39(1)	23(1)	39(1)	-10(1)	-3(1)	7(1)
C(10)	27(1)	33(1)	40(1)	-22(1)	2(1)	5(1)
C(11)	22(1)	47(1)	23(1)	-16(1)	5(1)	-8(1)
C(12)	17(1)	28(1)	22(1)	-6(1)	2(1)	-4(1)
C(13)	16(1)	16(1)	18(1)	-2(1)	1(1)	1(1)
C(14)	14(1)	17(1)	16(1)	1(1)	2(1)	3(1)
C(15)	20(1)	23(1)	19(1)	3(1)	5(1)	-2(1)
C(16)	31(1)	27(1)	24(1)	8(1)	6(1)	1(1)
C(17)	34(1)	36(1)	21(1)	2(1)	11(1)	1(1)
C(18)	18(1)	15(1)	17(1)	-1(1)	2(1)	3(1)
C(19)	20(1)	27(1)	27(1)	0(1)	1(1)	5(1)
C(20)	33(1)	18(1)	26(1)	-2(1)	-1(1)	4(1)
C(21)	18(1)	17(1)	19(1)	2(1)	2(1)	-3(1)
C(22)	23(1)	24(1)	34(1)	-1(1)	0(1)	-7(1)
C(23)	29(1)	18(1)	22(1)	1(1)	2(1)	0(1)
C(24)	16(1)	16(1)	21(1)	-1(1)	3(1)	0(1)
C(25)	17(1)	27(1)	21(1)	-3(1)	3(1)	2(1)
C(26)	19(1)	25(1)	28(1)	3(1)	1(1)	4(1)
O(1)	26(1)	25(1)	21(1)	-3(1)	1(1)	-8(1)
C(27)	29(1)	31(1)	28(1)	3(1)	-4(1)	-10(1)
C(28)	36(1)	22(1)	40(1)	-5(1)	-12(1)	-1(1)
C(29)	42(1)	36(1)	24(1)	-6(1)	1(1)	1(1)
C(30)	34(1)	32(1)	24(1)	-3(1)	6(1)	-4(1)
O(2)	30(1)	25(1)	24(1)	3(1)	-6(1)	7(1)
C(31)	26(1)	18(1)	37(1)	5(1)	3(1)	-1(1)
C(32)	30(1)	28(1)	58(2)	6(1)	-4(1)	8(1)
C(33)	32(1)	40(1)	38(1)	3(1)	-4(1)	8(1)
C(34)	38(1)	39(1)	24(1)	4(1)	-8(1)	10(1)

Table 18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2P^iPr_2)_2][Li(THF)_2]$ (36[Li]).

	x	y	z	U(eq)
H(2)	6616	4108	-102	24
H(3)	4789	4524	-605	29
H(4)	3241	3522	-745	30
H(5)	3547	2104	-360	29
H(6)	5361	1705	153	23
H(8)	7878	721	720	31
H(9)	8487	-398	74	41
H(10)	8889	-146	-1005	40
H(11)	8648	1252	-1435	37
H(12)	8024	2369	-790	27
H(13A)	7847	1756	1361	20
H(13B)	6462	1885	1196	20
H(14A)	8037	3864	602	18
H(14B)	8650	3406	24	18
H(15)	5524	2242	2261	24
H(16A)	7707	1697	2940	40
H(16B)	7018	1185	2346	40
H(16C)	6449	1263	3033	40
H(17A)	5611	2626	3384	45
H(17B)	5642	3477	2942	45
H(17C)	6837	3121	3319	45
H(18)	6451	3971	1132	20
H(19A)	4573	3590	1921	37
H(19B)	4763	3108	1247	37
H(19C)	4471	4121	1249	37
H(20A)	6039	5170	1742	39
H(20B)	7325	4810	1988	39
H(20C)	6220	4628	2407	39
H(21)	10475	4411	286	21
H(22A)	12109	5031	956	40
H(22B)	12311	4033	788	40
H(22C)	11926	4304	1494	40
H(23A)	9744	5002	1515	34
H(23B)	9017	5109	817	34
H(23C)	10211	5648	983	34
H(24)	10228	1923	581	21
H(25A)	11483	3130	-143	32
H(25B)	10179	2786	-366	32
H(25C)	11274	2129	-316	32
H(26A)	12184	1668	821	35
H(26B)	11763	2170	1444	35
H(26C)	12484	2673	921	35
H(27A)	10817	5223	2519	36
H(27B)	11572	4516	2951	36
H(28A)	10109	5852	3416	40
H(28B)	11394	5546	3731	40
H(29A)	9592	4969	4263	41
H(29B)	10632	4285	4147	41
H(30A)	9088	3615	3556	36
H(30B)	8450	4518	3356	36
H(31A)	10216	1465	1845	33
H(31B)	9494	1127	2438	33
H(32A)	11111	506	2928	47
H(32B)	11751	687	2269	47
H(33A)	12533	1425	3361	44
H(33B)	12628	1920	2675	44
H(34A)	10818	2128	3560	41
H(34B)	11509	2886	3210	41

Figure 5. Fully-labeled displacement ellipsoid representation of $[Ph_2B(CH_2P^tBu_2)_2][Li(OEt_2)]$ (**37**[Li]) (hydrogens and disordered *tert*-butyl and diethyl ether positions omitted for clarity).

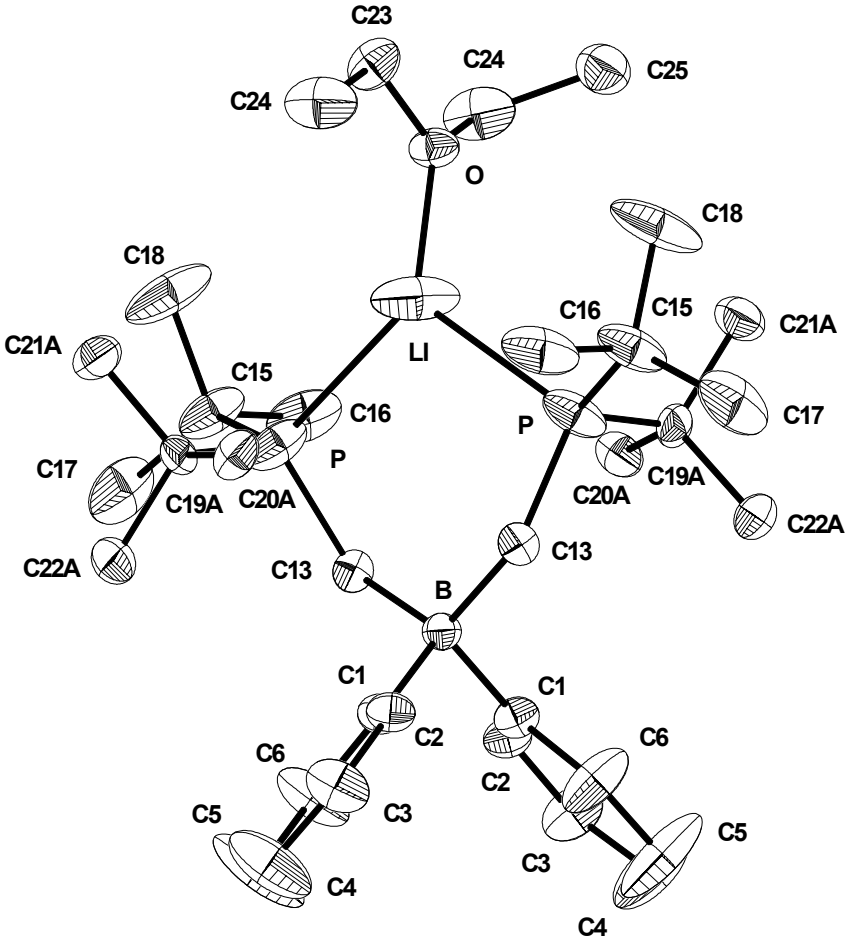

Table 19. Crystal data and structure refinement for $[Ph_2B(CH_2P^tBu_2)_2][Li(OEt_2)]$ (37[Li]).

Empirical formula	$C_{34}H_{60}BLiOP_2$
Formula weight	564.51
Crystal Habit	plate
Crystal Color	colorless
Crystal size	0.32 x 0.26 x 0.16 mm^3
Data Collection	
Data collection temperature	98(2) K
Unit cell dimensions	a = 16.295(3) Å
	b = 12.898(2) Å β = 105.480(3)°
	c = 17.470(3) Å
Volume	3538.6(11) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	C_2/c
Density (calculated)	1.060 g/cm^3
F(000)	1240
θ range for data collection	2.04 to 23.29°
Completeness to θ = 23.29°	99.6%
Index ranges	-18<=*h*<=18, -12<=*k*<=14, -19<=*l*<=14
Reflections collected	10511
Independent reflections	2544 [R(int) = 0.0727]
Absorption coefficient	0.146 mm^{-1}
Absorption correction	None
Structure solution and refinement	
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2544 / 0 / 229
Goodness-of-fit on F^2	1.879
Final R indices [I>2σ(I)]	R1 = 0.0517, wR2 = 0.0896
R indices (all data)	R1 = 0.0795, wR2 = 0.0952
Largest diff. peak and hole	0.286 and -0.321 $e.Å^{-3}$

Special refinement details

The structure contains two elements of disorder, which appear to be related. 1) A molecule of diethyl ether coordinated to the lithium atom is in two positions, related by an axis of symmetry. The two positions were refined as half occupied each. One of the positions is occupied by an atom from each molecule, thus making it a fully occupied site. Hydrogen positions were calculated at fixed positions and were recalculated after each series of least squares refinement cycles. 2) A *tert*-butyl group on the phosphine atom is disordered over two positions. The positions were split and were refined independently, each as half-occupied. It appears that the disorder in the *tert*-butyl group is related to the disorder in the diethyl ether molecule: the *tert*-butyl group is shifting along with the diethyl ether molecule to avoid interatomic contacts. The refinement of the two *tert*-butyl positions as half-occupied is based on attempts to refine using a free variable, which provided a free variable equal to one-half (within e.s.d.), which is consistent with the crystallographically imposed two-fold disorder in the diethyl ether molecule. It is possible that this disorder is propagated throughout the molecule, as evident by the large displacement ellipsoids present on other atoms.

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2P^tBu_2)_2][Li(OEt_2)]$ (37[Li]). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B	10000	6216(3)	2500	24(1)
Li	10000	3044(5)	2500	66(2)
P	8828(1)	4289(1)	1947(1)	42(1)
C(1)	9849(2)	7017(2)	1740(1)	26(1)
C(2)	10355(2)	7105(2)	1214(1)	29(1)
C(3)	10195(2)	7814(2)	598(2)	42(1)
C(4)	9512(2)	8464(3)	472(2)	71(1)
C(5)	8998(2)	8417(3)	987(2)	84(1)
C(6)	9175(2)	7711(2)	1603(2)	52(1)
C(13)	9135(1)	5514(2)	2471(1)	26(1)
C(15)	7895(2)	3826(2)	2311(2)	47(1)
C(16)	8182(2)	3855(2)	3223(2)	55(1)
C(17)	7079(2)	4456(2)	2040(2)	61(1)
C(18)	7713(2)	2680(2)	2077(2)	73(1)
C(19A)	8542(5)	4393(2)	938(3)	30(3)
C(20A)	9345(4)	4530(2)	672(3)	33(3)
C(21A)	8087(5)	3423(5)	503(5)	40(2)
C(22A)	7972(10)	5333(8)	660(8)	37(4)
C(19B)	8366(6)	4767(8)	786(5)	27(3)
C(20B)	9191(5)	4859(6)	486(5)	36(2)
C(21B)	7802(5)	3954(5)	277(5)	39(2)
C(22B)	7922(10)	5827(7)	637(10)	38(3)
O	9915(2)	1610(3)	2180(2)	31(1)
C(23)	10039(4)	826(5)	2774(3)	38(2)
C(24)	9966(2)	1237(2)	1433(2)	55(1)
C(25)	8975(4)	940(4)	962(3)	45(2)

Table 21. Selected bond lengths [Å] and angles [°] for $[Ph_2B(CH_2P^tBu_2)_2][Li(OEt_2)]$ (37[Li]).

B-Li	4.092(8)
Li-O	1.926(8)
Li-P	2.485(4)
O-Li-P	121.31(14)
O#1-Li-P	136.18(17)
P#1-Li-P	99.5(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+1/2

Table 22. Bond lengths [Å] and angles [°] for $[Ph_2B(CH_2P^tBu_2)_2][Li(Et_2O)]$ (37[Li]).

B-C(1)#1	1.648(3)	C(22B)-H(22E)	0.9800
B-C(1)	1.648(3)	C(22B)-H(22F)	0.9800
B-C(13)	1.665(3)	O-C(24)	1.414(4)
B-C(13)#1	1.665(3)	O-C(23)	1.423(5)
B-Li	4.092(8)	C(23)-C(23)#1	0.930(10)
Li-O	1.926(8)	C(23)-O#1	1.015(6)
Li-O#1	1.926(8)	C(23)-C(24)#1	1.486(6)
Li-P#1	2.485(4)	C(23)-H(23A)	0.9600
Li-P	2.485(4)	C(23)-H(23B)	0.9600
P-C(19A)	1.705(5)	C(24)-C(23)#1	1.486(6)
P-C(13)	1.828(2)	C(24)-C(25)	1.650(6)
P-C(15)	1.895(3)	C(24)-H(24D)	0.9600
P-C(19B)	2.061(9)	C(24)-H(24E)	0.9600
C(1)-C(6)	1.387(3)	C(25)-H(25A)	0.9601
C(1)-C(2)	1.394(3)	C(25)-H(25B)	0.9600
C(2)-C(3)	1.383(3)	C(25)-H(25C)	0.9599
C(2)-H(2)	0.9500		
C(3)-C(4)	1.363(4)	C(1)#1-B-C(1)	102.4(3)
C(3)-H(3)	0.9500	C(1)#1-B-C(13)	108.01(11)
C(4)-C(5)	1.384(4)	C(1)-B-C(13)	111.92(12)
C(4)-H(4)	0.9500	C(1)#1-B-C(13)#1	111.92(12)
C(5)-C(6)	1.380(4)	C(1)-B-C(13)#1	108.01(11)
C(5)-H(5)	0.9500	C(13)-B-C(13)#1	114.0(3)
C(6)-H(6)	0.9500	C(1)#1-B-Li	128.82(14)
C(13)-H(13A)	0.9900	C(1)-B-Li	128.82(14)
C(13)-H(13B)	0.9900	C(13)-B-Li	57.01(14)
C(15)-C(17)	1.522(4)	C(13)#1-B-Li	57.01(14)
C(15)-C(16)	1.536(4)	O-Li-O#1	32.5(2)
C(15)-C(18)	1.541(4)	O-Li-P#1	136.18(17)
C(16)-H(16A)	0.9800	O#1-Li-P#1	121.31(14)
C(16)-H(16B)	0.9800	O-Li-P	121.31(14)
C(16)-H(16C)	0.9800	O#1-Li-P	136.18(17)
C(17)-H(17A)	0.9800	P#1-Li-P	99.5(2)
C(17)-H(17B)	0.9800	O-Li-B	163.76(11)
C(17)-H(17C)	0.9800	O#1-Li-B	163.76(11)
C(18)-H(18A)	0.9800	P#1-Li-B	49.73(12)
C(18)-H(18B)	0.9800	P-Li-B	49.73(12)
C(18)-H(18C)	0.9800	C(19A)-P-C(13)	114.39(13)
C(19A)-C(20A)	1.5120(16)	C(19A)-P-C(15)	110.4(2)
C(19A)-C(22A)	1.525(11)	C(13)-P-C(15)	103.96(11)
C(19A)-C(21A)	1.546(9)	C(19A)-P-C(19B)	14.3(3)
C(20A)-H(20A)	0.9800	C(13)-P-C(19B)	102.3(3)
C(20A)-H(20B)	0.9800	C(15)-P-C(19B)	108.0(3)
C(20A)-H(20C)	0.9800	C(19A)-P-Li	115.0(2)
C(21A)-H(21A)	0.9800	C(13)-P-Li	106.55(14)
C(21A)-H(21B)	0.9800	C(15)-P-Li	105.53(13)
C(21A)-H(21C)	0.9800	C(19B)-P-Li	128.1(3)
C(22A)-H(22A)	0.9800	C(6)-C(1)-C(2)	114.5(2)
C(22A)-H(22B)	0.9800	C(6)-C(1)-B	119.0(2)
C(22A)-H(22C)	0.9800	C(2)-C(1)-B	126.5(2)
C(19B)-C(21B)	1.516(11)	C(3)-C(2)-C(1)	123.0(2)
C(19B)-C(22B)	1.536(12)	C(3)-C(2)-H(2)	118.5
C(19B)-C(20B)	1.573(9)	C(1)-C(2)-H(2)	118.5
C(20B)-H(20D)	0.9800	C(4)-C(3)-C(2)	120.5(2)
C(20B)-H(20E)	0.9800	C(4)-C(3)-H(3)	119.7
C(20B)-H(20F)	0.9800	C(2)-C(3)-H(3)	119.7
C(21B)-H(21D)	0.9800	C(3)-C(4)-C(5)	118.5(3)
C(21B)-H(21E)	0.9800	C(3)-C(4)-H(4)	120.7
C(21B)-H(21F)	0.9800	C(5)-C(4)-H(4)	120.7
C(22B)-H(22D)	0.9800	C(6)-C(5)-C(4)	120.0(3)

C(6)-C(5)-H(5)	120.0	C(19B)-C(20B)-H(20F)	109.5
C(4)-C(5)-H(5)	120.0	H(20D)-C(20B)-H(20F)	109.5
C(5)-C(6)-C(1)	123.4(2)	H(20E)-C(20B)-H(20F)	109.5
C(5)-C(6)-H(6)	118.3	C(19B)-C(21B)-H(21D)	109.5
C(1)-C(6)-H(6)	118.3	C(19B)-C(21B)-H(21E)	109.5
B-C(13)-P	127.02(16)	H(21D)-C(21B)-H(21E)	109.5
B-C(13)-H(13A)	105.6	C(19B)-C(21B)-H(21F)	109.5
P-C(13)-H(13A)	105.6	H(21D)-C(21B)-H(21F)	109.5
B-C(13)-H(13B)	105.6	H(21E)-C(21B)-H(21F)	109.5
P-C(13)-H(13B)	105.6	C(19B)-C(22B)-H(22D)	109.5
H(13A)-C(13)-H(13B)	106.1	C(19B)-C(22B)-H(22E)	109.5
C(17)-C(15)-C(16)	108.0(2)	H(22D)-C(22B)-H(22E)	109.5
C(17)-C(15)-C(18)	109.8(2)	C(19B)-C(22B)-H(22F)	109.5
C(16)-C(15)-C(18)	106.4(3)	H(22D)-C(22B)-H(22F)	109.5
C(17)-C(15)-P	116.1(2)	H(22E)-C(22B)-H(22F)	109.5
C(16)-C(15)-P	106.92(19)	C(24)-O-C(23)	113.5(3)
C(18)-C(15)-P	109.15(18)	C(24)-O-Li	125.2(3)
C(15)-C(16)-H(16A)	109.5	C(23)-O-Li	119.0(3)
C(15)-C(16)-H(16B)	109.5	C(23)#1-C(23)-O#1	93.9(4)
H(16A)-C(16)-H(16B)	109.5	C(23)#1-C(23)-O	45.4(2)
C(15)-C(16)-H(16C)	109.5	O#1-C(23)-O	49.0(4)
H(16A)-C(16)-H(16C)	109.5	C(23)#1-C(23)-C(24)#1	157.7(5)
H(16B)-C(16)-H(16C)	109.5	O#1-C(23)-C(24)#1	65.7(4)
C(15)-C(17)-H(17A)	109.5	O-C(23)-C(24)#1	113.0(4)
C(15)-C(17)-H(17B)	109.5	C(23)#1-C(23)-H(23A)	87.0
H(17A)-C(17)-H(17B)	109.5	O#1-C(23)-H(23A)	113.6
C(15)-C(17)-H(17C)	109.5	O-C(23)-H(23A)	109.0
H(17A)-C(17)-H(17C)	109.5	C(24)#1-C(23)-H(23A)	109.0
H(17B)-C(17)-H(17C)	109.5	C(23)#1-C(23)-H(23B)	79.3
C(15)-C(18)-H(18A)	109.5	O#1-C(23)-H(23B)	137.6
C(15)-C(18)-H(18B)	109.5	O-C(23)-H(23B)	109.0
H(18A)-C(18)-H(18B)	109.5	C(24)#1-C(23)-H(23B)	109.0
C(15)-C(18)-H(18C)	109.5	H(23A)-C(23)-H(23B)	107.8
H(18A)-C(18)-H(18C)	109.5	O-C(24)-C(23)#1	40.9(2)
H(18B)-C(18)-H(18C)	109.5	O-C(24)-C(25)	104.4(3)
C(20A)-C(19A)-C(22A)	108.3(6)	C(23)#1-C(24)-C(25)	97.7(4)
C(20A)-C(19A)-C(21A)	106.5(4)	O-C(24)-H(24D)	110.9
C(22A)-C(19A)-C(21A)	108.4(7)	C(23)#1-C(24)-H(24D)	76.4
C(20A)-C(19A)-P	107.8(2)	C(25)-C(24)-H(24D)	110.9
C(22A)-C(19A)-P	111.5(5)	O-C(24)-H(24E)	110.9
C(21A)-C(19A)-P	114.0(4)	C(23)#1-C(24)-H(24E)	145.7
C(21B)-C(19B)-C(22B)	109.4(8)	C(25)-C(24)-H(24E)	110.9
C(21B)-C(19B)-C(20B)	107.2(6)	H(24D)-C(24)-H(24E)	108.9
C(22B)-C(19B)-C(20B)	106.4(9)	C(24)-C(25)-H(25A)	109.5
C(21B)-C(19B)-P	112.0(6)	C(24)-C(25)-H(25B)	109.5
C(22B)-C(19B)-P	117.7(9)	H(25A)-C(25)-H(25B)	109.5
C(20B)-C(19B)-P	103.3(6)	C(24)-C(25)-H(25C)	109.5
C(19B)-C(20B)-H(20D)	109.5	H(25A)-C(25)-H(25C)	109.5
C(19B)-C(20B)-H(20E)	109.5	H(25B)-C(25)-H(25C)	109.5
H(20D)-C(20B)-H(20E)	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+1/2

Table 23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Ph_2B(CH_2P^tBu_2)_2][Li(Et_2O)]$ (37[Li]). 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}
B	22(2)	21(3)	28(3)	0	7(2)	0
Li	78(6)	30(5)	118(7)	0	72(5)	0
P	36(1)	39(1)	61(1)	-22(1)	32(1)	-17(1)
C(1)	30(2)	26(2)	26(2)	-1(1)	12(1)	4(1)
C(2)	34(2)	25(2)	31(2)	0(1)	14(1)	3(1)
C(3)	56(2)	47(2)	34(2)	12(2)	28(2)	12(2)
C(4)	89(3)	81(3)	59(2)	45(2)	47(2)	48(2)
C(5)	95(3)	98(3)	78(3)	62(2)	60(2)	73(2)
C(6)	62(2)	60(2)	48(2)	30(2)	38(2)	34(2)
C(13)	24(1)	29(2)	25(2)	-2(1)	9(1)	-1(1)
C(15)	43(2)	39(2)	72(2)	-23(2)	38(2)	-20(2)
C(16)	58(2)	41(2)	83(3)	-8(2)	51(2)	-20(2)
C(17)	36(2)	69(2)	91(3)	-24(2)	37(2)	-21(2)
C(18)	69(2)	51(2)	125(3)	-47(2)	72(2)	-40(2)
C(19A)	23(4)	27(6)	34(5)	-5(4)	-1(3)	10(4)
C(20A)	45(5)	35(6)	18(4)	2(4)	6(3)	-14(4)
C(21A)	35(5)	30(5)	52(6)	-12(4)	7(4)	-4(3)
C(22A)	42(6)	34(10)	30(5)	10(8)	-1(4)	1(8)
C(19B)	28(6)	19(6)	28(4)	2(4)	-1(4)	-3(5)
C(20B)	56(5)	27(4)	31(5)	-2(4)	22(4)	-12(4)
C(21B)	44(5)	31(6)	42(5)	-6(4)	12(4)	-10(4)
C(22B)	35(5)	26(8)	47(5)	9(6)	-1(4)	2(6)
O	44(2)	24(2)	27(2)	-1(2)	13(2)	0(2)
C(23)	49(4)	41(4)	26(4)	9(3)	15(4)	8(4)
C(24)	90(3)	42(2)	40(2)	1(2)	32(2)	5(2)
C(25)	50(4)	40(4)	42(4)	-4(3)	10(3)	-6(3)

Table 24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Ph_2B(CH_2P^tBu_2)_2][Li(Et_2O)]$ (37[Li]).

	x	y	z	U(eq)
H(2)	10832	6658	1282	35
H(3)	10564	7849	259	51
H(4)	9391	8937	40	85
H(5)	8525	8871	917	100
H(6)	8816	7699	1951	62
H(13A)	8647	5987	2269	31
H(13B)	9155	5371	3033	31
H(16A)	8204	4576	3405	82
H(16B)	8749	3542	3409	82
H(16C)	7777	3464	3437	82
H(17A)	6845	4378	1465	92
H(17B)	7204	5189	2168	92
H(17C)	6664	4207	2312	92
H(18A)	7280	2411	2321	110
H(18B)	8238	2275	2263	110
H(18C)	7506	2625	1498	110
H(20A)	9646	5154	918	50
H(20B)	9197	4600	93	50
H(20C)	9714	3924	833	50
H(21A)	7526	3354	603	61
H(21B)	8429	2805	700	61
H(21C)	8019	3495	-69	61
H(22A)	7457	5272	846	56
H(22B)	7812	5364	79	56
H(22C)	8280	5966	877	56
H(20D)	9036	5088	-69	54
H(20E)	9473	4182	527	54
H(20F)	9580	5365	814	54
H(21D)	7247	3945	395	58
H(21E)	8070	3271	393	58
H(21F)	7724	4119	-285	58
H(22D)	7380	5794	779	58
H(22E)	7814	6009	74	58
H(22F)	8287	6355	962	58
H(23A)	10574	488	2814	46
H(23B)	9598	316	2614	46
H(24A)	10119	678	3943	82
H(24B)	10482	1737	3736	82
H(24C)	9495	1563	3534	82
H(24D)	10327	637	1494	66
H(24E)	10186	1762	1151	66
H(25A)	8956	679	443	67
H(25B)	8767	421	1256	67
H(25C)	8626	1549	912	67

Figure 6. Fully-labeled displacement ellipsoid representation of [(*m,m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (**38**[Tl]) (hydrogens omitted for clarity).

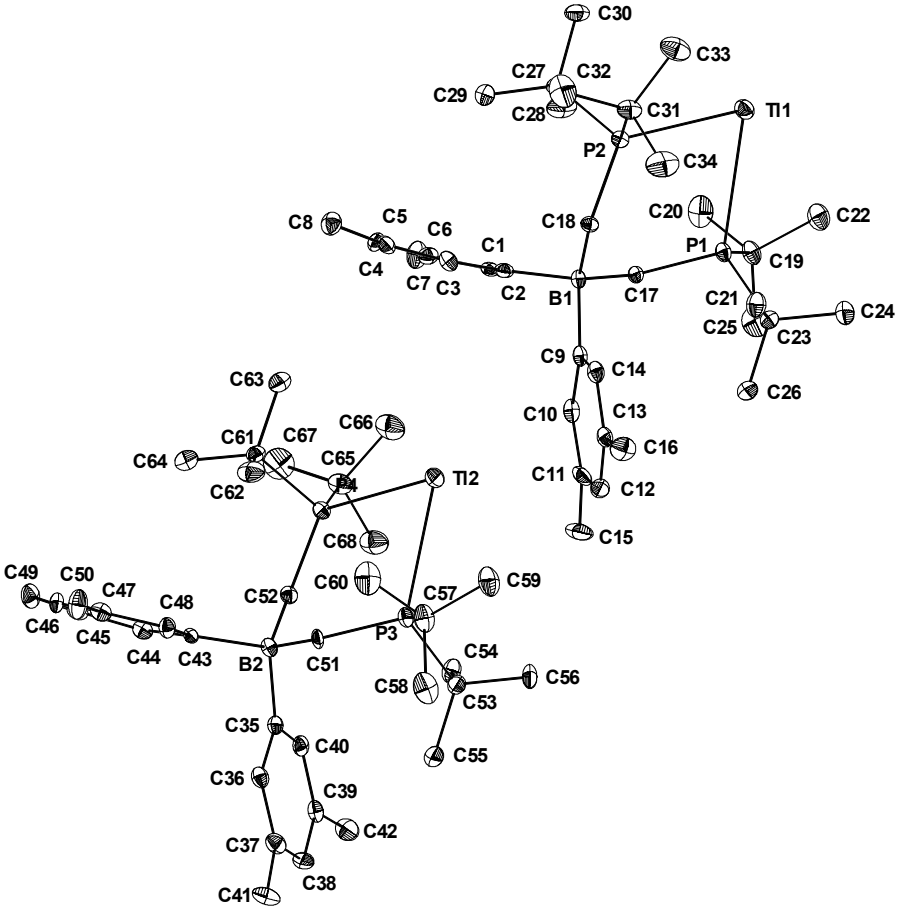

Table 25. Crystal data and structure refinement for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]).

Empirical formula	$C_{38}H_{34}BP_2Tl$	
Formula weight	767.77	
Crystallization solvent	Petroleum ether / THF	
Crystal Habit	plate	
Crystal Color	colorless	
Crystal size	0.23 x 0.15 x 0.07 mm^3	
Data Collection		
Data collection temperature	98(2) K	
Unit cell dimensions	a = 8.4192(6) Å	α= 95.5850(10)°
	b = 12.6996(9) Å	β= 98.2930(10)°
	c = 15.6565(11) Å	γ = 104.5320(10)°
Volume	1587.85(19) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (#2)	
Density (calculated)	1.606 g/cm^3	
F(000)	756	
θ range for data collection	1.33 to 28.53°	
Completeness to θ = 28.53°	86.5%	
Index ranges	-11<=*h*<=11, -16<=*k*<=12, -19<=*l*<=20	
Reflections collected	10036	
Independent reflections	6970 [R(int) = 0.0364]	
Absorption coefficient	5.213 mm^{-1}	
Absorption correction	Integration	
Structure solution and Refinement		
Primary solution method	Direct methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Calculated	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6970 / 0 / 379	
Goodness-of-fit on F^2	1.286	
Final R indices [I>2σ(I)]	R1 = 0.0277, wR2 = 0.0622	
R indices (all data)	R1 = 0.0323, wR2 = 0.0635	
Largest diff. peak and hole	1.670 and -1.263 e.$Å^{-3}$	

Special refinement details: Face-centered absorption correction was applied to the integrated data. All remaining electron density (> 1 e / $Å^3$) resides near the thallium atom.

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tl	7207(1)	8618(1)	7388(1)	18(1)
P(1)	-929(1)	7242(1)	8388(1)	13(1)
P(2)	3942(1)	6874(1)	6786(1)	14(1)
B	2064(5)	8290(3)	7658(2)	13(1)
C(1)	3842(4)	9257(3)	7945(2)	13(1)
C(2)	4486(4)	10045(3)	7423(2)	14(1)
C(3)	5960(4)	10876(3)	7697(2)	16(1)
C(4)	6872(4)	10951(3)	8528(2)	20(1)
C(5)	6318(4)	10171(3)	9046(2)	19(1)
C(6)	4850(4)	9341(3)	8764(2)	15(1)
C(7)	824(4)	8571(3)	6856(2)	15(1)
C(8)	-310(4)	7739(3)	6241(2)	21(1)
C(9)	-1459(5)	7963(4)	5588(2)	28(1)
C(10)	-1469(5)	9044(4)	5526(2)	29(1)
C(11)	-381(5)	9884(4)	6118(3)	27(1)
C(12)	718(4)	9635(3)	6771(2)	19(1)
C(13)	1080(4)	8257(3)	8519(2)	13(1)
C(14)	2440(4)	7074(3)	7471(2)	13(1)
C(15)	-462(4)	5936(3)	8578(2)	16(1)
C(16)	926(5)	5876(3)	9147(2)	19(1)
C(17)	1231(5)	4873(3)	9260(2)	25(1)
C(18)	130(6)	3917(3)	8818(3)	31(1)
C(19)	-1267(6)	3958(3)	8264(3)	32(1)
C(20)	-1566(5)	4960(3)	8132(2)	23(1)
C(21)	-1804(4)	7529(3)	9369(2)	14(1)
C(22)	-3393(5)	6865(3)	9424(2)	23(1)
C(23)	-4147(5)	7069(4)	10126(3)	28(1)
C(24)	-3381(5)	7931(3)	10782(3)	26(1)
C(25)	-1820(5)	8589(3)	10735(2)	25(1)
C(26)	-1036(5)	8401(3)	10032(2)	20(1)
C(27)	3863(4)	5418(3)	6734(2)	16(1)
C(28)	4785(5)	4973(3)	6192(2)	21(1)
C(29)	4822(5)	3886(3)	6170(2)	25(1)
C(30)	3966(5)	3221(3)	6700(2)	24(1)
C(31)	3088(5)	3648(3)	7255(2)	25(1)
C(32)	3022(5)	4738(3)	7264(2)	21(1)
C(33)	3027(4)	6996(3)	5672(2)	17(1)
C(34)	3522(5)	8007(3)	5383(2)	20(1)
C(35)	2798(5)	8178(3)	4564(2)	23(1)
C(36)	1615(5)	7330(4)	4033(2)	27(1)
C(37)	1156(5)	6309(4)	4296(2)	28(1)
C(38)	1863(5)	6132(3)	5116(2)	25(1)

Table 27. Selected bond lengths [Å] and angles [°] for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]).

Tl-P(2)	3.0231(9)	Tl-P(1)#1	3.0283(9)
Tl-C(1)	3.342(3)	Tl-C(7)#1	3.284(3)
Tl-C(2)	3.261(3)	Tl-C(8)#1	3.272(4)
Tl-C(3)	3.309(3)	Tl-C(9)#1	3.289(4)
Tl-C(4)	3.403(4)	Tl-C(10)#1	3.313(4)
Tl-C(5)	3.390(4)	Tl-C(11)#1	3.288(4)
Tl-C(6)	3.345(3)	Tl-C(12)#1	3.239(3)
		P(2)-Tl-P(1)#1	97.80(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z

Table 28. Bond lengths [Å] and angles [°] for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]).

Tl-P(2)	3.0231(9)	C(15)-C(20)	1.398(5)
Tl-P(1)#1	3.0283(9)	C(16)-C(17)	1.383(5)
Tl-C(12)#1	3.239(3)	C(16)-H(16)	0.9500
Tl-C(2)	3.261(3)	C(17)-C(18)	1.378(6)
Tl-C(8)#1	3.272(4)	C(17)-H(17)	0.9500
Tl-C(7)#1	3.284(3)	C(18)-C(19)	1.373(6)
Tl-C(11)#1	3.288(4)	C(18)-H(18)	0.9500
Tl-C(9)#1	3.289(4)	C(19)-C(20)	1.386(6)
Tl-C(3)	3.309(3)	C(19)-H(19)	0.9500
Tl-C(10)#1	3.313(4)	C(20)-H(20)	0.9500
Tl-C(1)	3.342(3)	C(21)-C(26)	1.395(5)
Tl-C(6)	3.345(3)	C(21)-C(22)	1.410(5)
Tl-C(5)	3.390(4)	C(21)-Tl#2	3.592(3)
Tl-C(4)	3.403(4)	C(22)-C(23)	1.380(5)
Tl-C(21)#1	3.592(3)	C(22)-H(22)	0.9500
Tl-C(13)#1	3.636(3)	C(23)-C(24)	1.380(6)
P(1)-C(13)	1.822(3)	C(23)-H(23)	0.9500
P(1)-C(15)	1.839(4)	C(24)-C(25)	1.386(6)
P(1)-C(21)	1.841(3)	C(24)-H(24)	0.9500
P(1)-Tl#2	3.0283(9)	C(25)-C(26)	1.393(5)
P(2)-C(14)	1.820(3)	C(25)-H(25)	0.9500
P(2)-C(27)	1.827(4)	C(26)-H(26)	0.9500
P(2)-C(33)	1.839(4)	C(27)-C(32)	1.393(5)
B-C(7)	1.640(5)	C(27)-C(28)	1.400(5)
B-C(1)	1.652(5)	C(28)-C(29)	1.385(5)
B-C(14)	1.660(5)	C(28)-H(28)	0.9500
B-C(13)	1.680(5)	C(29)-C(30)	1.387(6)
C(1)-C(2)	1.407(5)	C(29)-H(29)	0.9500
C(1)-C(6)	1.411(5)	C(30)-C(31)	1.375(5)
C(2)-C(3)	1.392(5)	C(30)-H(30)	0.9500
C(2)-H(2)	0.9500	C(31)-C(32)	1.399(5)
C(3)-C(4)	1.394(5)	C(31)-H(31)	0.9500
C(3)-H(3)	0.9500	C(32)-H(32)	0.9500
C(4)-C(5)	1.374(5)	C(33)-C(34)	1.388(5)
C(4)-H(4)	0.9500	C(33)-C(38)	1.397(5)
C(5)-C(6)	1.390(5)	C(34)-C(35)	1.399(5)
C(5)-H(5)	0.9500	C(34)-H(34)	0.9500
C(6)-H(6)	0.9500	C(35)-C(36)	1.376(6)
C(7)-C(12)	1.394(5)	C(35)-H(35)	0.9500
C(7)-C(8)	1.409(5)	C(36)-C(37)	1.378(6)
C(7)-Tl#2	3.284(3)	C(36)-H(36)	0.9500
C(8)-C(9)	1.404(5)	C(37)-C(38)	1.399(5)
C(8)-Tl#2	3.272(4)	C(37)-H(37)	0.9500
C(8)-H(8)	0.9500	C(38)-H(38)	0.9500
C(9)-C(10)	1.387(6)		
C(9)-Tl#2	3.289(4)	P(2)-Tl-P(1)#1	97.80(2)
C(9)-H(9)	0.9500	P(2)-Tl-C(12)#1	141.02(7)
C(10)-C(11)	1.381(6)	P(1)#1-Tl-C(12)#1	85.03(7)
C(10)-Tl#2	3.313(4)	P(2)-Tl-C(2)	77.72(7)
C(10)-H(10)	0.9500	P(1)#1-Tl-C(2)	145.70(6)
C(11)-C(12)	1.392(5)	C(12)#1-Tl-C(2)	119.90(9)
C(11)-Tl#2	3.288(4)	P(2)-Tl-C(8)#1	102.30(7)
C(11)-H(11)	0.9500	P(1)#1-Tl-C(8)#1	68.82(7)
C(12)-Tl#2	3.239(3)	C(12)#1-Tl-C(8)#1	42.58(10)
C(12)-H(12)	0.9500	C(2)-Tl-C(8)#1	145.48(9)
C(13)-Tl#2	3.636(3)	P(2)-Tl-C(7)#1	126.48(7)
C(13)-H(13A)	0.9900	P(1)#1-Tl-C(7)#1	64.32(6)
C(13)-H(13B)	0.9900	C(12)#1-Tl-C(7)#1	24.66(9)
C(14)-H(14A)	0.9900	C(2)-Tl-C(7)#1	144.34(9)
C(14)-H(14B)	0.9900	C(8)#1-Tl-C(7)#1	24.81(9)
C(15)-C(16)	1.387(5)	P(2)-Tl-C(11)#1	125.87(8)

P(1)#1-Tl-C(11)#1	107.94(7)	P(1)#1-Tl-C(4)	116.54(6)
C(12)#1-Tl-C(11)#1	24.61(9)	C(12)#1-Tl-C(4)	98.27(9)
C(2)-Tl-C(11)#1	101.72(9)	C(2)-Tl-C(4)	42.32(9)
C(8)#1-Tl-C(11)#1	49.84(10)	C(8)#1-Tl-C(4)	140.85(9)
C(7)#1-Tl-C(11)#1	43.88(9)	C(7)#1-Tl-C(4)	118.65(9)
P(2)-Tl-C(9)#1	91.07(8)	C(11)#1-Tl-C(4)	95.46(10)
P(1)#1-Tl-C(9)#1	91.96(8)	C(9)#1-Tl-C(4)	136.75(10)
C(12)#1-Tl-C(9)#1	49.95(10)	C(3)-Tl-C(4)	23.92(8)
C(2)-Tl-C(9)#1	121.86(9)	C(10)#1-Tl-C(4)	112.79(10)
C(8)#1-Tl-C(9)#1	24.72(9)	C(1)-Tl-C(4)	50.11(8)
C(7)#1-Tl-C(9)#1	44.09(9)	C(6)-Tl-C(4)	41.81(9)
C(11)#1-Tl-C(9)#1	42.73(11)	C(5)-Tl-C(4)	23.35(9)
P(2)-Tl-C(3)	102.18(6)	P(2)-Tl-C(21)#1	93.99(6)
P(1)#1-Tl-C(3)	140.39(6)	P(1)#1-Tl-C(21)#1	30.82(5)
C(12)#1-Tl-C(3)	99.67(9)	C(12)#1-Tl-C(21)#1	106.44(8)
C(2)-Tl-C(3)	24.46(9)	C(2)-Tl-C(21)#1	114.95(8)
C(8)#1-Tl-C(3)	137.09(9)	C(8)#1-Tl-C(21)#1	99.54(8)
C(7)#1-Tl-C(3)	124.04(9)	C(7)#1-Tl-C(21)#1	91.22(8)
C(11)#1-Tl-C(3)	87.30(10)	C(11)#1-Tl-C(21)#1	131.04(9)
C(9)#1-Tl-C(3)	121.20(10)	C(9)#1-Tl-C(21)#1	122.70(9)
P(2)-Tl-C(10)#1	102.13(8)	C(3)-Tl-C(21)#1	113.25(8)
P(1)#1-Tl-C(10)#1	111.34(7)	C(10)#1-Tl-C(21)#1	141.35(9)
C(12)#1-Tl-C(10)#1	42.86(9)	C(1)-Tl-C(21)#1	94.27(8)
C(2)-Tl-C(10)#1	102.79(9)	C(6)-Tl-C(21)#1	72.94(8)
C(8)#1-Tl-C(10)#1	42.94(10)	C(5)-Tl-C(21)#1	71.79(8)
C(7)#1-Tl-C(10)#1	51.07(9)	C(4)-Tl-C(21)#1	91.19(8)
C(11)#1-Tl-C(10)#1	24.15(11)	P(2)-Tl-C(13)#1	127.14(6)
C(9)#1-Tl-C(10)#1	24.26(11)	P(1)#1-Tl-C(13)#1	30.00(6)
C(3)-Tl-C(10)#1	97.46(10)	C(12)#1-Tl-C(13)#1	59.06(8)
P(2)-Tl-C(1)	64.34(6)	C(2)-Tl-C(13)#1	144.89(8)
P(1)#1-Tl-C(1)	123.56(6)	C(8)#1-Tl-C(13)#1	61.22(8)
C(12)#1-Tl-C(1)	143.07(9)	C(7)#1-Tl-C(13)#1	44.83(8)
C(2)-Tl-C(1)	24.56(8)	C(11)#1-Tl-C(13)#1	83.59(8)
C(8)#1-Tl-C(1)	161.55(9)	C(9)#1-Tl-C(13)#1	85.59(8)
C(7)#1-Tl-C(1)	167.51(9)	C(3)-Tl-C(13)#1	124.29(8)
C(11)#1-Tl-C(1)	126.27(9)	C(10)#1-Tl-C(13)#1	95.83(8)
C(9)#1-Tl-C(1)	137.72(9)	C(1)-Tl-C(13)#1	136.68(8)
C(3)-Tl-C(1)	43.49(9)	C(6)-Tl-C(13)#1	112.35(8)
C(10)#1-Tl-C(1)	124.38(9)	C(5)-Tl-C(13)#1	97.93(8)
P(2)-Tl-C(6)	78.28(6)	C(4)-Tl-C(13)#1	102.93(8)
P(1)#1-Tl-C(6)	103.66(6)	C(21)#1-Tl-C(13)#1	47.78(7)
C(12)#1-Tl-C(6)	139.04(9)	C(13)-P(1)-C(15)	106.03(16)
C(2)-Tl-C(6)	42.04(8)	C(13)-P(1)-C(21)	106.10(16)
C(8)#1-Tl-C(6)	172.48(9)	C(15)-P(1)-C(21)	100.14(15)
C(7)#1-Tl-C(6)	152.27(9)	C(13)-P(1)-Tl#2	93.80(11)
C(11)#1-Tl-C(6)	135.67(10)	C(15)-P(1)-Tl#2	152.82(12)
C(9)#1-Tl-C(6)	162.07(9)	C(21)-P(1)-Tl#2	91.74(11)
C(3)-Tl-C(6)	49.07(9)	C(14)-P(2)-C(27)	105.05(16)
C(10)#1-Tl-C(6)	144.49(9)	C(14)-P(2)-C(33)	106.17(15)
C(1)-Tl-C(6)	24.36(8)	C(27)-P(2)-C(33)	103.52(16)
P(2)-Tl-C(5)	102.09(7)	C(14)-P(2)-Tl	110.02(12)
P(1)#1-Tl-C(5)	100.90(6)	C(27)-P(2)-Tl	120.61(11)
C(12)#1-Tl-C(5)	115.61(9)	C(33)-P(2)-Tl	110.43(12)
C(2)-Tl-C(5)	48.68(9)	C(7)-B-C(1)	112.3(3)
C(8)#1-Tl-C(5)	154.61(9)	C(7)-B-C(14)	114.2(3)
C(7)#1-Tl-C(5)	129.84(9)	C(1)-B-C(14)	109.7(3)
C(11)#1-Tl-C(5)	117.88(10)	C(7)-B-C(13)	106.4(3)
C(9)#1-Tl-C(5)	160.05(11)	C(1)-B-C(13)	107.0(3)
C(3)-Tl-C(5)	41.62(9)	C(14)-B-C(13)	106.8(3)
C(10)#1-Tl-C(5)	136.11(11)	C(2)-C(1)-C(6)	114.6(3)
C(1)-Tl-C(5)	42.76(8)	C(2)-C(1)-B	124.8(3)
C(6)-Tl-C(5)	23.81(9)	C(6)-C(1)-B	120.6(3)
P(2)-Tl-C(4)	114.45(6)	C(2)-C(1)-Tl	74.50(18)

C(6)-C(1)-Tl	77.93(19)	C(11)-C(12)-Tl#2	79.7(2)
B-C(1)-Tl	116.1(2)	C(7)-C(12)-Tl#2	79.5(2)
C(3)-C(2)-C(1)	123.4(3)	C(11)-C(12)-H(12)	118.2
C(3)-C(2)-Tl	79.7(2)	C(7)-C(12)-H(12)	118.2
C(1)-C(2)-Tl	80.94(19)	Tl#2-C(12)-H(12)	112.5
C(3)-C(2)-H(2)	118.3	B-C(13)-P(1)	116.5(2)
C(1)-C(2)-H(2)	118.3	B-C(13)-Tl#2	96.70(18)
Tl-C(2)-H(2)	110.8	P(1)-C(13)-Tl#2	56.21(9)
C(2)-C(3)-C(4)	119.7(3)	B-C(13)-H(13A)	108.2
C(2)-C(3)-Tl	75.9(2)	P(1)-C(13)-H(13A)	108.2
C(4)-C(3)-Tl	81.8(2)	Tl#2-C(13)-H(13A)	65.7
C(2)-C(3)-H(3)	120.1	B-C(13)-H(13B)	108.2
C(4)-C(3)-H(3)	120.1	P(1)-C(13)-H(13B)	108.2
Tl-C(3)-H(3)	112.6	Tl#2-C(13)-H(13B)	155.0
C(5)-C(4)-C(3)	118.7(3)	H(13A)-C(13)-H(13B)	107.3
C(5)-C(4)-Tl	77.8(2)	B-C(14)-P(2)	120.9(2)
C(3)-C(4)-Tl	74.2(2)	B-C(14)-H(14A)	107.1
C(5)-C(4)-H(4)	120.7	P(2)-C(14)-H(14A)	107.1
C(3)-C(4)-H(4)	120.7	B-C(14)-H(14B)	107.1
Tl-C(4)-H(4)	118.2	P(2)-C(14)-H(14B)	107.1
C(4)-C(5)-C(6)	121.2(3)	H(14A)-C(14)-H(14B)	106.8
C(4)-C(5)-Tl	78.8(2)	C(16)-C(15)-C(20)	118.6(4)
C(6)-C(5)-Tl	76.3(2)	C(16)-C(15)-P(1)	123.0(3)
C(4)-C(5)-H(5)	119.4	C(20)-C(15)-P(1)	118.3(3)
C(6)-C(5)-H(5)	119.4	C(17)-C(16)-C(15)	120.8(4)
Tl-C(5)-H(5)	116.0	C(17)-C(16)-H(16)	119.6
C(5)-C(6)-C(1)	122.4(3)	C(15)-C(16)-H(16)	119.6
C(5)-C(6)-Tl	79.9(2)	C(18)-C(17)-C(16)	120.0(4)
C(1)-C(6)-Tl	77.71(19)	C(18)-C(17)-H(17)	120.0
C(5)-C(6)-H(6)	118.8	C(16)-C(17)-H(17)	120.0
C(1)-C(6)-H(6)	118.8	C(19)-C(18)-C(17)	120.1(4)
Tl-C(6)-H(6)	113.7	C(19)-C(18)-H(18)	119.9
C(12)-C(7)-C(8)	115.1(3)	C(17)-C(18)-H(18)	119.9
C(12)-C(7)-B	122.8(3)	C(18)-C(19)-C(20)	120.4(4)
C(8)-C(7)-B	121.9(3)	C(18)-C(19)-H(19)	119.8
C(12)-C(7)-Tl#2	75.86(19)	C(20)-C(19)-H(19)	119.8
C(8)-C(7)-Tl#2	77.09(19)	C(19)-C(20)-C(15)	120.1(4)
B-C(7)-Tl#2	111.75(19)	C(19)-C(20)-H(20)	120.0
C(9)-C(8)-C(7)	122.6(4)	C(15)-C(20)-H(20)	120.0
C(9)-C(8)-Tl#2	78.3(2)	C(26)-C(21)-C(22)	118.3(3)
C(7)-C(8)-Tl#2	78.1(2)	C(26)-C(21)-P(1)	123.9(3)
C(9)-C(8)-H(8)	118.7	C(22)-C(21)-P(1)	117.7(3)
C(7)-C(8)-H(8)	118.7	C(26)-C(21)-Tl#2	108.7(2)
Tl#2-C(8)-H(8)	115.2	C(22)-C(21)-Tl#2	100.1(2)
C(10)-C(9)-C(8)	119.4(4)	P(1)-C(21)-Tl#2	57.43(9)
C(10)-C(9)-Tl#2	78.8(2)	C(23)-C(22)-C(21)	120.4(4)
C(8)-C(9)-Tl#2	77.0(2)	C(23)-C(22)-H(22)	119.8
C(10)-C(9)-H(9)	120.3	C(21)-C(22)-H(22)	119.8
C(8)-C(9)-H(9)	120.3	C(24)-C(23)-C(22)	121.1(4)
Tl#2-C(9)-H(9)	114.5	C(24)-C(23)-H(23)	119.5
C(11)-C(10)-C(9)	119.9(4)	C(22)-C(23)-H(23)	119.5
C(11)-C(10)-Tl#2	76.9(2)	C(23)-C(24)-C(25)	119.0(3)
C(9)-C(10)-Tl#2	76.9(2)	C(23)-C(24)-H(24)	120.5
C(11)-C(10)-H(10)	120.1	C(25)-C(24)-H(24)	120.5
C(9)-C(10)-H(10)	120.1	C(24)-C(25)-C(26)	121.0(4)
Tl#2-C(10)-H(10)	116.8	C(24)-C(25)-H(25)	119.5
C(10)-C(11)-C(12)	119.5(4)	C(26)-C(25)-H(25)	119.5
C(10)-C(11)-Tl#2	78.9(2)	C(25)-C(26)-C(21)	120.2(4)
C(12)-C(11)-Tl#2	75.7(2)	C(25)-C(26)-H(26)	119.9
C(10)-C(11)-H(11)	120.3	C(21)-C(26)-H(26)	119.9
C(12)-C(11)-H(11)	120.3	C(32)-C(27)-C(28)	117.6(3)
Tl#2-C(11)-H(11)	115.8	C(32)-C(27)-P(2)	122.7(3)
C(11)-C(12)-C(7)	123.6(4)	C(28)-C(27)-P(2)	119.5(3)

C(29)-C(28)-C(27)	121.0(4)	C(38)-C(33)-P(2)	123.4(3)
C(29)-C(28)-H(28)	119.5	C(33)-C(34)-C(35)	120.6(4)
C(27)-C(28)-H(28)	119.5	C(33)-C(34)-H(34)	119.7
C(28)-C(29)-C(30)	120.5(3)	C(35)-C(34)-H(34)	119.7
C(28)-C(29)-H(29)	119.8	C(36)-C(35)-C(34)	119.7(4)
C(30)-C(29)-H(29)	119.8	C(36)-C(35)-H(35)	120.1
C(31)-C(30)-C(29)	119.6(4)	C(34)-C(35)-H(35)	120.1
C(31)-C(30)-H(30)	120.2	C(35)-C(36)-C(37)	120.5(4)
C(29)-C(30)-H(30)	120.2	C(35)-C(36)-H(36)	119.8
C(30)-C(31)-C(32)	119.9(4)	C(37)-C(36)-H(36)	119.8
C(30)-C(31)-H(31)	120.0	C(36)-C(37)-C(38)	120.2(4)
C(32)-C(31)-H(31)	120.0	C(36)-C(37)-H(37)	119.9
C(27)-C(32)-C(31)	121.3(3)	C(38)-C(37)-H(37)	119.9
C(27)-C(32)-H(32)	119.3	C(33)-C(38)-C(37)	119.8(4)
C(31)-C(32)-H(32)	119.3	C(33)-C(38)-H(38)	120.1
C(34)-C(33)-C(38)	119.1(3)	C(37)-C(38)-H(38)	120.1
C(34)-C(33)-P(2)	117.5(3)		

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x-1,y,z

Table 29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]). 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}
Tl	12(1)	19(1)	24(1)	7(1)	5(1)	6(1)
P(1)	12(1)	14(1)	13(1)	3(1)	2(1)	3(1)
P(2)	13(1)	18(1)	12(1)	3(1)	4(1)	6(1)
B	11(2)	15(2)	13(2)	3(2)	2(1)	3(2)
C(1)	10(2)	16(2)	14(2)	2(1)	2(1)	5(1)
C(2)	14(2)	15(2)	16(2)	3(1)	4(1)	8(1)
C(3)	18(2)	13(2)	21(2)	7(1)	7(1)	4(1)
C(4)	13(2)	15(2)	28(2)	1(2)	2(1)	-1(1)
C(5)	17(2)	24(2)	16(2)	2(2)	-1(1)	6(2)
C(6)	16(2)	17(2)	15(2)	6(1)	5(1)	5(1)
C(7)	11(2)	23(2)	15(2)	6(1)	8(1)	6(1)
C(8)	19(2)	26(2)	19(2)	6(2)	7(1)	7(2)
C(9)	16(2)	47(3)	18(2)	2(2)	1(2)	6(2)
C(10)	17(2)	57(3)	21(2)	20(2)	5(2)	17(2)
C(11)	20(2)	39(3)	33(2)	24(2)	14(2)	17(2)
C(12)	13(2)	24(2)	22(2)	9(2)	6(1)	6(2)
C(13)	13(2)	11(2)	16(2)	4(1)	5(1)	3(1)
C(14)	15(2)	14(2)	11(2)	2(1)	3(1)	4(1)
C(15)	22(2)	15(2)	13(2)	3(1)	9(1)	5(2)
C(16)	21(2)	21(2)	18(2)	8(2)	9(1)	8(2)
C(17)	29(2)	29(2)	24(2)	14(2)	13(2)	14(2)
C(18)	54(3)	18(2)	30(2)	10(2)	24(2)	17(2)
C(19)	51(3)	10(2)	31(2)	0(2)	13(2)	0(2)
C(20)	31(2)	18(2)	16(2)	0(2)	5(2)	-2(2)
C(21)	14(2)	17(2)	15(2)	7(1)	4(1)	8(1)
C(22)	17(2)	29(2)	24(2)	8(2)	5(2)	7(2)
C(23)	18(2)	40(3)	34(2)	15(2)	13(2)	13(2)
C(24)	35(2)	32(2)	25(2)	12(2)	17(2)	23(2)
C(25)	41(2)	20(2)	22(2)	6(2)	12(2)	15(2)
C(26)	26(2)	20(2)	19(2)	7(2)	10(2)	9(2)
C(27)	15(2)	21(2)	13(2)	2(1)	1(1)	7(2)
C(28)	19(2)	24(2)	19(2)	2(2)	4(1)	7(2)
C(29)	25(2)	28(2)	21(2)	-6(2)	3(2)	13(2)
C(30)	30(2)	20(2)	24(2)	-2(2)	-3(2)	13(2)
C(31)	32(2)	23(2)	24(2)	6(2)	8(2)	10(2)
C(32)	24(2)	22(2)	20(2)	4(2)	9(2)	12(2)
C(33)	15(2)	24(2)	16(2)	2(2)	6(1)	9(2)
C(34)	23(2)	24(2)	17(2)	1(2)	5(2)	11(2)
C(35)	31(2)	23(2)	22(2)	8(2)	9(2)	14(2)
C(36)	26(2)	45(3)	14(2)	9(2)	5(2)	17(2)
C(37)	19(2)	42(3)	18(2)	8(2)	0(2)	1(2)
C(38)	21(2)	30(2)	21(2)	8(2)	5(2)	2(2)

Table 30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [(*m*,*m*-$Me_2Ph)_2B(CH_2P^tBu_2)_2$][Tl] (38[Tl]).

	x	y	z	U(eq)
H(2)	3884	10009	6854	17
H(3)	6342	11390	7320	20
H(4)	7858	11530	8733	23
H(5)	6950	10200	9606	23
H(6)	4512	8811	9137	18
H(8)	-296	6997	6270	25
H(9)	-2224	7380	5193	33
H(10)	-2222	9206	5078	35
H(11)	-382	10626	6080	32
H(12)	1436	10222	7181	22
H(13A)	912	8993	8667	16
H(13B)	1823	8121	9022	16
H(14A)	1363	6538	7212	16
H(14B)	2802	6864	8045	16
H(16)	1678	6532	9462	23
H(17)	2198	4844	9643	30
H(18)	339	3229	8897	37
H(19)	-2033	3296	7969	38
H(20)	-2523	4983	7737	28
H(22)	-3948	6274	8975	27
H(23)	-5210	6608	10158	34
H(24)	-3916	8071	11259	31
H(25)	-1276	9176	11188	30
H(26)	25	8869	10003	24
H(28)	5395	5422	5833	25
H(29)	5438	3595	5790	30
H(30)	3986	2474	6679	29
H(31)	2527	3203	7632	30
H(32)	2390	5021	7640	25
H(34)	4359	8587	5743	25
H(35)	3123	8877	4375	28
H(36)	1111	7449	3480	32
H(37)	355	5724	3920	33
H(38)	1553	5425	5294	29