ORGANOMETALLICS
Organometallics, 1996, 15(3), 958-964, DOI:10.1021/om950588w

Table 1. Crystal data for 2,6-Mes*PhH.

L964-1

Identification code	bs10
Empirical formula	$C_{42}H_{62}$
Formula weight	566.92
Crystal size	0.4 x 0.3 x 0.25 mm
Crystal habit	blocks
Crystal color	colorless
Crystal system	triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 6.260(2) Å α = 78.98(5)°
	b = 10.557(4) Å β = 84.08(5)°
	c = 28.79(2) Å γ = 75.79(3)°
Volume	1808(2) Å^3
Z	2
Density (calculated)	1.042 Mg•m^3
Absorption coefficient	0.422 mm^{-1}
F(000)	628
Absorption correction[1]	XABS2
Max. and min. transmission	0.92 and 0.87

1) Parkin, S. R., Moezzi, B. Hope, H. (1995). XABS2: an empirical absorption correction program. J. Appl. Cryst., 28, 53-56.

Table 2. Data collection for 2,6-Mes*PhH.

L964-2

Diffractometer	Syntex $P2_1$
Temperature	143(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
θ range for data collection	1.57 to 57.04°
Scan type	$2\theta-\theta$
Index ranges	$-6 \leq h \leq 6$, $-11 \leq k \leq 11$, $0 \leq \ell \leq 31$
Reflections collected	5424
Independent reflections	4883 (R_{int} = 0.065)
Observed [I>2σ(I)] reflections	2902
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable

Table 3. Solution and refinement of 2,6-Mes*PhH.

L964-3

System for solution	SHELXTL 5 (Sheldrick, 1995)
Structure solution	direct
System for refinement	SHELXTL 5 (Sheldrick, 1995)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	Riding model, fixed thermal parameters
Extinction correction	none
Data / restraints / parameters	4882 / 6 / 428
Goodness-of-fit on F^2	0.921
Final R indices [$I>2\sigma(I)$]	R1 = 0.0831, wR2 = 0.1998
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.1278P)^2 + 3.35P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.1407, wR2 = 0.2553
Largest diff. peak and hole	0.464 and -0.343 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) Goodness-of-Fit $= [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections

and N is the number of parameters refined.

Table 5. Bond lengths [Å] for 2,6-Mes*PhH.

L964-4

C(1)-C(6)	1.391(6)	C(1)-C(2)	1.401(6)
C(2)-C(3)	1.385(7)	C(2)-C(25)	1.517(6)
C(3)-C(4)	1.375(7)	C(4)-C(5)	1.383(7)
C(5)-C(6)	1.389(7)	C(6)-C(7)	1.525(7)
C(7)-C(12)	1.412(7)	C(7)-C(8)	1.429(7)
C(8)-C(9)	1.405(7)	C(8)-C(17)	1.557(7)
C(9)-C(10)	1.366(7)	C(10)-C(11)	1.376(7)
C(10)-C(21)	1.531(7)	C(11)-C(12)	1.409(7)
C(12)-C(13)	1.566(7)	C(13)-C(16)	1.511(7)
C(13)-C(15)	1.529(7)	C(13)-C(14)	1.556(8)
C(17)-C(18)	1.534(8)	C(17)-C(19)	1.541(7)
C(17)-C(20)	1.539(8)	C(21)-C(22X)	1.432(11)
C(21)-C(24)	1.465(12)	C(21)-C(22)	1.488(11)
C(21)-C(23X)	1.548(12)	C(21)-C(24X)	1.665(11)
C(21)-C(23)	1.675(11)	C(25)-C(30)	1.418(6)
C(25)-C(26)	1.439(6)	C(26)-C(27)	1.393(6)
C(26)-C(35)	1.553(6)	C(27)-C(28)	1.374(6)
C(28)-C(29)	1.382(6)	C(28)-C(39)	1.533(6)
C(29)-C(30)	1.404(6)	C(30)-C(31)	1.561(6)
C(31)-C(34)	1.528(7)	C(31)-C(33)	1.538(6)
C(31)-C(32)	1.539(7)	C(35)-C(38)	1.532(7)
C(35)-C(36)	1.538(7)	C(35)-C(37)	1.541(7)
C(39)-C(41)	1.529(7)	C(39)-C(42)	1.532(7)
C(39)-C(40)	1.539(7)		

Table 6. Bond angles [°] for 2,6-Mes*PhH.

L964-5

C(6)-C(1)-C(2)	123.6(5)	C(3)-C(2)-C(1)	115.9(4)
C(3)-C(2)-C(25)	118.8(4)	C(1)-C(2)-C(25)	125.2(4)
C(4)-C(3)-C(2)	122.0(4)	C(3)-C(4)-C(5)	120.8(5)
C(4)-C(5)-C(6)	119.8(5)	C(5)-C(6)-C(1)	117.9(4)
C(5)-C(6)-C(7)	123.4(4)	C(1)-C(6)-C(7)	118.7(4)
C(12)-C(7)-C(8)	119.7(4)	C(12)-C(7)-C(6)	120.5(4)
C(8)-C(7)-C(6)	119.6(4)	C(9)-C(8)-C(7)	117.3(5)
C(9)-C(8)-C(17)	113.0(4)	C(7)-C(8)-C(17)	129.7(5)
C(10)-C(9)-C(8)	124.4(5)	C(9)-C(10)-C(11)	116.4(5)
C(9)-C(10)-C(21)	121.9(5)	C(11)-C(10)-C(21)	121.7(5)
C(10)-C(11)-C(12)	124.2(5)	C(11)-C(12)-C(7)	117.5(5)
C(11)-C(12)-C(13)	113.8(4)	C(7)-C(12)-C(13)	128.7(4)
C(16)-C(13)-C(15)	106.9(5)	C(16)-C(13)-C(14)	107.0(4)
C(15)-C(13)-C(14)	108.6(5)	C(16)-C(13)-C(12)	118.3(4)
C(15)-C(13)-C(12)	108.2(4)	C(14)-C(13)-C(12)	107.5(4)
C(18)-C(17)-C(19)	105.6(5)	C(18)-C(17)-C(20)	108.8(5)
C(19)-C(17)-C(20)	109.0(5)	C(18)-C(17)-C(8)	116.9(4)
C(19)-C(17)-C(8)	107.3(4)	C(20)-C(17)-C(8)	108.9(5)
C(24)-C(21)-C(22)	117.1(8)	C(22X)-C(21)-C(10)	112.2(6)
C(24)-C(21)-C(10)	111.3(6)	C(22)-C(21)-C(10)	110.2(6)
C(22X)-C(21)-C(23X)	117.0(8)	C(10)-C(21)-C(23X)	109.2(6)
C(22X)-C(21)-C(24X)	105.9(7)	C(10)-C(21)-C(24X)	110.5(6)
C(23X)-C(21)-C(24X)	101.2(7)	C(24)-C(21)-C(23)	105.2(8)
C(22)-C(21)-C(23)	102.6(7)	C(10)-C(21)-C(23)	109.8(6)
C(30)-C(25)-C(26)	119.3(4)	C(30)-C(25)-C(2)	120.3(4)
C(26)-C(25)-C(2)	120.1(4)	C(27)-C(26)-C(25)	117.5(4)
C(27)-C(26)-C(35)	116.8(4)	C(25)-C(26)-C(35)	125.6(4)
C(28)-C(27)-C(26)	124.6(4)	C(27)-C(28)-C(29)	116.6(4)
C(27)-C(28)-C(39)	120.6(4)	C(29)-C(28)-C(39)	122.8(4)
C(28)-C(29)-C(30)	123.7(4)	C(29)-C(30)-C(25)	118.2(4)
C(29)-C(30)-C(31)	116.0(4)	C(25)-C(30)-C(31)	125.7(4)
C(34)-C(31)-C(33)	105.0(4)	C(34)-C(31)-C(32)	110.4(4)
C(33)-C(31)-C(32)	105.4(4)	C(34)-C(31)-C(30)	112.7(4)
C(33)-C(31)-C(30)	112.6(4)	C(32)-C(31)-C(30)	110.3(4)
C(38)-C(35)-C(36)	105.6(4)	C(38)-C(35)-C(37)	110.4(4)
C(36)-C(35)-C(37)	105.2(4)	C(38)-C(35)-C(26)	109.9(4)
C(36)-C(35)-C(26)	112.7(4)	C(37)-C(35)-C(26)	112.8(4)
C(41)-C(39)-C(42)	107.9(5)	C(41)-C(39)-C(28)	110.4(4)
C(42)-C(39)-C(28)	112.1(4)	C(41)-C(39)-C(40)	109.6(4)
C(42)-C(39)-C(40)	108.0(4)	C(28)-C(39)-C(40)	108.7(4)

L964-6

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2,6-Mes*PhH.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	17(3)	22(2)	29(3)	-8(2)	2(2)	-3(2)
C(2)	23(3)	18(2)	25(2)	-8(2)	0(2)	-2(2)
C(3)	28(3)	27(3)	25(3)	-4(2)	0(2)	-6(2)
C(4)	18(3)	39(3)	37(3)	-6(2)	1(2)	-9(2)
C(5)	25(3)	30(3)	29(3)	-1(2)	-5(2)	-3(2)
C(6)	20(3)	24(2)	27(3)	-8(2)	3(2)	-2(2)
C(7)	15(3)	35(3)	30(3)	-3(2)	-5(2)	-5(2)
C(8)	41(3)	37(3)	27(3)	-2(2)	-6(2)	-11(3)
C(9)	45(4)	37(3)	32(3)	0(2)	-9(3)	-15(3)
C(10)	34(3)	48(3)	26(3)	3(2)	-6(2)	-17(3)
C(11)	26(3)	45(3)	25(3)	-5(2)	0(2)	-7(2)
C(12)	18(3)	35(3)	31(3)	-8(2)	-6(2)	-5(2)
C(13)	34(3)	32(3)	30(3)	-7(2)	-6(2)	-9(2)
C(14)	65(5)	51(4)	53(4)	-7(3)	5(3)	-6(3)
C(15)	83(5)	52(4)	44(3)	-10(3)	-19(3)	-23(4)
C(16)	50(4)	42(3)	55(4)	-15(3)	-3(3)	-19(3)
C(17)	47(4)	35(3)	34(3)	1(2)	-7(3)	-3(3)
C(18)	65(4)	32(3)	40(3)	-13(2)	-1(3)	4(3)
C(19)	93(6)	36(3)	51(4)	-10(3)	-15(4)	5(3)
C(20)	88(5)	47(3)	42(3)	-9(3)	-9(3)	-29(4)
C(21)	51(4)	54(4)	29(3)	3(3)	-4(3)	-23(3)
C(22)	63(9)	42(8)	32(6)	-9(5)	6(6)	-9(6)
C(23)	95(12)	49(8)	38(7)	-9(6)	25(7)	-37(8)
C(24)	38(8)	55(9)	59(8)	6(7)	4(6)	-28(7)
C(22X)	40(7)	61(8)	38(6)	-4(6)	10(5)	-22(6)
C(23X)	40(8)	61(9)	49(7)	-9(6)	14(6)	-25(6)
C(24X)	63(9)	58(8)	37(6)	-15(5)	19(6)	-18(6)
C(25)	20(3)	23(2)	28(3)	-2(2)	1(2)	-8(2)
C(26)	19(3)	26(2)	24(2)	-7(2)	4(2)	-7(2)
C(27)	22(3)	25(3)	28(3)	-8(2)	3(2)	-7(2)
C(28)	18(3)	29(3)	27(3)	-5(2)	6(2)	-9(2)
C(29)	25(3)	27(3)	29(3)	0(2)	0(2)	-3(2)
C(30)	19(3)	23(2)	29(3)	-4(2)	1(2)	-5(2)
C(31)	27(3)	22(2)	34(3)	-5(2)	0(2)	-7(2)
C(32)	51(4)	35(3)	39(3)	-16(2)	3(3)	-6(3)
C(33)	56(4)	24(3)	46(3)	-8(2)	-16(3)	-3(3)
C(34)	41(4)	34(3)	40(3)	-13(2)	-3(3)	-9(3)
C(35)	29(3)	28(3)	26(3)	-6(2)	1(2)	-9(2)
C(36)	48(4)	35(3)	40(3)	-15(2)	-5(3)	2(3)
C(37)	31(3)	31(3)	40(3)	-9(2)	3(2)	0(2)
C(38)	38(3)	23(3)	42(3)	-8(2)	0(3)	-10(2)
C(39)	32(3)	31(3)	29(3)	-3(2)	-9(2)	-4(2)
C(40)	45(4)	39(3)	29(3)	-5(2)	-8(3)	-5(3)
C(41)	39(3)	52(3)	39(3)	1(3)	-18(3)	-15(3)
C(42)	49(4)	40(3)	38(3)	-2(2)	-11(3)	0(3)

L9647

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2,6-Mes*PhH.

	x	y	z	U(eq)
H(1)	2059(8)	5111(4)	2446(2)	27
H(3A)	-2579(8)	4041(4)	3387(2)	33
H(4A)	-5089(8)	4733(5)	2816(2)	37
H(5A)	-4096(8)	5674(5)	2057(2)	35
H(9A)	1262(9)	8737(5)	1084(2)	45
H(11A)	2562(8)	5222(5)	707(2)	38
H(14A)	3987(21)	3220(28)	1084(8)	88
H(14B)	3160(12)	1996(9)	1373(15)	88
H(14C)	3808(25)	2998(33)	1639(8)	88
H(15A)	614(42)	4012(39)	628(2)	86
H(15B)	-1737(24)	4163(34)	889(7)	86
H(15C)	-187(65)	2750(7)	889(7)	86
H(16A)	-77(42)	3194(32)	2055(2)	70
H(16B)	-342(49)	2177(9)	1746(8)	70
H(16C)	-2108(12)	3520(25)	1741(7)	70
H(18A)	-3791(35)	7944(35)	2191(3)	71
H(18B)	-3194(50)	9027(11)	2425(8)	71
H(18C)	-1788(18)	7562(27)	2515(6)	71
H(19A)	-3720(41)	9406(16)	1433(13)	94
H(19B)	-1621(22)	9940(31)	1234(7)	94
H(19C)	-3036(63)	10454(17)	1671(6)	94
H(20A)	1632(42)	9417(37)	1737(2)	85
H(20B)	1749(39)	8366(11)	2204(12)	85
H(20C)	170(12)	9776(27)	2190(12)	85
H(22A)	958(46)	8084(69)	-32(14)	70
H(22B)	2444(126)	6673(14)	-71(16)	70
H(22C)	3249(80)	7944(76)	-319(4)	70
H(23A)	1916(30)	9672(16)	348(33)	88
H(23B)	4278(129)	9489(25)	91(19)	88
H(23C)	4010(146)	9296(15)	646(17)	88
H(24A)	6696(26)	7296(60)	149(17)	75
H(24B)	6064(24)	5978(21)	408(31)	75
H(24C)	6401(40)	7007(73)	704(15)	75
H(22D)	1009(77)	8301(28)	-15(23)	69
H(22E)	3093(36)	8864(55)	-203(13)	69
H(22F)	1619(110)	9357(31)	231(10)	69
H(23D)	6384(69)	7077(31)	758(21)	73
H(23E)	5257(21)	8594(47)	703(24)	73
H(23F)	6610(57)	8012(75)	271(5)	73
H(24D)	5615(103)	5664(38)	264(11)	79
H(24E)	5357(114)	6706(21)	-206(15)	79
H(24F)	3433(25)	6009(54)	-3(24)	79
H(27A)	3279(8)	4892(4)	4282(2)	30

L964-8

H(29A)	4901(8)	1343(5)	3917(2)	34
H(32A)	5424(21)	1992(34)	2710(2)	62
H(32B)	3141(34)	2783(17)	2514(5)	62
H(32C)	3977(52)	1271(19)	2487(5)	62
H(33A)	5601(18)	236(9)	3412(12)	64
H(33B)	4130(52)	-407(9)	3162(6)	64
H(33C)	3435(35)	-98(16)	3675(6)	64
H(34A)	-313(20)	2177(15)	2909(9)	56
H(34B)	-279(21)	1308(32)	3416(2)	56
H(34C)	606(9)	637(19)	2971(11)	56
H(36A)	2671(10)	6874(30)	4079(8)	62
H(36B)	490(50)	6581(24)	4348(3)	62
H(36C)	432(51)	7929(8)	4002(6)	62
H(37A)	-2213(8)	6476(30)	3342(5)	53
H(37B)	-2460(9)	7569(9)	3656(11)	53
H(37C)	-2406(10)	6099(23)	3896(7)	53
H(38A)	3223(14)	7026(27)	3228(5)	50
H(38B)	943(37)	8046(7)	3160(7)	50
H(38C)	1474(48)	6770(22)	2926(2)	50
H(40A)	3146(35)	2114(28)	5056(6)	57
H(40B)	3519(44)	3522(6)	5068(6)	57
H(40C)	5104(12)	2250(31)	5326(2)	57
H(41A)	6632(9)	4301(8)	4589(12)	63
H(41B)	8353(37)	3351(27)	4301(6)	63
H(41C)	8287(40)	3080(22)	4857(7)	63
H(42A)	6039(11)	545(7)	4619(13)	66
H(42B)	7858(49)	816(13)	4898(7)	66
H(42C)	8054(43)	1040(8)	4342(7)	66

L964-9

Table 1. Crystal data for 2,6-Tripp$_2$PhLi(Et$_2$O).

Identification code	BS06
Empirical formula	$C_{40}H_{59}LiO$
Formula weight	562.81
Crystal size	0.5 x 0.4 x 0.4 mm
Crystal habit	colorless
Crystal color	blocks
Crystal system	$P2_1/n$
Space group	monoclinic
Unit cell dimensions	a = 8.765(3) Å
	b = 17.178(8) Å
	c = 24.267(14) Å
	β = 93.84(4)°
Volume	3646(3) Å^3
Z	4
Density (calculated)	1.025 Mg*m^{-3}
Absorption coefficient	0.433 mm^{-1}
F(000)	1240
Absorption correction(1)	XABS2
Max. and min. trans. coeff.	0.87 and 0.84

1) Parkin, S. R., Moezzi, B., Hope, H. (1995). J. Appl. Cryst., 28, 53-56. XABS2: an empirical absorption correction program.

L964-10

Table 2. Data collection for 2,6-Tripp$_2$PhLi(Et$_2$O).

Diffractometer	Syntex P2$_1$
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
2θ-range, data collection	3.15 to 57.05°
Scan type	2θ-θ
Index ranges	$-9 \leq h \leq 9$, $0 \leq k \leq 18$, $0 \leq l \leq 26$
Reflections collected	5517
Independent reflections	4929 (R(int) = 0.037)
Standard reflections	2 (measured every 198 reflections)
Stability of standards	stable

L964-11

Table 3. Solution and refinement of 2,6-Tripp$_2$PhLi(Et$_2$O).

System for solution	SHELXTL 5 (Sheldrick, 1995)
Structure solution	direct
System for refinement	SHELXTL 5 (Sheldrick, 1995)
Hydrogen atoms	riding model, fixed thermal parameters
Data/ restraints/ parameters	4928 / 0 / 520
Final R indices (1) [I>2σ(I)]	R1 = 0.0618,
	wR2 = 0.1381
Reflections observed	3598
R indices (all data)	R1 = 0.0898,
	wR2 = 0.1574
Goodness-of-fit (2) on F^2	1.022
Largest diff. peak and hole	0.302 and -0.338 eÅ^{-3}

1) $R1 = \sum||Fo|-|Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) Goodness-of-Fit = $[\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$ where M is the number of reflections and N is the number of parameters refined.

L964-12

Table 5. Bond lengths [Å] for 2,6-Tripp$_2$PhLi(Et$_2$O).

O(1)-C(37)	1.416(5)
O(1)-C(39)	1.430(5)
O(1)-Li(1)	1.850(7)
Li(1)-C(1)	2.017(7)
Li(1)-H(14A)	2.60(5)
Li(1)-H(38C)	2.73(5)
Li(1)-H(40C)	2.76(7)
Li(1)-H(38B)	2.77(6)
Li(1)-H(40B)	2.81(5)
Li(1)-C(37)	2.866(8)
Li(1)-C(39)	2.885(8)
Li(1)-H(32A)	2.92(4)
Li(1)-C(38)	2.933(9)
Li(1)-C(40)	2.949(10)
C(1)-C(6)	1.408(4)
C(1)-C(2)	1.416(4)
C(2)-C(3)	1.394(4)
C(2)-C(22)	1.502(4)
C(3)-C(4)	1.378(4)
C(4)-C(5)	1.378(4)
C(5)-C(6)	1.397(4)
C(6)-C(7)	1.509(4)
C(7)-C(8)	1.409(4)
C(7)-C(12)	1.414(4)
C(8)-C(9)	1.390(4)
C(8)-C(16)	1.528(4)
C(9)-C(10)	1.387(4)
C(10)-C(11)	1.384(4)
C(10)-C(19)	1.518(4)
C(11)-C(12)	1.391(4)
C(12)-C(13)	1.523(4)
C(13)-C(15)	1.523(4)
C(13)-C(14)	1.529(5)
C(16)-C(17)	1.519(4)
C(16)-C(18)	1.524(4)
C(19)-C(21)	1.521(5)
C(19)-C(20)	1.527(5)

L964-13

C(22)-C(23)	1.407(4)
C(22)-C(27)	1.408(4)
C(23)-C(24)	1.392(4)
C(23)-C(31)	1.524(4)
C(24)-C(25)	1.389(5)
C(25)-C(26)	1.384(5)
C(25)-C(34)	1.519(5)
C(26)-C(27)	1.388(4)
C(27)-C(28)	1.518(4)
C(28)-C(30)	1.508(6)
C(28)-C(29)	1.517(6)
C(31)-C(33)	1.518(4)
C(31)-C(32)	1.530(5)
C(34)-C(35)	1.413(6)
C(34)-C(36)	1.414(6)
C(37)-C(38)	1.481(7)
C(39)-C(40)	1.441(7)

Table 6. Bond angles [°] for 2,6-Tripp$_2$PhLi(Et$_2$O).

C(37)-O(1)-C(39)	114.9(3)
C(37)-O(1)-Li(1)	122.1(3)
C(39)-O(1)-Li(1)	122.6(3)
O(1)-Li(1)-C(1)	171.9(5)
O(1)-Li(1)-H(14A)	79.7(10)
C(1)-Li(1)-H(14A)	92.2(10)
O(1)-Li(1)-H(38C)	66.2(11)
C(1)-Li(1)-H(38C)	110.8(12)
H(14A)-Li(1)-H(38C)	70.1(14)
O(1)-Li(1)-H(40C)	63(2)
C(1)-Li(1)-H(40C)	120(2)
H(14A)-Li(1)-H(40C)	103(2)
H(38C)-Li(1)-H(40C)	130(2)
O(1)-Li(1)-H(38B)	63.7(12)
C(1)-Li(1)-H(38B)	118.2(13)
H(14A)-Li(1)-H(38B)	102(2)
H(38C)-Li(1)-H(38B)	33(2)
H(40C)-Li(1)-H(38B)	115(2)
O(1)-Li(1)-H(40B)	66.2(11)

L964-14

C(1)-Li(1)-H(40B)	111.3(11)
H(14A)-Li(1)-H(40B)	68.5(14)
H(38C)-Li(1)-H(40B)	120.7(14)
H(40C)-Li(1)-H(40B)	35(2)
H(38B)-Li(1)-H(40B)	130(2)
O(1)-Li(1)-C(37)	24.7(2)
C(1)-Li(1)-C(37)	152.9(4)
H(14A)-Li(1)-C(37)	78.2(10)
H(38C)-Li(1)-C(37)	42.1(11)
H(40C)-Li(1)-C(37)	88(2)
H(38B)-Li(1)-C(37)	42.0(12)
H(40B)-Li(1)-C(37)	88.9(10)
O(1)-Li(1)-C(39)	24.7(2)
C(1)-Li(1)-C(39)	154.4(4)
H(14A)-Li(1)-C(39)	80.3(10)
H(38C)-Li(1)-C(39)	89.7(11)
H(40C)-Li(1)-C(39)	41(2)
H(38B)-Li(1)-C(39)	87.3(12)
H(40B)-Li(1)-C(39)	43.2(11)
C(37)-Li(1)-C(39)	49.3(2)
O(1)-Li(1)-H(32A)	89.0(8)
C(1)-Li(1)-H(32A)	99.1(8)
H(14A)-Li(1)-H(32A)	168.6(13)
H(38C)-Li(1)-H(32A)	105.3(13)
H(40C)-Li(1)-H(32A)	72(2)
H(38B)-Li(1)-H(32A)	72.5(14)
H(40B)-Li(1)-H(32A)	107.1(13)
C(37)-Li(1)-H(32A)	91.4(8)
C(39)-Li(1)-H(32A)	89.5(8)
O(1)-Li(1)-C(38)	54.1(2)
C(1)-Li(1)-C(38)	124.9(3)
H(14A)-Li(1)-C(38)	83.4(10)
H(38C)-Li(1)-C(38)	18.7(11)
H(40C)-Li(1)-C(38)	115(2)
H(38B)-Li(1)-C(38)	19.4(12)
H(40B)-Li(1)-C(38)	117.5(10)
C(37)-Li(1)-C(38)	29.6(2)
C(39)-Li(1)-C(38)	78.8(2)

L964-15

H(32A)-Li(1)-C(38)	89.9(8)
O(1)-Li(1)-C(40)	53.3(2)
C(1)-Li(1)-C(40)	126.7(4)
H(14A)-Li(1)-C(40)	83.8(10)
H(38C)-Li(1)-C(40)	117.2(11)
H(40C)-Li(1)-C(40)	20(2)
H(38B)-Li(1)-C(40)	114.5(12)
H(40B)-Li(1)-C(40)	20.8(11)
C(37)-Li(1)-C(40)	77.9(2)
C(39)-Li(1)-C(40)	28.6(2)
H(32A)-Li(1)-C(40)	89.5(8)
C(38)-Li(1)-C(40)	107.4(2)
C(6)-C(1)-C(2)	115.1(2)
C(6)-C(1)-Li(1)	123.6(3)
C(2)-C(1)-Li(1)	121.2(3)
C(3)-C(2)-C(1)	122.6(3)
C(3)-C(2)-C(22)	119.4(2)
C(1)-C(2)-C(22)	118.0(2)
C(3)-C(2)-Li(1)	157.5(2)
C(1)-C(2)-Li(1)	35.0(2)
C(22)-C(2)-Li(1)	83.0(2)
C(4)-C(3)-C(2)	119.9(3)
C(3)-C(4)-C(5)	119.8(3)
C(4)-C(5)-C(6)	120.2(3)
C(5)-C(6)-C(1)	122.3(2)
C(5)-C(6)-C(7)	118.5(2)
C(1)-C(6)-C(7)	119.2(2)
C(5)-C(6)-Li(1)	155.8(2)
C(1)-C(6)-Li(1)	33.6(2)
C(7)-C(6)-Li(1)	85.6(2)
C(8)-C(7)-C(12)	118.6(2)
C(8)-C(7)-C(6)	120.9(2)
C(12)-C(7)-C(6)	120.5(2)
C(9)-C(8)-C(7)	119.8(3)
C(9)-C(8)-C(16)	119.5(2)
C(7)-C(8)-C(16)	120.6(2)
C(10)-C(9)-C(8)	122.1(3)
C(11)-C(10)-C(9)	117.5(3)

L964-16

C(11)-C(10)-C(19)	121.7(3)
C(9)-C(10)-C(19)	120.7(3)
C(10)-C(11)-C(12)	122.8(3)
C(11)-C(12)-C(7)	119.1(3)
C(11)-C(12)-C(13)	118.6(3)
C(7)-C(12)-C(13)	122.3(2)
C(15)-C(13)-C(12)	111.8(3)
C(15)-C(13)-C(14)	110.4(3)
C(12)-C(13)-C(14)	110.9(3)
C(17)-C(16)-C(18)	110.7(3)
C(17)-C(16)-C(8)	113.6(2)
C(18)-C(16)-C(8)	110.1(2)
C(10)-C(19)-C(21)	111.5(3)
C(10)-C(19)-C(20)	111.4(3)
C(21)-C(19)-C(20)	110.4(3)
C(23)-C(22)-C(27)	118.9(3)
C(23)-C(22)-C(2)	119.7(2)
C(27)-C(22)-C(2)	121.3(3)
C(24)-C(23)-C(22)	119.1(3)
C(24)-C(23)-C(31)	119.2(3)
C(22)-C(23)-C(31)	121.6(2)
C(25)-C(24)-C(23)	122.8(3)
C(26)-C(25)-C(24)	117.1(3)
C(26)-C(25)-C(34)	121.1(3)
C(24)-C(25)-C(34)	121.8(3)
C(25)-C(26)-C(27)	122.6(3)
C(26)-C(27)-C(22)	119.6(3)
C(26)-C(27)-C(28)	118.9(3)
C(22)-C(27)-C(28)	121.5(3)
C(30)-C(28)-C(29)	110.3(5)
C(30)-C(28)-C(27)	112.4(3)
C(29)-C(28)-C(27)	111.7(3)
C(33)-C(31)-C(23)	110.2(2)
C(33)-C(31)-C(32)	111.3(3)
C(23)-C(31)-C(32)	112.5(3)
C(35)-C(34)-C(36)	123.0(4)
C(35)-C(34)-C(25)	115.1(3)
C(36)-C(34)-C(25)	116.0(3)

L964-17

O(1)-C(37)-C(38)	110.5(4)
O(1)-C(37)-Li(1)	33.1(2)
C(38)-C(37)-Li(1)	77.7(3)
C(37)-C(38)-Li(1)	72.7(3)
O(1)-C(39)-C(40)	110.8(4)
O(1)-C(39)-Li(1)	32.7(2)
C(40)-C(39)-Li(1)	78.2(3)
C(39)-C(40)-Li(1)	73.2(3)

L964-18

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2,6-Tripp$_2$PhLi(Et$_2$O). The anisotropic displacement factor exponent takes the form: $-2(\pi)^2[h^2a^{2*}U_{11} + ... + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13	U12
O(1)	28(1)	44(2)	69(2)	9(1)	12(1)	12(1)
Li(1)	38(4)	55(4)	104(6)	-14(4)	6(4)	18(3)
C(1)	16(2)	22(2)	20(2)	0(1)	-1(1)	-2(1)
C(2)	16(2)	23(2)	20(1)	1(1)	1(1)	-2(1)
C(3)	20(2)	33(2)	21(2)	5(1)	-4(1)	4(1)
C(4)	15(2)	36(2)	29(2)	1(1)	2(1)	9(2)
C(5)	20(2)	31(2)	19(2)	-3(1)	4(1)	1(1)
C(6)	15(2)	17(1)	21(2)	2(1)	0(1)	-3(1)
C(7)	15(2)	22(2)	20(1)	-1(1)	3(1)	2(1)
C(8)	16(2)	21(2)	23(2)	-1(1)	-2(1)	-1(1)
C(9)	26(2)	23(2)	25(2)	-3(1)	-7(1)	-3(1)
C(10)	25(2)	25(2)	22(2)	2(1)	-4(1)	3(1)
C(11)	29(2)	17(2)	25(2)	3(1)	-1(1)	1(1)
C(12)	24(2)	22(2)	20(2)	-2(1)	1(1)	-2(1)
C(13)	31(2)	24(2)	25(2)	1(1)	-6(1)	-5(1)
C(14)	51(3)	34(2)	41(2)	-14(2)	8(2)	-10(2)
C(15)	40(2)	28(2)	36(2)	0(2)	0(2)	-10(2)
C(16)	27(2)	21(2)	26(2)	5(1)	-9(1)	-2(1)
C(17)	45(2)	22(2)	34(2)	1(2)	-8(2)	0(2)
C(18)	43(2)	31(2)	46(2)	10(2)	7(2)	-1(2)
C(19)	40(2)	27(2)	28(2)	2(1)	-11(2)	3(2)
C(20)	57(3)	55(2)	40(2)	9(2)	-13(2)	23(2)
C(21)	73(3)	49(2)	24(2)	7(2)	-1(2)	11(2)
C(22)	20(2)	23(2)	18(1)	5(1)	1(1)	2(1)
C(23)	24(2)	28(2)	24(2)	4(1)	4(1)	2(1)
C(24)	37(2)	38(2)	34(2)	5(2)	16(2)	-8(2)
C(25)	62(3)	34(2)	28(2)	-2(2)	19(2)	-8(2)
C(26)	52(2)	28(2)	23(2)	-3(1)	5(2)	-4(2)
C(27)	32(2)	27(2)	21(2)	5(1)	2(1)	0(1)
C(28)	38(2)	30(2)	22(2)	0(1)	2(1)	-8(2)
C(29)	61(4)	128(5)	75(4)	55(4)	-33(3)	-54(4)
C(30)	70(4)	38(3)	147(6)	25(3)	43(4)	-14(3)

L964-19

C(31)	26(2)	34(2)	26(2)	3(1)	5(1)	-8(2)
C(32)	32(2)	51(3)	49(2)	8(2)	-3(2)	-11(2)
C(33)	44(2)	34(2)	35(2)	-4(2)	2(2)	-6(2)
C(34)	136(5)	39(2)	53(3)	-10(2)	62(3)	-13(3)
C(35)	146(5)	79(3)	72(3)	12(3)	74(3)	46(4)
C(36)	160(5)	66(3)	52(3)	1(2)	64(3)	-9(3)
C(37)	69(3)	124(5)	72(3)	0(3)	10(3)	56(3)
C(38)	47(3)	91(4)	75(3)	2(3)	6(3)	24(3)
C(39)	44(3)	78(3)	78(3)	6(3)	0(2)	30(2)
C(40)	52(3)	95(5)	100(4)	-28(4)	1(3)	15(3)

L964-20

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2,6-Tripp$_2$PhLi(Et$_2$O).

	x	y	z	U(eq)
H(3)	605(33)	3210(16)	1027(12)	24(8)
H(4)	-327(38)	3399(18)	1907(12)	31(9)
H(5)	1007(33)	2911(16)	2693(12)	26(8)
H(9)	5824(35)	2677(17)	3858(12)	30(8)
H(11)	4218(30)	514(17)	3522(10)	18(7)
H(13)	2011	1012	2294	32
H(14A)	4378(53)	454(26)	2066(18)	85(15)
H(14B)	3090(40)	-221(21)	2073(14)	49(10)
H(14C)	4321(47)	-135(24)	2590(17)	68(13)
H(15A)	2019(39)	-104(20)	3170(13)	42(10)
H(15B)	785(36)	-69(19)	2669(12)	34(9)
H(15C)	831(44)	619(23)	3122(15)	60(12)
H(16)	3823	3619	2730	30
H(17A)	4704(34)	4610(19)	3325(12)	33(8)
H(17B)	5593(39)	3946(18)	3713(13)	33(9)
H(17C)	3812(41)	3959(19)	3714(14)	44(10)
H(18A)	6032(9)	3238(8)	2340(4)	43(10)
H(18B)	7001(5)	3374(10)	2898(3)	29(8)
H(18C)	6274(12)	4084(2)	2571(7)	43(10)
H(19)	6533(38)	1713(19)	4483(13)	41(9)
H(20A)	7444(22)	460(9)	4596(3)	77
H(20B)	7612(19)	709(5)	3982(8)	77
H(20C)	6291(5)	145(4)	4127(10)	77
H(21A)	5176(5)	931(14)	5084(3)	73
H(21B)	4036(18)	666(10)	4595(5)	73
H(21C)	4046(18)	1534(5)	4795(8)	73
H(24)	5716(39)	3202(19)	-13(13)	37(9)
H(26)	2839(37)	1438(19)	-382(13)	38(9)
H(28)	881	1565	874	36
H(29A)	-6(61)	1453(31)	-260(22)	106(20)
H(29B)	-464(86)	2160(46)	118(30)	186(34)
H(29C)	-1052(52)	1239(25)	193(16)	70(13)
H(30A)	802(45)	245(22)	595(14)	51(11)

L964-21

H(30B)	2255(63)	632(31)	874(22)	106(22)
H(30C)	2046(75)	445(35)	142(27)	146(26)
H(31)	4501	3576	1328	35
H(32A)	7030(44)	3055(24)	1228(15)	63(12)
H(32B)	7061(41)	3982(21)	1353(14)	49(10)
H(32C)	7196(40)	3666(19)	748(15)	44(10)
H(33A)	3390(4)	4437(5)	682(8)	56
H(33B)	4911(20)	4475(6)	378(4)	56
H(33C)	4854(21)	4818(2)	975(4)	56
H(34)	3798(95)	2037(46)	-1204(32)	217(34)
H(35A)	4834(20)	1070(3)	-850(15)	144
H(35B)	6512(22)	1377(9)	-744(13)	144
H(35C)	5709(44)	1403(8)	-1341(3)	144
H(36A)	6523(21)	3025(12)	-906(10)	135
H(36B)	4844(20)	3306(6)	-1054(14)	135
H(36C)	5688(42)	2795(7)	-1474(4)	135
H(37A)	7241	110	1302	106
H(37B)	8280	740	1045	106
H(38A)	6127(65)	395(34)	430(24)	125(22)
H(38B)	6098(66)	1336(35)	630(23)	123(23)
H(38C)	5107(62)	670(28)	859(20)	94(18)
H(39A)	9213	1234	1958	80
H(39B)	8312	537	2201	80
H(40A)	8537(80)	1463(38)	2870(27)	148(27)
H(40B)	6835(62)	1397(27)	2714(19)	92(16)
H(40C)	7820(86)	2100(47)	2411(30)	182(35)

L964-22

Table 1. Crystal data for 2,6-Tripp2PhCu(SMe2).

Identification code	bs19
Empirical formula	$C_{38}H_{55}CuS$
Formula weight	607.42
Crystal size	0.40 x 0.40 x 0.25 mm
Crystal habit	blocks
Crystal color	colorless
Crystal system	orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 8.7740(10) Å α = 90°
	b = 15.974(4) Å β = 90°
	c = 24.860(6) Å γ = 90°
Volume	3484.3(13) $Å^3$
Z	4
Density (calculated)	1.158 $Mg \cdot m^3$
Absorption coefficient	1.595 mm^{-1}
F(000)	1312
Absorption correction[1]	XABS2
Max. and min. transmission	0.72 and 0.55

1) Parkin, S. R., Moezzi, B. Hope, H. (1995). XABS2: an empirical absorption correction program. J. Appl. Cryst., 28, 53–56.

L964-23

Table 2. Data collection for 2,6-Tripp2PhCu(SMe2).

Diffractometer	Syntex $P2_1$
Temperature	143(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
θ range for data collection	3.29 to 57.04°
Scan type	$2\theta-\theta$
Index ranges	$0 \le h \le 9$, $0 \le k \le 17$, $0 \le \ell \le 27$
Reflections collected	2716
Independent reflections	2688 (R_{int} = 0.0299)
Observed [$I>2\sigma(I)$] reflections	2385
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable

L964-24

Table 3. Solution and refinement of 2,6-Tripp2PhCu(SMe2).

System for solution	SHELXTL 5 (Sheldrick, 1995)
Structure solution	direct
System for refinement	SHELXTL 5 (Sheldrick, 1995)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding model, fixed thermal parameters
Extinction correction	none
Data / restraints / parameters	2682 / 0 / 360
Goodness-of-fit on F^2	1.053
Final R indices [$I>2\sigma(I)$]	R1 = 0.0495, wR2 = 0.1226
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0692P)^2 + 4.96P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0592, wR2 = 0.1429
Absolute structure parameter	0.42(5)
Largest diff. peak and hole	0.318 and -0.550 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) Goodness-of-Fit = $[\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections

and N is the number of parameters refined.

L964-25

Table 5. Bond lengths [Å] for 2,6-Tripp2PhCu(SMe2).

Cu(1)-C(1)	1.894(6)	Cu(1)-S(1)	2.177(2)
S(1)-C(38)	1.799(8)	S(1)-C(37)	1.810(8)
C(1)-C(2)	1.414(9)	C(1)-C(6)	1.428(9)
C(2)-C(3)	1.394(9)	C(2)-C(22)	1.504(9)
C(3)-C(4)	1.380(8)	C(4)-C(5)	1.383(9)
C(5)-C(6)	1.395(9)	C(6)-C(7)	1.494(9)
C(7)-C(8)	1.393(9)	C(7)-C(12)	1.420(9)
C(8)-C(9)	1.396(9)	C(8)-C(16)	1.541(9)
C(9)-C(10)	1.395(9)	C(10)-C(11)	1.380(10)
C(10)-C(19)	1.520(9)	C(11)-C(12)	1.388(9)
C(12)-C(13)	1.513(10)	C(13)-C(14)	1.533(11)
C(13)-C(15)	1.533(10)	C(16)-C(17)	1.535(9)
C(16)-C(18)	1.539(10)	C(19)-C(21)	1.517(10)
C(19)-C(20)	1.520(11)	C(22)-C(23)	1.405(9)
C(22)-C(27)	1.426(9)	C(23)-C(24)	1.398(9)
C(23)-C(31)	1.516(9)	C(24)-C(25)	1.389(9)
C(25)-C(26)	1.370(9)	C(25)-C(34)	1.516(9)
C(26)-C(27)	1.387(9)	C(27)-C(28)	1.513(9)
C(28)-C(29)	1.523(10)	C(28)-C(30)	1.546(9)
C(31)-C(33)	1.530(9)	C(31)-C(32)	1.544(10)
C(34)-C(35)	1.508(10)	C(34)-C(36)	1.513(10)

Table 6. Bond angles [°] for 2,6-Tripp2PhCu(SMe2).

L964-26

C(1)-Cu(1)-S(1)	176.3(2)	C(38)-S(1)-C(37)	98.1(4)
C(38)-S(1)-Cu(1)	104.9(3)	C(37)-S(1)-Cu(1)	103.4(3)
C(2)-C(1)-C(6)	116.8(5)	C(2)-C(1)-Cu(1)	122.0(5)
C(6)-C(1)-Cu(1)	121.2(5)	C(3)-C(2)-C(1)	121.5(6)
C(3)-C(2)-C(22)	120.9(6)	C(1)-C(2)-C(22)	117.6(6)
C(4)-C(3)-C(2)	119.8(6)	C(3)-C(4)-C(5)	121.0(6)
C(4)-C(5)-C(6)	119.9(6)	C(5)-C(6)-C(1)	121.0(6)
C(5)-C(6)-C(7)	121.2(6)	C(1)-C(6)-C(7)	117.8(5)
C(8)-C(7)-C(12)	118.8(6)	C(8)-C(7)-C(6)	121.4(6)
C(12)-C(7)-C(6)	119.8(6)	C(7)-C(8)-C(9)	120.2(6)
C(7)-C(8)-C(16)	120.8(6)	C(9)-C(8)-C(16)	119.0(6)
C(10)-C(9)-C(8)	121.5(6)	C(11)-C(10)-C(9)	117.6(6)
C(11)-C(10)-C(19)	121.3(6)	C(9)-C(10)-C(19)	121.1(6)
C(10)-C(11)-C(12)	122.8(7)	C(11)-C(12)-C(7)	119.1(6)
C(11)-C(12)-C(13)	120.2(6)	C(7)-C(12)-C(13)	120.6(6)
C(12)-C(13)-C(14)	111.4(6)	C(12)-C(13)-C(15)	112.0(6)
C(14)-C(13)-C(15)	110.3(7)	C(17)-C(16)-C(18)	110.3(6)
C(17)-C(16)-C(8)	113.1(5)	C(18)-C(16)-C(8)	110.7(6)
C(21)-C(19)-C(20)	110.2(7)	C(21)-C(19)-C(10)	112.0(6)
C(20)-C(19)-C(10)	111.6(6)	C(23)-C(22)-C(27)	118.1(6)
C(23)-C(22)-C(2)	120.6(6)	C(27)-C(22)-C(2)	121.2(6)
C(24)-C(23)-C(22)	120.2(6)	C(24)-C(23)-C(31)	118.4(6)
C(22)-C(23)-C(31)	121.3(6)	C(25)-C(24)-C(23)	121.7(7)
C(26)-C(25)-C(24)	117.6(6)	C(26)-C(25)-C(34)	120.1(6)
C(24)-C(25)-C(34)	122.3(6)	C(25)-C(26)-C(27)	123.5(6)
C(26)-C(27)-C(22)	118.9(6)	C(26)-C(27)-C(28)	120.3(6)
C(22)-C(27)-C(28)	120.8(5)	C(27)-C(28)-C(29)	112.9(5)
C(27)-C(28)-C(30)	110.3(6)	C(29)-C(28)-C(30)	110.3(6)
C(23)-C(31)-C(33)	109.8(5)	C(23)-C(31)-C(32)	112.4(6)
C(33)-C(31)-C(32)	110.5(6)	C(35)-C(34)-C(36)	110.8(7)
C(35)-C(34)-C(25)	114.4(6)	C(36)-C(34)-C(25)	109.3(6)

L964-27

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2,6-Tripp2PhCu(SMe2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	14(1)	15(1)	14(1)	1(1)	-1(1)	-4(1)
S(1)	16(1)	21(1)	22(1)	-1(1)	-1(1)	-6(1)
C(1)	16(3)	12(3)	5(3)	0(3)	2(3)	2(3)
C(2)	19(4)	3(3)	13(3)	4(3)	0(3)	6(3)
C(3)	17(3)	7(3)	9(3)	3(3)	-2(3)	1(3)
C(4)	13(3)	8(3)	22(3)	3(3)	4(3)	-1(3)
C(6)	11(3)	13(3)	12(3)	1(3)	-1(3)	3(3)
C(7)	15(4)	14(4)	9(3)	4(3)	3(3)	-1(3)
C(8)	9(3)	16(3)	11(3)	1(3)	3(3)	-4(3)
C(9)	13(3)	26(4)	17(3)	4(3)	-4(3)	6(4)
C(10)	19(4)	17(4)	15(3)	3(3)	-2(3)	3(3)
C(11)	23(4)	14(4)	25(4)	-5(3)	1(3)	1(4)
C(12)	15(3)	13(4)	20(4)	5(3)	-5(3)	-2(3)
C(13)	19(4)	14(4)	24(4)	-9(3)	-7(3)	8(3)
C(14)	30(5)	81(7)	50(5)	4(5)	9(5)	25(6)
C(15)	35(5)	21(4)	70(6)	14(4)	-22(5)	9(4)
C(16)	20(4)	22(4)	15(3)	-2(3)	-5(3)	9(3)
C(17)	28(4)	20(4)	32(4)	-6(3)	6(4)	3(4)
C(18)	37(5)	29(5)	29(4)	3(4)	9(4)	11(4)
C(19)	26(4)	31(4)	16(4)	2(3)	-15(3)	6(4)
C(20)	30(5)	76(7)	24(4)	2(5)	-10(4)	-24(5)
C(21)	37(5)	58(6)	15(4)	4(4)	-4(4)	-9(6)
C(22)	7(3)	12(4)	12(3)	-1(3)	0(3)	-2(3)
C(23)	26(4)	8(3)	13(3)	2(3)	-5(3)	1(3)
C(24)	19(4)	19(4)	7(3)	2(3)	3(3)	4(4)
C(25)	19(4)	10(4)	11(3)	0(3)	-4(3)	-6(3)
C(26)	21(4)	11(4)	14(3)	-4(3)	-1(3)	2(3)
C(27)	16(3)	14(4)	3(3)	-4(3)	0(3)	-4(3)
C(28)	13(3)	7(3)	15(3)	-2(3)	8(3)	2(3)
C(29)	15(4)	32(4)	29(4)	-1(4)	2(3)	4(4)
C(30)	21(5)	24(4)	39(5)	-10(4)	6(4)	3(4)
C(31)	20(4)	19(4)	11(3)	0(3)	0(3)	5(4)
C(32)	16(4)	23(4)	30(4)	4(3)	-4(3)	1(3)
C(33)	31(4)	15(4)	29(4)	-1(3)	-2(4)	10(4)
C(34)	19(4)	19(4)	14(3)	4(3)	1(3)	-2(3)
C(35)	34(5)	44(5)	38(5)	25(4)	16(4)	0(5)
C(36)	50(5)	41(5)	26(4)	5(4)	-4(4)	-12(5)

L964-28 21.

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2,6-Tripp2PhCu(SMe2).

	x	y	z	U(eq)
H(3A)	451(8)	4161(4)	1612(2)	14
H(4A)	-341(7)	3602(4)	2429(3)	17
H(5A)	928(7)	3932(4)	3223(3)	17
H(9A)	6075(9)	4406(4)	4181(2)	22
H(11A)	3346(8)	6416(5)	4324(3)	25
H(13A)	1107(8)	5967(4)	3151(3)	23
H(14A)	-60(50)	5603(7)	3978(19)	80
H(14B)	-679(29)	6487(36)	3769(12)	80
H(14C)	554(29)	6452(37)	4243(10)	80
H(15A)	2727(47)	7145(5)	3094(17)	63
H(15B)	2307(62)	7399(12)	3699(7)	63
H(15C)	1029(18)	7433(10)	3240(22)	63
H(16A)	4143(8)	3519(4)	3048(3)	22
H(17A)	4332(23)	2856(20)	3901(14)	41
H(17B)	6111(38)	3076(14)	3921(14)	41
H(17C)	5476(56)	2441(8)	3476(3)	41
H(18A)	6196(19)	4276(23)	2688(13)	47
H(18B)	6711(34)	3324(9)	2773(16)	47
H(18C)	7249(19)	4029(30)	3189(4)	47
H(19A)	6393(8)	5253(5)	4940(3)	29
H(20A)	7236(52)	6612(22)	5086(10)	65
H(20B)	5958(10)	6980(9)	4692(23)	65
H(20C)	7318(48)	6424(15)	4454(15)	65
H(21A)	5167(10)	5960(34)	5637(5)	55
H(21B)	3994(45)	5324(14)	5361(14)	55
H(21C)	3898(43)	6303(24)	5230(10)	55
H(24A)	5472(9)	5223(4)	520(2)	18
H(26A)	1872(8)	6762(4)	549(3)	18
H(28A)	57(8)	5827(4)	1685(2)	14
H(29A)	-1818(16)	6534(28)	1198(4)	38
H(29B)	-1061(36)	5839(9)	819(13)	38
H(29C)	-601(24)	6803(21)	751(11)	38
H(30A)	1485(41)	6992(9)	1993(14)	42
H(30B)	-248(17)	7265(16)	1896(16)	42
H(30C)	1033(53)	7510(10)	1466(4)	42
H(31A)	4481(8)	4078(4)	1704(2)	20
H(32A)	6765(8)	4916(17)	1627(15)	34
H(32B)	7082(13)	4491(28)	1054(3)	34
H(32C)	7105(12)	3933(13)	1589(16)	34
H(33A)	3549(12)	3361(18)	953(14)	38
H(33B)	5221(42)	3015(10)	1084(11)	38
H(33C)	4971(49)	3657(11)	597(5)	38
H(34A)	4190(8)	7140(5)	24(3)	21

L964-29

H(35A)	6235(19)	6687(28)	-502(13)	58
H(35B)	6139(16)	5777(7)	-234(21)	58
H(35C)	6611(10)	6568(31)	124(10)	58
H(36A)	3565(44)	6635(25)	-820(7)	58
H(36B)	2234(11)	6390(32)	-409(8)	58
H(36C)	3446(46)	5699(11)	-595(14)	58
H(37A)	9077(18)	6284(11)	2709(19)	48
H(37B)	8289(42)	5478(17)	2447(11)	48
H(37C)	7781(27)	5789(26)	3032(9)	48
H(38A)	7344(26)	7680(25)	2976(15)	56
H(38B)	6222(63)	7023(5)	3258(5)	56
H(38C)	5554(42)	7711(24)	2854(11)	56