Electronic Supporting Information

Hydrotris(3-mesitylpyrazolyl)borato-copper(I) alkyne complexes: synthesis, structural characterization and rationalization of their activities as alkyne cyclopropenation catalysts.

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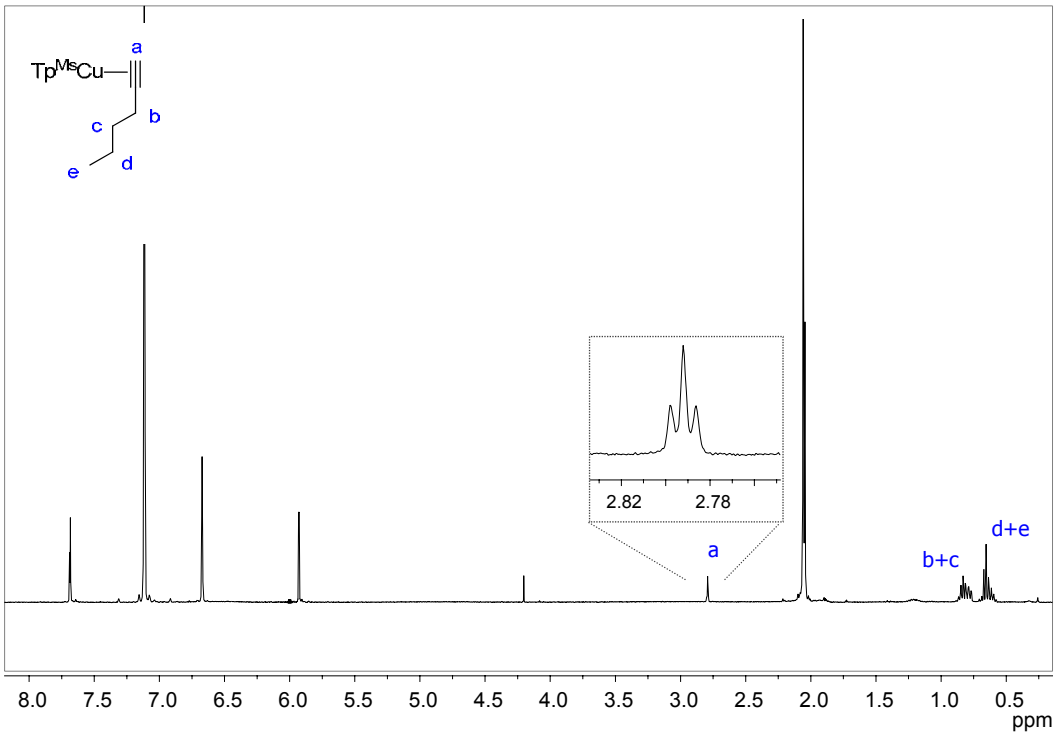


Figure 2. ^{13}C NMR spectrum of $Tp^{Ms}Cu$(1-hexyne), **1**, in C_6D_6 (100 MHz).

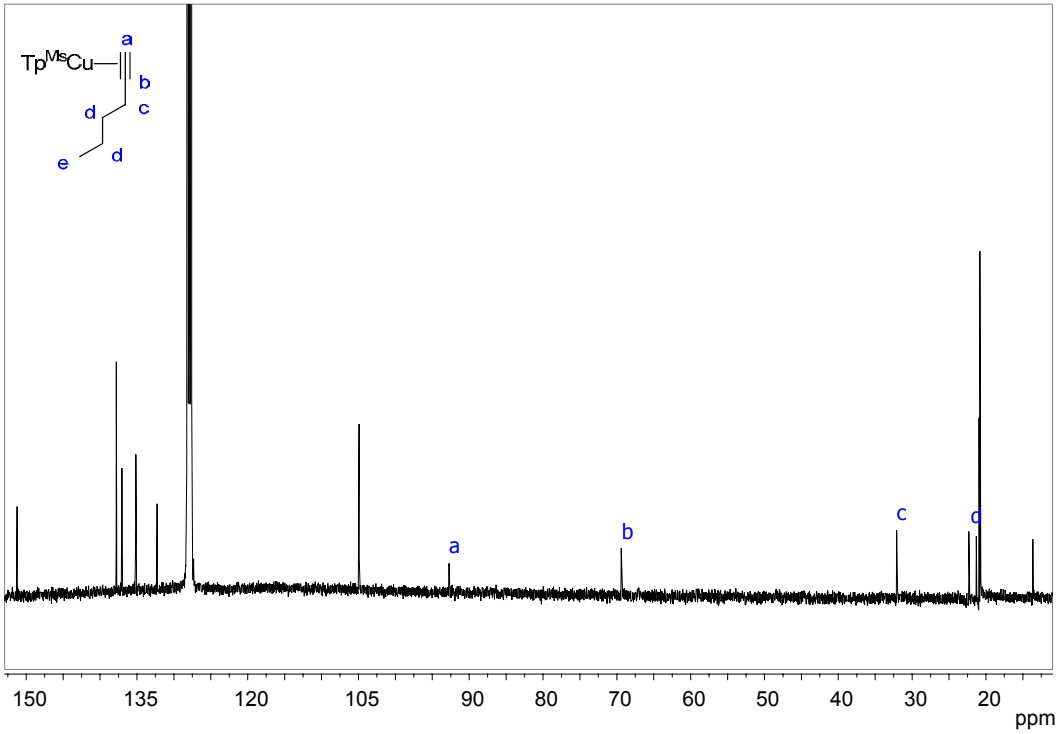


Figure 3. ^{1}H NMR spectrum of Tp^{Ms}Cu(phenylacetylene), **2**, in C_6D_6 (400 MHz).

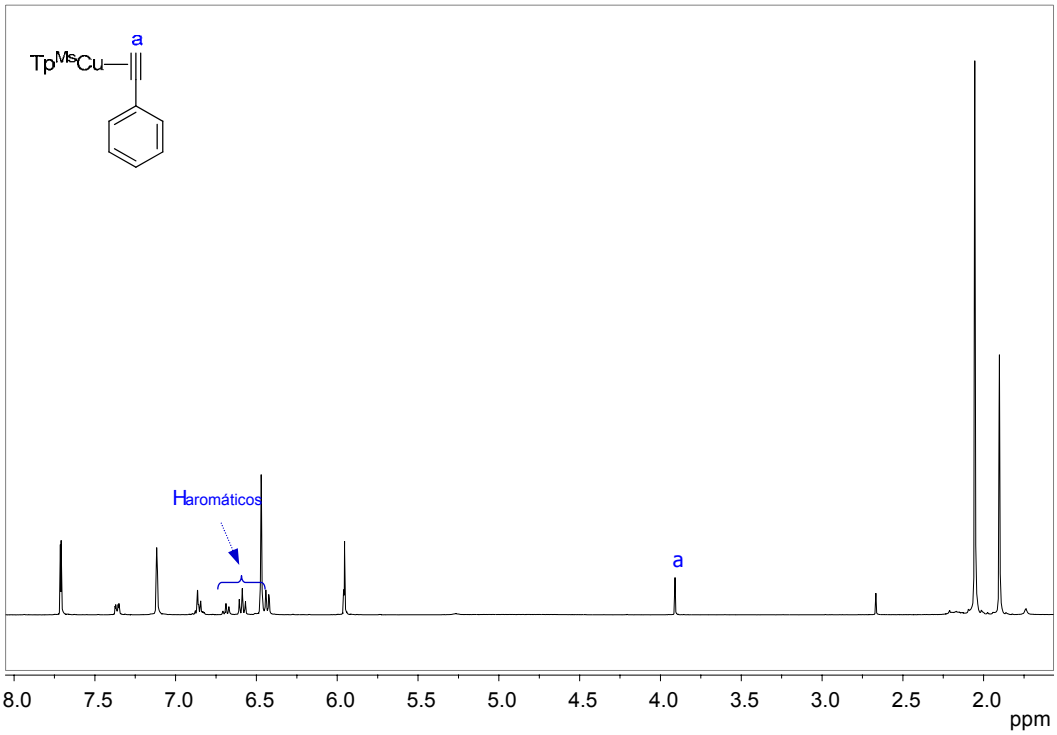


Figure 4. ^{13}C NMR spectrum of Tp^{Ms}Cu(phenylacetylene), **2**, in C_6D_6 (100 MHz).

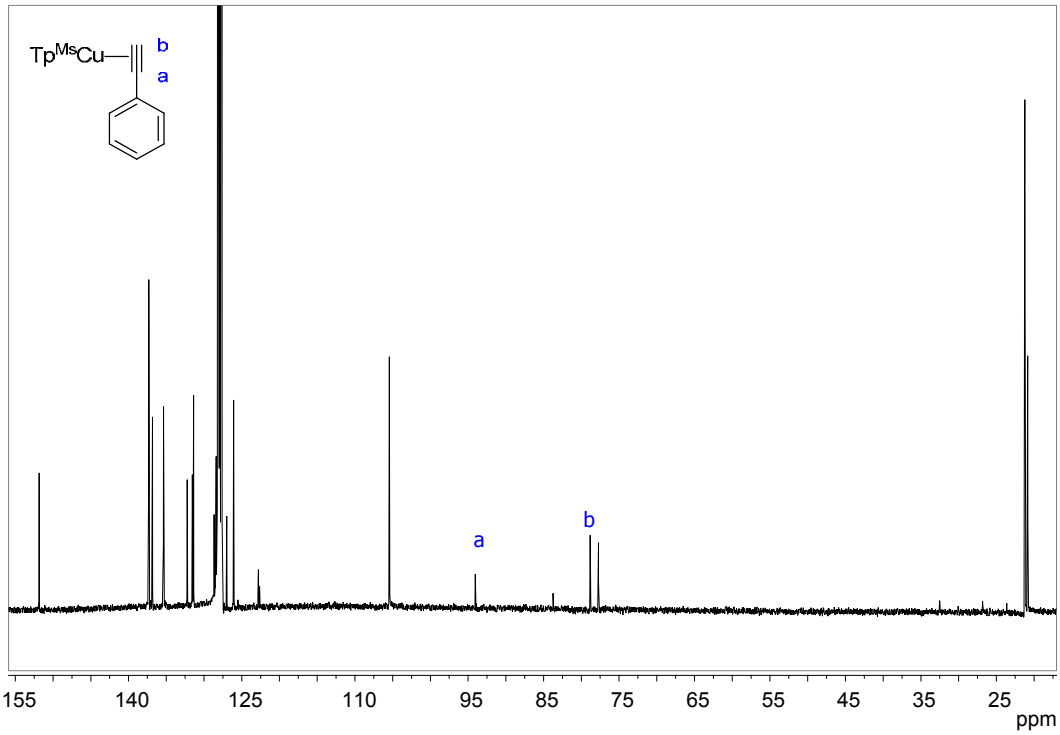


Figure 5. ^{1}H NMR spectrum of Tp^{Ms}Cu(ethyl propiolate), **3**, in $CDCl_3$ (400 MHz).

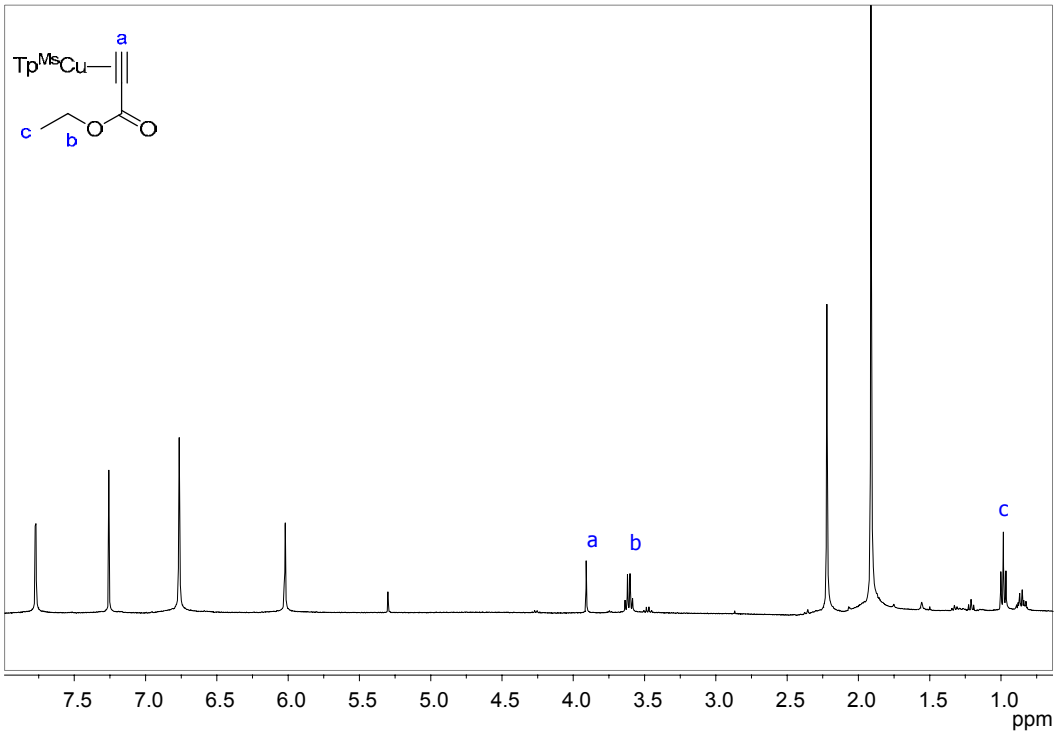


Figure 6. ^{13}C NMR spectrum of Tp^{Ms}Cu(ethyl propiolate), **3**, in $CDCl_3$ (100 MHz).

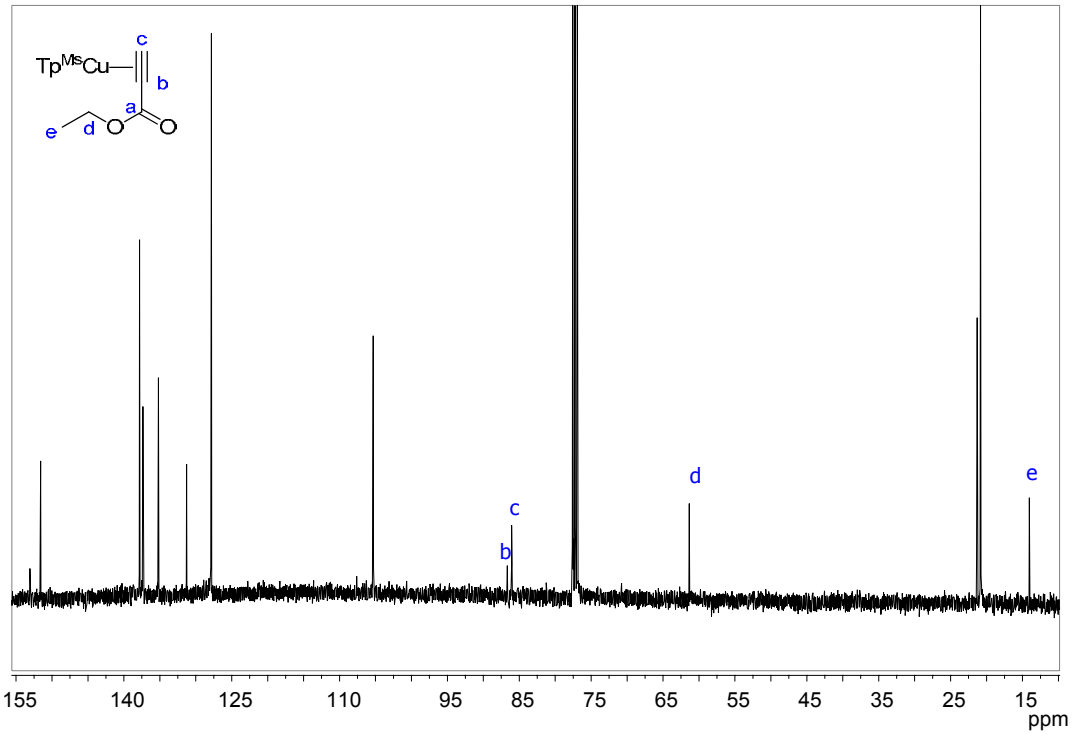
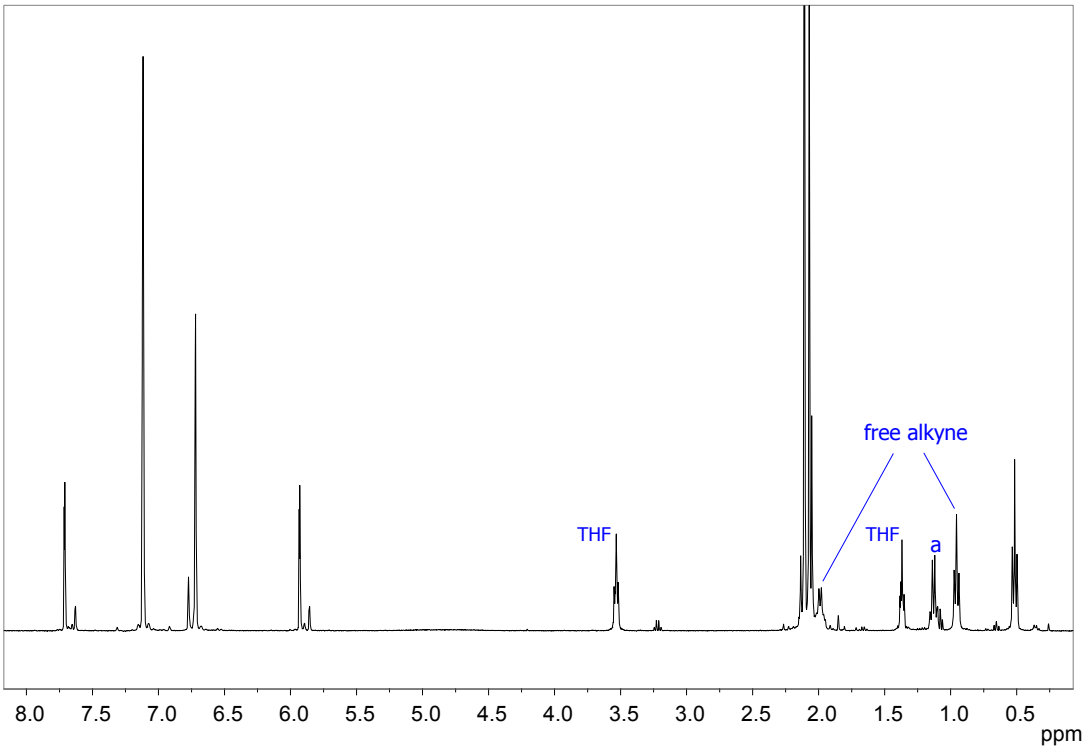


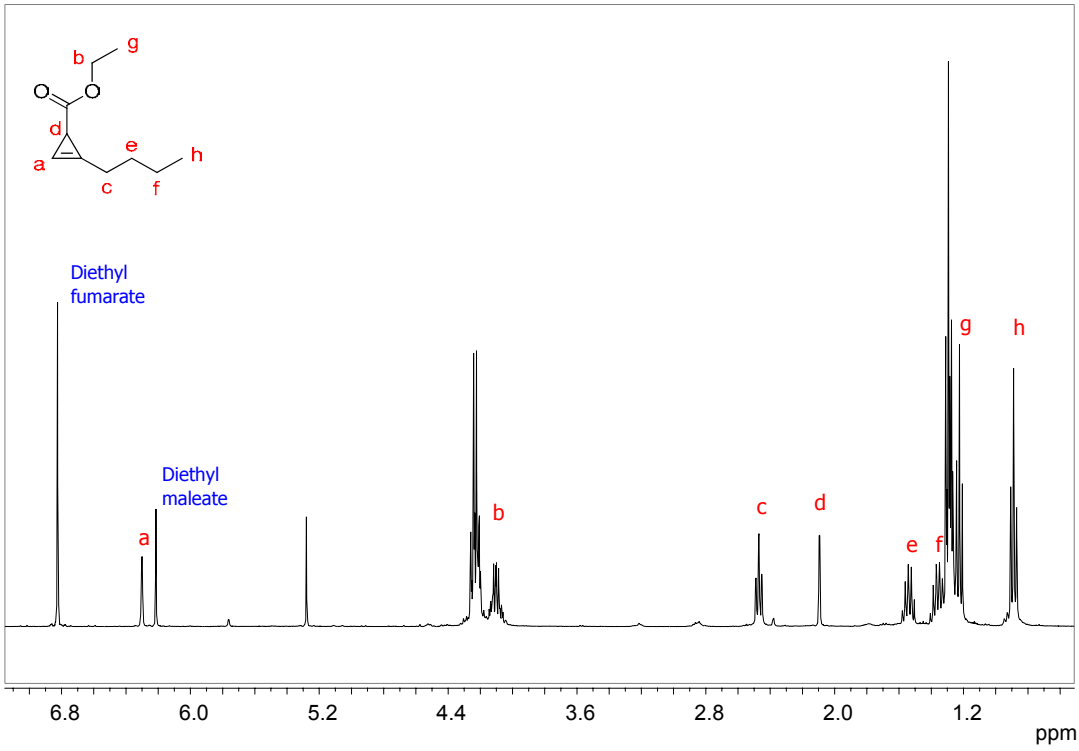
Figure 7. ^{1}H NMR spectrum of $Tp^{Ms}Cu$(3-hexyne), **4**, in C_6D_6 (400 MHz).



II. ^{1}H NMR spectra and GC of the final cyclopropanation reaction mixtures.

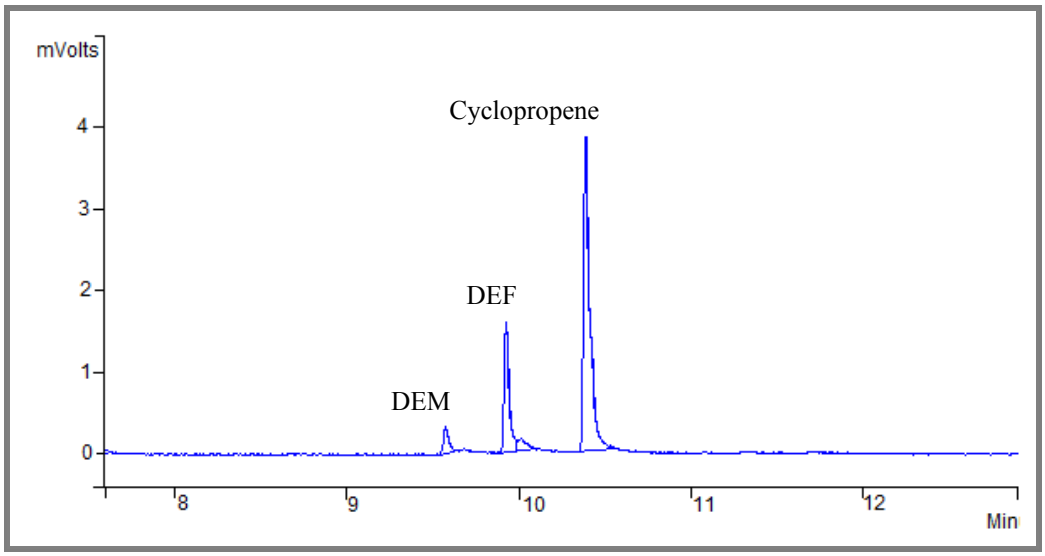
a) Ethyl 2-butylcycloprop-2-enecarboxylate.

Figure 8. ^{1}H NMR spectrum of the final cyclopropenation reaction mixture of 1-hexyne with EDA in the presence of $Tp^{Br3}Cu(CNMe)$ as catalyst in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (d, ^{3}J = 1.4 Hz, 1H), 4.11 (q, ^{3}J = 7.1 Hz, 2H), 2.47 (t, ^{3}J = 7.4 Hz, 2H), 2.09 (d, ^{3}J = 1.5 Hz, 1H), 1.54 (m, 2H), 1.35 (m, 2H), 1.23 (t, ^{3}J = 7.1 Hz, 3H), 0.89 (t, ^{3}J = 7.3 Hz, 3H).

Figure 9. GC chromatogram of the reaction mixture after total consumption of EDA obtained from the cyclopropenation reaction of 1-hexyne.

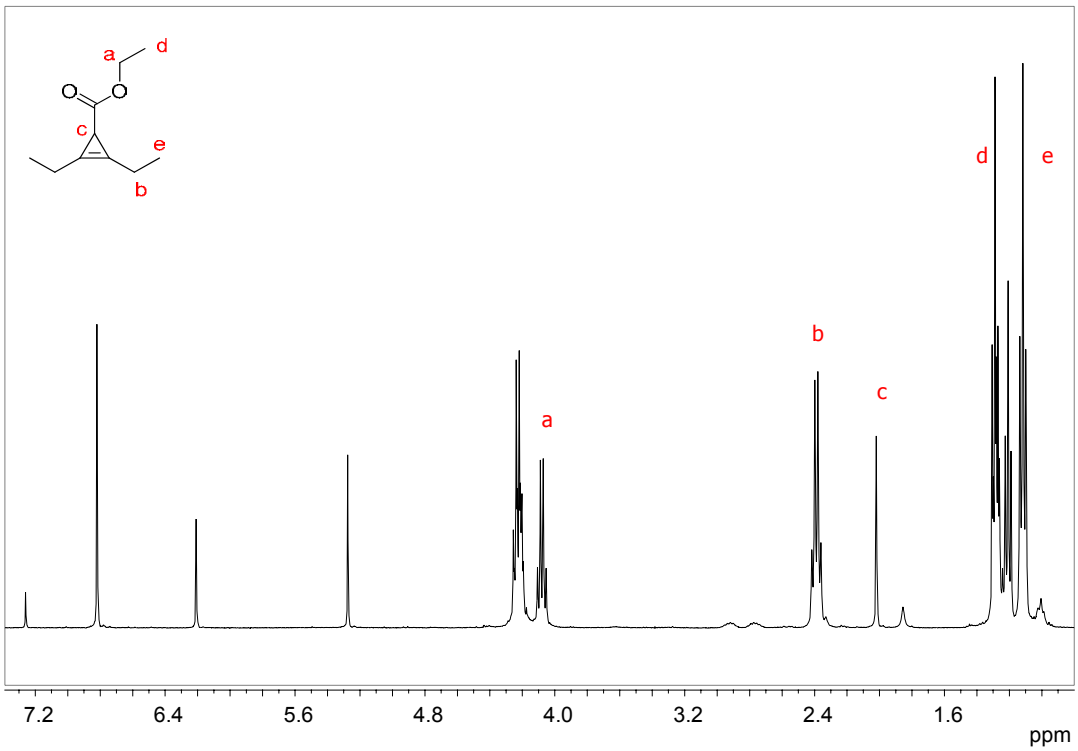


- Column: CP-Sil 8CB (Varian Capilary Column: 30m, 0.25 mm, 0.25 μm CP8751)
- Detector: FID
- T_0: 50 ºC
- T_f: 250 ºC
- Rate: 10 ºC/min
- Injector temperature: 225 ºC
- Detector temperature: 255 ºC

Products	**t_R (min)**
Diethyl maleate (DEM)	9.5
Diethyl fumarate (DEF)	9.9
Cyclopropene	10.4

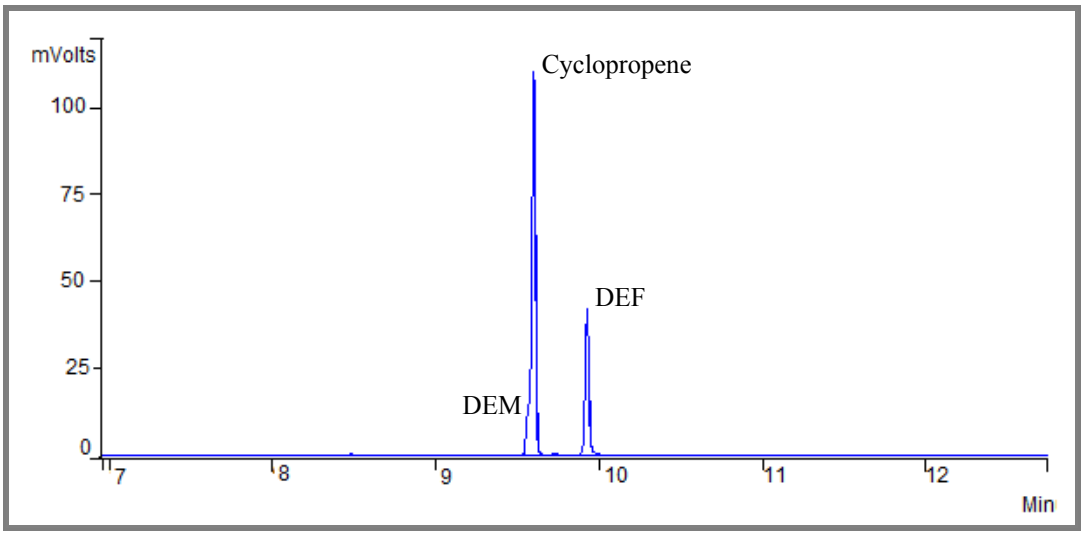
b) Ethyl 2,3-diethylcycloprop-2-enecarboxylate.

Figure 10. ^{1}H NMR spectrum of the final cyclopropenation reaction mixture reaction of 3-hexyne with EDA in the presence of $Tp^{Br3}Cu(CNMe)$ as catalyst in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 4.08 (q, ^{3}J = 7.1 Hz, 2H), 2.39 (q, ^{3}J = 7.5 Hz, 2H), 2.01 (s, 1H), 1.29 (t, ^{3}J = 7.1 Hz, 3H), 1.12 (t, ^{3}J = 7.4 Hz, 3H).

Figure 11. GC chromatogram of the reaction mixture after total consumption of EDA obtained from the cyclopropenation reaction of 3-hexyne.

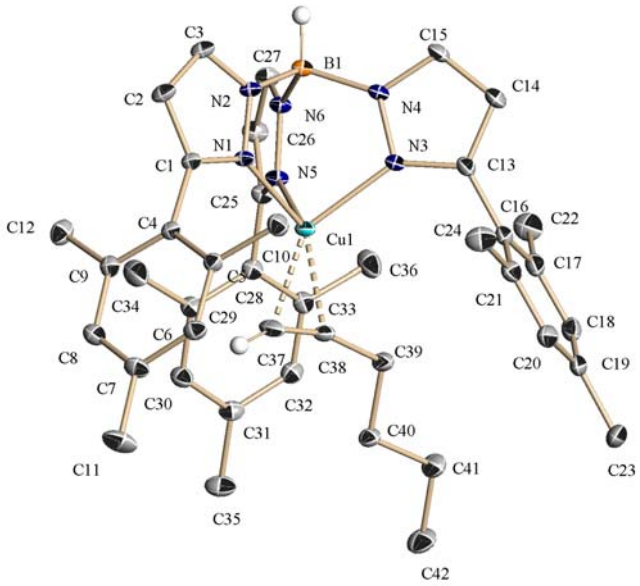


- Column: CP-Sil 8CB (Varian Capilary Column: 30m, 0.25 mm, 0.25 μm CP8751)
- Detector: FID
- T_0: 60 ºC
- T_f: 250 ºC
- Rate: 10 ºC/min
- Injector temperature: 225 ºC
- Detector temperature: 255 ºC

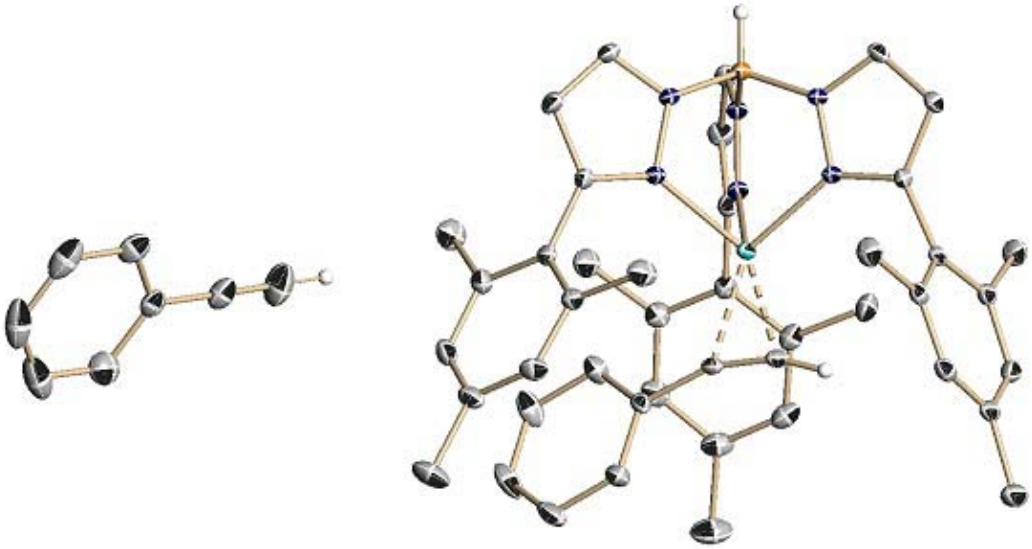
Products	**t_R (min)**
Diethyl maleate (DEM)	9.5
Diethyl fumarate (DEF)	9.9
Cyclopropene	9.6

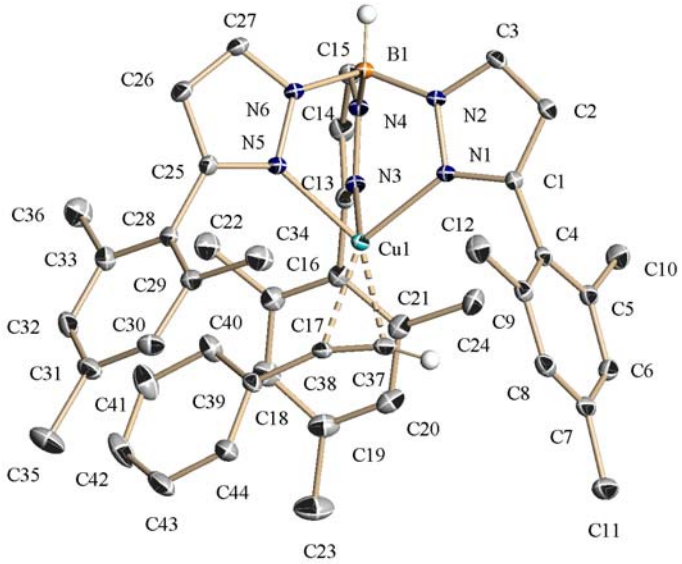
III. X Ray crystal structure analysis for 1-3.

Crystal data for **1**: $C_{87}H_{106}B_2C_{l6}Cu_2N_{12}$, M = 1681.26, triclinic, $P\bar{1}$ **,** a = 11.1908(5), b = 12.0506(5), c = 16.6731(7) Å, α = 77.7080(9)°, β = 83.1730(10)°, γ = 89.2120(10)°, V = 2181.19(16) $Å^3$, Z = 1, D_c = 1.280 Mg/m^3, absorption coefficient 0.722 mm^{-1}, T = 173(2) K, colourless prisms; 13139 independent measured reflections (R_{int} = 0.0266), F^2 refinement, final R indices [I>2sigma(I)] R1 = 0.0481, wR2 = 0.1287, R indices (all data) R1 = 0.0664, wR2 = 0.1437.

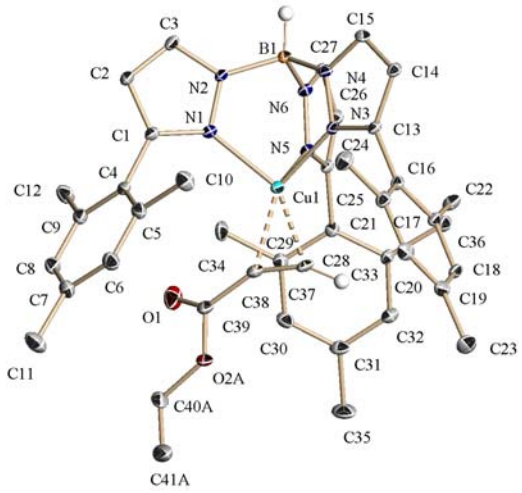


Crystal data for **2**: $C_{52}H_{52}BCuN_6$ [$C_{44}H_{46}BCuN_6$, C_8H_6], M = 835.35, monoclinic, $P2_1/n$, a = 9.1406(6), b = 20.6632(15), c = 23.8733(17) Å, α = 90°, β= 97.186(2)°, γ = 90°, V = 4473.6(5) $Å^3$, Z = 4, D_c = 1.240 Mg/m^3, absorption coefficient 0.531 mm^{-1}, T = 173(2) K, colourless prisms; 13516 independent measured reflections (R_{int} = 0.0652), F^2 refinement, final R indices [I>2sigma(I)] R1 = 0.0463, wR2 = 0.1001, R indices (all data) R1 = 0.0769, wR2 = 0.1142. In this case, a free phenylacetylene molecule was observed in the unit cell.





Crystal data for **3**: $C_{165}H_{186}B_4Cl_2Cu_4N_{24}O_8$ [4($C_{41}H_{46}BCuN_6O_2$), CH_2Cl_2], M = 3001.68, triclinic, $P\bar{1}$, a = 9.0009(7), b = 11.2392(9), c = 38.765(3) Å, α = 97.899(2)°, β= 97.186(2)°, γ = 90°, V = 3875.5(5) Å^3, Z = 1, D_c = 1.286 Mg/m^3, absorption coefficient 0.641 mm^{-1}, T = 100(2) K, colourless prisms; 23921 independent measured reflections (R_{int} = 0.0544), F^2 refinement, final R indices [I>2sigma(I)] R1 = 0.0776, wR2 = 0.1802, R indices (all data) R1 = 0.1021, wR2 = 0.1900. The two different molecules in the cell unti are shown.



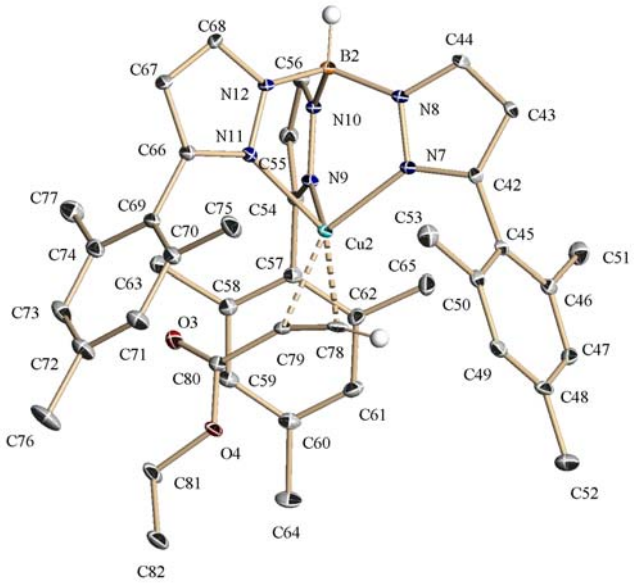


Table 1. Crystal data and structure refinement for $Tp^{Ms}Cu$(1-hexyne), **1.**

Empirical formula	$C_{87}H_{106}B_2C_{l6}Cu_2N_{12}$	
	$[2(C_{42}H_{50}BCuN_6), 3(CH_2C_{l2})]$	
Formula weight	1681.26	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.1908(5) Å	α= 77.7080(9)°.
	b = 12.0506(5) Å	β= 83.1730(10)°.
	c = 16.6731(7) Å	γ = 89.2120(10)°.
Volume	2181.19(16) $Å^3$	
Z	1	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.722 mm^{-1}	
F(000)	882	
Crystal size	0.50 x 0.48 x 0.45 mm^3	
Theta range for data collection	1.73 to 30.53°.	
Index ranges	-15<=h<=10, -15<=k<=17, -23<=l<=22	
Reflections collected	51665	
Independent reflections	13139 [R(int) = 0.0266]	
Completeness to theta = 30.53°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7371 and 0.7142	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13139 / 1 / 509	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.1287	
R indices (all data)	R1 = 0.0664, wR2 = 0.1437	
Largest diff. peak and hole	1.055 and -1.047 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ea18410a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1159(1)	2628(1)	7345(1)	25(1)
N(1)	1059(1)	4234(1)	6724(1)	23(1)
N(2)	1851(1)	4547(1)	6024(1)	23(1)
N(3)	3042(1)	2606(1)	7193(1)	24(1)
N(4)	3539(1)	3226(1)	6446(1)	25(1)
N(5)	1299(1)	2038(1)	6169(1)	25(1)
N(6)	2086(1)	2682(1)	5565(1)	24(1)
C(1)	328(2)	5119(2)	6767(1)	24(1)
C(2)	654(2)	6013(2)	6089(1)	31(1)
C(3)	1617(2)	5610(2)	5641(1)	28(1)
C(4)	-657(2)	5027(1)	7459(1)	23(1)
C(5)	-406(2)	5107(2)	8248(1)	26(1)
C(6)	-1338(2)	4933(2)	8896(1)	30(1)
C(7)	-2499(2)	4673(2)	8786(1)	33(1)
C(8)	-2740(2)	4622(2)	7997(1)	32(1)
C(9)	-1838(2)	4805(2)	7326(1)	27(1)
C(10)	849(2)	5362(2)	8402(1)	35(1)
C(11)	-3484(2)	4469(3)	9506(2)	53(1)
C(12)	-2142(2)	4750(2)	6477(1)	38(1)
C(13)	3960(2)	2209(2)	7616(1)	27(1)
C(14)	5056(2)	2583(2)	7145(1)	37(1)
C(15)	4753(2)	3217(2)	6409(1)	32(1)
C(16)	3767(2)	1428(2)	8440(1)	28(1)
C(17)	3885(2)	253(2)	8491(1)	34(1)
C(18)	3719(2)	-475(2)	9263(2)	40(1)
C(19)	3439(2)	-81(2)	9983(2)	40(1)
C(20)	3343(2)	1084(2)	9920(1)	40(1)
C(21)	3508(2)	1846(2)	9159(1)	33(1)
C(22)	4166(3)	-218(2)	7723(2)	51(1)
C(23)	3241(2)	-889(3)	10815(2)	56(1)
C(24)	3423(3)	3107(2)	9116(2)	48(1)
C(25)	921(2)	1195(2)	5852(1)	25(1)
C(26)	1466(2)	1295(2)	5036(1)	33(1)

C(27)	2194(2)	2243(2)	4884(1)	30(1)
C(28)	26(2)	338(2)	6337(1)	25(1)
C(29)	-1177(2)	644(2)	6485(1)	29(1)
C(30)	-2017(2)	-177(2)	6923(1)	32(1)
C(31)	-1696(2)	-1291(2)	7215(1)	31(1)
C(32)	-499(2)	-1581(2)	7064(1)	31(1)
C(33)	370(2)	-788(2)	6626(1)	29(1)
C(34)	-1576(2)	1840(2)	6187(2)	47(1)
C(35)	-2624(2)	-2167(2)	7675(2)	45(1)
C(36)	1652(2)	-1157(2)	6472(2)	46(1)
C(37)	-290(2)	2229(2)	8172(1)	36(1)
C(38)	352(2)	1403(2)	8255(1)	27(1)
C(39)	853(2)	270(2)	8545(1)	34(1)
C(40)	-101(2)	-597(2)	9003(1)	30(1)
C(41)	471(2)	-1737(2)	9334(2)	43(1)
C(42)	-459(3)	-2620(2)	9778(2)	50(1)
B(1)	2761(2)	3690(2)	5745(1)	24(1)
Cl(1)	4031(1)	6303(1)	7973(1)	69(1)
Cl(2)	4647(1)	6445(1)	6206(1)	99(1)
C(43)	3794(3)	5771(3)	7102(2)	60(1)
Cl(3)	5315(2)	859(2)	5428(1)	156(1)
C(44)	4680(17)	258(14)	4557(7)	201(10)

Table 3. Bond lengths [Å] and angles [°] for $Tp^{Ms}Cu$(1-hexyne), **1.**

Cu(1)-C(37)	1.991(2)	C(11)-H(11A)	0.9800
Cu(1)-N(1)	2.0002(15)	C(11)-H(11B)	0.9800
Cu(1)-C(38)	2.0127(18)	C(11)-H(11C)	0.9800
Cu(1)-N(3)	2.0930(15)	C(12)-H(12A)	0.9800
Cu(1)-N(5)	2.2124(15)	C(12)-H(12B)	0.9800
N(1)-C(1)	1.344(2)	C(12)-H(12C)	0.9800
N(1)-N(2)	1.3654(19)	C(13)-C(14)	1.400(3)
N(2)-C(3)	1.341(2)	C(13)-C(16)	1.485(3)
N(2)-B(1)	1.544(2)	C(14)-C(15)	1.377(3)
N(3)-C(13)	1.340(2)	C(14)-H(14)	0.9500
N(3)-N(4)	1.368(2)	C(15)-H(15)	0.9500
N(4)-C(15)	1.352(2)	C(16)-C(21)	1.394(3)
N(4)-B(1)	1.544(3)	C(16)-C(17)	1.406(3)
N(5)-C(25)	1.336(2)	C(17)-C(18)	1.390(3)
N(5)-N(6)	1.366(2)	C(17)-C(22)	1.506(4)
N(6)-C(27)	1.345(2)	C(18)-C(19)	1.383(4)
N(6)-B(1)	1.540(2)	C(18)-H(18)	0.9500
C(1)-C(2)	1.402(2)	C(19)-C(20)	1.389(4)
C(1)-C(4)	1.486(2)	C(19)-C(23)	1.509(3)
C(2)-C(3)	1.380(3)	C(20)-C(21)	1.394(3)
C(2)-H(2)	0.9500	C(20)-H(20)	0.9500
C(3)-H(3)	0.9500	C(21)-C(24)	1.507(3)
C(4)-C(5)	1.401(3)	C(22)-H(22A)	0.9800
C(4)-C(9)	1.404(3)	C(22)-H(22B)	0.9800
C(5)-C(6)	1.393(3)	C(22)-H(22C)	0.9800
C(5)-C(10)	1.505(3)	C(23)-H(23A)	0.9800
C(6)-C(7)	1.382(3)	C(23)-H(23B)	0.9800
C(6)-H(6)	0.9500	C(23)-H(23C)	0.9800
C(7)-C(8)	1.388(3)	C(24)-H(24A)	0.9800
C(7)-C(11)	1.510(3)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.398(3)	C(24)-H(24C)	0.9800
C(8)-H(8)	0.9500	C(25)-C(26)	1.404(3)
C(9)-C(12)	1.508(3)	C(25)-C(28)	1.484(2)
C(10)-H(10A)	0.9800	C(26)-C(27)	1.373(3)
C(10)-H(10B)	0.9800	C(26)-H(26)	0.9500
C(10)-H(10C)	0.9800	C(27)-H(27)	0.9500

C(28)-C(29)	1.398(3)	C(43)-H(43A)	0.9900
C(28)-C(33)	1.404(3)	C(43)-H(43B)	0.9900
C(29)-C(30)	1.397(3)	Cl(3)-C(44)#1	1.342(18)
C(29)-C(34)	1.501(3)	Cl(3)-C(44)	1.96(2)
C(30)-C(31)	1.385(3)	C(44)-Cl(3)#1	1.342(18)
C(30)-H(30)	0.9500	C(44)-H(44A)	0.9900
C(31)-C(32)	1.387(3)	C(44)-H(44B)	0.9900
C(31)-C(35)	1.510(3)		
C(32)-C(33)	1.397(3)	C(37)-Cu(1)-N(1)	110.03(7)
C(32)-H(32)	0.9500	C(37)-Cu(1)-C(38)	35.26(8)
C(33)-C(36)	1.505(3)	N(1)-Cu(1)-C(38)	145.24(7)
C(34)-H(34A)	0.9800	C(37)-Cu(1)-N(3)	143.61(8)
C(34)-H(34B)	0.9800	N(1)-Cu(1)-N(3)	94.42(6)
C(34)-H(34C)	0.9800	C(38)-Cu(1)-N(3)	115.49(7)
C(35)-H(35A)	0.9800	C(37)-Cu(1)-N(5)	120.00(8)
C(35)-H(35B)	0.9800	N(1)-Cu(1)-N(5)	90.00(6)
C(35)-H(35C)	0.9800	C(38)-Cu(1)-N(5)	108.81(7)
C(36)-H(36A)	0.9800	N(3)-Cu(1)-N(5)	85.29(6)
C(36)-H(36B)	0.9800	C(1)-N(1)-N(2)	106.94(14)
C(36)-H(36C)	0.9800	C(1)-N(1)-Cu(1)	136.58(12)
C(37)-C(38)	1.213(3)	N(2)-N(1)-Cu(1)	116.21(11)
C(37)-H(37)	0.903(17)	C(3)-N(2)-N(1)	109.48(14)
C(38)-C(39)	1.474(3)	C(3)-N(2)-B(1)	129.60(15)
C(39)-C(40)	1.520(3)	N(1)-N(2)-B(1)	120.72(14)
C(39)-H(39A)	0.9900	C(13)-N(3)-N(4)	106.61(14)
C(39)-H(39B)	0.9900	C(13)-N(3)-Cu(1)	140.09(13)
C(40)-C(41)	1.528(3)	N(4)-N(3)-Cu(1)	113.22(11)
C(40)-H(40A)	0.9900	C(15)-N(4)-N(3)	109.73(16)
C(40)-H(40B)	0.9900	C(15)-N(4)-B(1)	128.32(16)
C(41)-C(42)	1.509(3)	N(3)-N(4)-B(1)	121.41(14)
C(41)-H(41A)	0.9900	C(25)-N(5)-N(6)	106.58(14)
C(41)-H(41B)	0.9900	C(25)-N(5)-Cu(1)	140.74(13)
C(42)-H(42A)	0.9800	N(6)-N(5)-Cu(1)	112.49(10)
C(42)-H(42B)	0.9800	C(27)-N(6)-N(5)	109.92(15)
C(42)-H(42C)	0.9800	C(27)-N(6)-B(1)	129.64(16)
B(1)-H(1)	1.0000	N(5)-N(6)-B(1)	120.28(14)
Cl(1)-C(43)	1.756(3)	N(1)-C(1)-C(2)	109.74(16)
Cl(2)-C(43)	1.722(3)	N(1)-C(1)-C(4)	119.73(15)

C(2)-C(1)-C(4)	130.52(17)	C(9)-C(12)-H(12B)	109.5
C(3)-C(2)-C(1)	104.86(17)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-H(2)	127.6	C(9)-C(12)-H(12C)	109.5
C(1)-C(2)-H(2)	127.6	H(12A)-C(12)-H(12C)	109.5
N(2)-C(3)-C(2)	108.99(16)	H(12B)-C(12)-H(12C)	109.5
N(2)-C(3)-H(3)	125.5	N(3)-C(13)-C(14)	110.05(17)
C(2)-C(3)-H(3)	125.5	N(3)-C(13)-C(16)	121.99(16)
C(5)-C(4)-C(9)	120.04(16)	C(14)-C(13)-C(16)	127.84(17)
C(5)-C(4)-C(1)	120.48(16)	C(15)-C(14)-C(13)	105.37(17)
C(9)-C(4)-C(1)	119.41(16)	C(15)-C(14)-H(14)	127.3
C(6)-C(5)-C(4)	118.91(17)	C(13)-C(14)-H(14)	127.3
C(6)-C(5)-C(10)	120.11(17)	N(4)-C(15)-C(14)	108.23(17)
C(4)-C(5)-C(10)	120.97(16)	N(4)-C(15)-H(15)	125.9
C(7)-C(6)-C(5)	122.06(18)	C(14)-C(15)-H(15)	125.9
C(7)-C(6)-H(6)	119.0	C(21)-C(16)-C(17)	120.03(19)
C(5)-C(6)-H(6)	119.0	C(21)-C(16)-C(13)	121.03(18)
C(6)-C(7)-C(8)	118.37(18)	C(17)-C(16)-C(13)	118.92(18)
C(6)-C(7)-C(11)	120.7(2)	C(18)-C(17)-C(16)	118.8(2)
C(8)-C(7)-C(11)	120.9(2)	C(18)-C(17)-C(22)	120.2(2)
C(7)-C(8)-C(9)	121.60(18)	C(16)-C(17)-C(22)	121.0(2)
C(7)-C(8)-H(8)	119.2	C(19)-C(18)-C(17)	122.1(2)
C(9)-C(8)-H(8)	119.2	C(19)-C(18)-H(18)	118.9
C(8)-C(9)-C(4)	118.95(18)	C(17)-C(18)-H(18)	118.9
C(8)-C(9)-C(12)	119.84(18)	C(18)-C(19)-C(20)	118.1(2)
C(4)-C(9)-C(12)	121.21(18)	C(18)-C(19)-C(23)	121.2(2)
C(5)-C(10)-H(10A)	109.5	C(20)-C(19)-C(23)	120.7(3)
C(5)-C(10)-H(10B)	109.5	C(19)-C(20)-C(21)	121.8(2)
H(10A)-C(10)-H(10B)	109.5	C(19)-C(20)-H(20)	119.1
C(5)-C(10)-H(10C)	109.5	C(21)-C(20)-H(20)	119.1
H(10A)-C(10)-H(10C)	109.5	C(20)-C(21)-C(16)	119.1(2)
H(10B)-C(10)-H(10C)	109.5	C(20)-C(21)-C(24)	120.3(2)
C(7)-C(11)-H(11A)	109.5	C(16)-C(21)-C(24)	120.55(19)
C(7)-C(11)-H(11B)	109.5	C(17)-C(22)-H(22A)	109.5
H(11A)-C(11)-H(11B)	109.5	C(17)-C(22)-H(22B)	109.5
C(7)-C(11)-H(11C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(11A)-C(11)-H(11C)	109.5	C(17)-C(22)-H(22C)	109.5
H(11B)-C(11)-H(11C)	109.5	H(22A)-C(22)-H(22C)	109.5
C(9)-C(12)-H(12A)	109.5	H(22B)-C(22)-H(22C)	109.5

C(19)-C(23)-H(23A)	109.5	C(28)-C(33)-C(36)	121.42(18)
C(19)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34A)	109.5
H(23A)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34B)	109.5
C(19)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(23A)-C(23)-H(23C)	109.5	C(29)-C(34)-H(34C)	109.5
H(23B)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24A)	109.5	H(34B)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35A)	109.5
H(24A)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35B)	109.5
C(21)-C(24)-H(24C)	109.5	H(35A)-C(35)-H(35B)	109.5
H(24A)-C(24)-H(24C)	109.5	C(31)-C(35)-H(35C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(35A)-C(35)-H(35C)	109.5
N(5)-C(25)-C(26)	109.94(16)	H(35B)-C(35)-H(35C)	109.5
N(5)-C(25)-C(28)	121.27(16)	C(33)-C(36)-H(36A)	109.5
C(26)-C(25)-C(28)	128.77(16)	C(33)-C(36)-H(36B)	109.5
C(27)-C(26)-C(25)	105.17(16)	H(36A)-C(36)-H(36B)	109.5
C(27)-C(26)-H(26)	127.4	C(33)-C(36)-H(36C)	109.5
C(25)-C(26)-H(26)	127.4	H(36A)-C(36)-H(36C)	109.5
N(6)-C(27)-C(26)	108.39(17)	H(36B)-C(36)-H(36C)	109.5
N(6)-C(27)-H(27)	125.8	C(38)-C(37)-Cu(1)	73.33(13)
C(26)-C(27)-H(27)	125.8	C(38)-C(37)-H(37)	162.3(18)
C(29)-C(28)-C(33)	119.66(17)	Cu(1)-C(37)-H(37)	124.2(18)
C(29)-C(28)-C(25)	119.78(17)	C(37)-C(38)-C(39)	163.5(2)
C(33)-C(28)-C(25)	120.53(17)	C(37)-C(38)-Cu(1)	71.42(13)
C(30)-C(29)-C(28)	119.34(18)	C(39)-C(38)-Cu(1)	125.04(14)
C(30)-C(29)-C(34)	119.55(18)	C(38)-C(39)-C(40)	112.86(17)
C(28)-C(29)-C(34)	121.12(18)	C(38)-C(39)-H(39A)	109.0
C(31)-C(30)-C(29)	121.88(19)	C(40)-C(39)-H(39A)	109.0
C(31)-C(30)-H(30)	119.1	C(38)-C(39)-H(39B)	109.0
C(29)-C(30)-H(30)	119.1	C(40)-C(39)-H(39B)	109.0
C(30)-C(31)-C(32)	118.10(18)	H(39A)-C(39)-H(39B)	107.8
C(30)-C(31)-C(35)	120.9(2)	C(39)-C(40)-C(41)	110.86(18)
C(32)-C(31)-C(35)	121.0(2)	C(39)-C(40)-H(40A)	109.5
C(31)-C(32)-C(33)	121.87(18)	C(41)-C(40)-H(40A)	109.5
C(31)-C(32)-H(32)	119.1	C(39)-C(40)-H(40B)	109.5
C(33)-C(32)-H(32)	119.1	C(41)-C(40)-H(40B)	109.5
C(32)-C(33)-C(28)	119.14(18)	H(40A)-C(40)-H(40B)	108.1
C(32)-C(33)-C(36)	119.43(18)	C(42)-C(41)-C(40)	111.9(2)

C(42)-C(41)-H(41A)	109.2
C(40)-C(41)-H(41A)	109.2
C(42)-C(41)-H(41B)	109.2
C(40)-C(41)-H(41B)	109.2
H(41A)-C(41)-H(41B)	107.9
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(6)-B(1)-N(2)	109.88(14)
N(6)-B(1)-N(4)	108.15(15)
N(2)-B(1)-N(4)	109.43(14)
N(6)-B(1)-H(1)	109.8
N(2)-B(1)-H(1)	109.8
N(4)-B(1)-H(1)	109.8
Cl(2)-C(43)-Cl(1)	113.79(16)
Cl(2)-C(43)-H(43A)	108.8
Cl(1)-C(43)-H(43A)	108.8
Cl(2)-C(43)-H(43B)	108.8
Cl(1)-C(43)-H(43B)	108.8
H(43A)-C(43)-H(43B)	107.7
C(44)#1-Cl(3)-C(44)	58.9(8)
Cl(3)#1-C(44)-Cl(3)	121.1(8)
Cl(3)#1-C(44)-H(44A)	107.1
Cl(3)-C(44)-H(44A)	107.1
Cl(3)#1-C(44)-H(44B)	107.1
Cl(3)-C(44)-H(44B)	107.1
H(44A)-C(44)-H(44B)	106.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Tp^{Ms}Cu$(1-hexyne), **1**. 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}
Cu(1)	25(1)	23(1)	24(1)	0(1)	5(1)	-1(1)
N(1)	24(1)	23(1)	20(1)	-4(1)	3(1)	-1(1)
N(2)	27(1)	22(1)	19(1)	-3(1)	3(1)	-3(1)
N(3)	21(1)	25(1)	25(1)	-3(1)	1(1)	-3(1)
N(4)	22(1)	26(1)	25(1)	-6(1)	3(1)	-4(1)
N(5)	27(1)	24(1)	23(1)	-7(1)	3(1)	-7(1)
N(6)	26(1)	24(1)	23(1)	-7(1)	3(1)	-4(1)
C(1)	28(1)	22(1)	21(1)	-4(1)	-1(1)	1(1)
C(2)	44(1)	22(1)	24(1)	0(1)	1(1)	3(1)
C(3)	39(1)	21(1)	22(1)	-2(1)	2(1)	-3(1)
C(4)	27(1)	19(1)	22(1)	-4(1)	-1(1)	3(1)
C(5)	27(1)	25(1)	25(1)	-6(1)	-2(1)	2(1)
C(6)	35(1)	31(1)	24(1)	-8(1)	0(1)	2(1)
C(7)	32(1)	33(1)	34(1)	-10(1)	8(1)	-2(1)
C(8)	26(1)	32(1)	38(1)	-10(1)	-1(1)	-2(1)
C(9)	29(1)	22(1)	29(1)	-7(1)	-4(1)	2(1)
C(10)	30(1)	47(1)	30(1)	-10(1)	-5(1)	0(1)
C(11)	43(1)	67(2)	47(1)	-20(1)	20(1)	-11(1)
C(12)	45(1)	37(1)	34(1)	-9(1)	-14(1)	-2(1)
C(13)	21(1)	28(1)	32(1)	-6(1)	-2(1)	-1(1)
C(14)	20(1)	44(1)	42(1)	-3(1)	-1(1)	-4(1)
C(15)	21(1)	38(1)	35(1)	-8(1)	4(1)	-5(1)
C(16)	19(1)	32(1)	32(1)	-2(1)	-6(1)	-1(1)
C(17)	25(1)	33(1)	43(1)	-4(1)	-7(1)	1(1)
C(18)	28(1)	32(1)	55(1)	4(1)	-9(1)	3(1)
C(19)	22(1)	49(1)	42(1)	10(1)	-10(1)	-1(1)
C(20)	31(1)	53(1)	33(1)	-2(1)	-7(1)	-3(1)
C(21)	25(1)	37(1)	35(1)	-5(1)	-5(1)	-2(1)
C(22)	51(1)	40(1)	61(2)	-16(1)	1(1)	2(1)
C(23)	35(1)	68(2)	49(1)	23(1)	-11(1)	-3(1)
C(24)	57(2)	39(1)	46(1)	-12(1)	2(1)	-7(1)
C(25)	26(1)	23(1)	28(1)	-9(1)	-2(1)	-1(1)
C(26)	39(1)	33(1)	30(1)	-16(1)	1(1)	-6(1)

C(27)	35(1)	32(1)	24(1)	-10(1)	2(1)	-3(1)
C(28)	28(1)	22(1)	28(1)	-10(1)	-3(1)	-3(1)
C(29)	29(1)	23(1)	35(1)	-7(1)	-2(1)	-1(1)
C(30)	29(1)	30(1)	37(1)	-8(1)	1(1)	-2(1)
C(31)	37(1)	27(1)	30(1)	-7(1)	0(1)	-7(1)
C(32)	39(1)	23(1)	33(1)	-6(1)	-7(1)	-1(1)
C(33)	30(1)	25(1)	34(1)	-10(1)	-6(1)	1(1)
C(34)	35(1)	27(1)	74(2)	-1(1)	-1(1)	4(1)
C(35)	48(1)	35(1)	48(1)	-4(1)	7(1)	-13(1)
C(36)	34(1)	33(1)	70(2)	-11(1)	-5(1)	4(1)
C(37)	30(1)	29(1)	42(1)	1(1)	12(1)	-1(1)
C(38)	27(1)	27(1)	25(1)	-1(1)	3(1)	-4(1)
C(39)	32(1)	28(1)	36(1)	3(1)	3(1)	3(1)
C(40)	32(1)	24(1)	31(1)	-1(1)	-1(1)	-2(1)
C(41)	44(1)	29(1)	50(1)	3(1)	-2(1)	3(1)
C(42)	59(2)	30(1)	55(2)	5(1)	-7(1)	-5(1)
B(1)	25(1)	22(1)	23(1)	-6(1)	3(1)	-4(1)
Cl(1)	71(1)	68(1)	76(1)	-32(1)	-10(1)	-16(1)
Cl(2)	79(1)	131(1)	73(1)	-7(1)	21(1)	-47(1)
C(43)	61(2)	61(2)	60(2)	-25(1)	13(1)	-22(1)
Cl(3)	258(3)	120(1)	104(1)	-39(1)	-51(1)	-26(1)
C(44)	270(20)	183(14)	95(8)	45(9)	60(10)	154(14)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Tp^{Ms}Cu(1-hexyne), **1.**

	x	y	z	U(eq)
H(2)	291	6737	5965	37
H(3)	2046	6020	5142	34
H(6)	-1171	4996	9430	36
H(8)	-3537	4459	7911	39
H(10A)	856	5365	8989	53
H(10B)	1110	6109	8068	53
H(10C)	1397	4780	8251	53
H(11A)	-4114	5036	9399	80
H(11B)	-3148	4531	10011	80
H(11C)	-3830	3707	9574	80
H(12A)	-2994	4549	6511	57
H(12B)	-1646	4174	6266	57
H(12C)	-1982	5492	6103	57
H(14)	5841	2431	7300	44
H(15)	5303	3584	5955	38
H(18)	3800	-1269	9298	48
H(20)	3160	1368	10410	48
H(22A)	3645	136	7310	76
H(22B)	4026	-1041	7861	76
H(22C)	5010	-55	7499	76
H(23A)	2756	-1541	10774	83
H(23B)	2819	-497	11222	83
H(23C)	4020	-1154	10990	83
H(24A)	4139	3489	8782	71
H(24B)	3370	3252	9675	71
H(24C)	2703	3398	8862	71
H(26)	1356	811	4669	39
H(27)	2690	2538	4382	36
H(30)	-2833	35	7024	39
H(32)	-263	-2340	7264	38
H(34A)	-1321	2323	6541	71
H(34B)	-2455	1852	6209	71

H(34C)	-1214	2124	5616	71
H(35A)	-3175	-1832	8058	68
H(35B)	-2220	-2817	7987	68
H(35C)	-3079	-2423	7279	68
H(36A)	1771	-1882	6849	68
H(36B)	2198	-581	6567	68
H(36C)	1823	-1248	5899	68
H(37)	-890(20)	2710(20)	8252(17)	43
H(39A)	1465	333	8915	40
H(39B)	1260	-1	8063	40
H(40A)	-687	-703	8624	36
H(40B)	-540	-313	9468	36
H(41A)	925	-2010	8868	52
H(41B)	1048	-1630	9719	52
H(42A)	-929	-2342	10228	74
H(42B)	-56	-3324	10006	74
H(42C)	-997	-2768	9389	74
H(1)	3288	4072	5237	28
H(43A)	3981	4952	7208	72
H(43B)	2932	5850	7021	72
H(44A)	3835	508	4544	242
H(44B)	5131	640	4025	242

Table 6. Torsion angles [°] for $Tp^{Ms}Cu$(1-hexyne), **1**.

C(37)-Cu(1)-N(1)-C(1)	6.7(2)
C(38)-Cu(1)-N(1)-C(1)	4.4(3)
N(3)-Cu(1)-N(1)-C(1)	-145.91(18)
N(5)-Cu(1)-N(1)-C(1)	128.81(18)
C(37)-Cu(1)-N(1)-N(2)	-166.42(13)
C(38)-Cu(1)-N(1)-N(2)	-168.71(13)
N(3)-Cu(1)-N(1)-N(2)	41.01(13)
N(5)-Cu(1)-N(1)-N(2)	-44.26(12)
C(1)-N(1)-N(2)-C(3)	0.2(2)
Cu(1)-N(1)-N(2)-C(3)	175.22(12)
C(1)-N(1)-N(2)-B(1)	-175.05(15)
Cu(1)-N(1)-N(2)-B(1)	0.0(2)
C(37)-Cu(1)-N(3)-C(13)	7.4(3)
N(1)-Cu(1)-N(3)-C(13)	140.5(2)
C(38)-Cu(1)-N(3)-C(13)	-21.2(2)
N(5)-Cu(1)-N(3)-C(13)	-129.8(2)
C(37)-Cu(1)-N(3)-N(4)	-168.55(14)
N(1)-Cu(1)-N(3)-N(4)	-35.40(12)
C(38)-Cu(1)-N(3)-N(4)	162.85(12)
N(5)-Cu(1)-N(3)-N(4)	54.23(12)
C(13)-N(3)-N(4)-C(15)	-0.2(2)
Cu(1)-N(3)-N(4)-C(15)	177.04(12)
C(13)-N(3)-N(4)-B(1)	172.00(16)
Cu(1)-N(3)-N(4)-B(1)	-10.7(2)
C(37)-Cu(1)-N(5)-C(25)	-27.7(2)
N(1)-Cu(1)-N(5)-C(25)	-141.0(2)
C(38)-Cu(1)-N(5)-C(25)	9.2(2)
N(3)-Cu(1)-N(5)-C(25)	124.5(2)
C(37)-Cu(1)-N(5)-N(6)	158.17(12)
N(1)-Cu(1)-N(5)-N(6)	44.88(12)
C(38)-Cu(1)-N(5)-N(6)	-164.91(12)
N(3)-Cu(1)-N(5)-N(6)	-49.56(12)
C(25)-N(5)-N(6)-C(27)	-0.1(2)
Cu(1)-N(5)-N(6)-C(27)	176.02(13)
C(25)-N(5)-N(6)-B(1)	-175.93(16)
Cu(1)-N(5)-N(6)-B(1)	0.2(2)

N(2)-N(1)-C(1)-C(2)	-0.1(2)
Cu(1)-N(1)-C(1)-C(2)	-173.62(14)
N(2)-N(1)-C(1)-C(4)	178.70(15)
Cu(1)-N(1)-C(1)-C(4)	5.2(3)
N(1)-C(1)-C(2)-C(3)	0.0(2)
C(4)-C(1)-C(2)-C(3)	-178.64(19)
N(1)-N(2)-C(3)-C(2)	-0.2(2)
B(1)-N(2)-C(3)-C(2)	174.50(18)
C(1)-C(2)-C(3)-N(2)	0.1(2)
N(1)-C(1)-C(4)-C(5)	76.5(2)
C(2)-C(1)-C(4)-C(5)	-105.0(2)
N(1)-C(1)-C(4)-C(9)	-100.4(2)
C(2)-C(1)-C(4)-C(9)	78.1(3)
C(9)-C(4)-C(5)-C(6)	1.6(3)
C(1)-C(4)-C(5)-C(6)	-175.31(16)
C(9)-C(4)-C(5)-C(10)	-179.03(17)
C(1)-C(4)-C(5)-C(10)	4.0(3)
C(4)-C(5)-C(6)-C(7)	0.8(3)
C(10)-C(5)-C(6)-C(7)	-178.60(19)
C(5)-C(6)-C(7)-C(8)	-2.2(3)
C(5)-C(6)-C(7)-C(11)	178.9(2)
C(6)-C(7)-C(8)-C(9)	1.2(3)
C(11)-C(7)-C(8)-C(9)	-179.8(2)
C(7)-C(8)-C(9)-C(4)	1.0(3)
C(7)-C(8)-C(9)-C(12)	-179.55(19)
C(5)-C(4)-C(9)-C(8)	-2.5(3)
C(1)-C(4)-C(9)-C(8)	174.47(17)
C(5)-C(4)-C(9)-C(12)	178.12(18)
C(1)-C(4)-C(9)-C(12)	-4.9(3)
N(4)-N(3)-C(13)-C(14)	0.6(2)
Cu(1)-N(3)-C(13)-C(14)	-175.53(16)
N(4)-N(3)-C(13)-C(16)	-175.82(17)
Cu(1)-N(3)-C(13)-C(16)	8.1(3)
N(3)-C(13)-C(14)-C(15)	-0.7(2)
C(16)-C(13)-C(14)-C(15)	175.4(2)
N(3)-N(4)-C(15)-C(14)	-0.2(2)
B(1)-N(4)-C(15)-C(14)	-171.74(18)
C(13)-C(14)-C(15)-N(4)	0.5(2)

N(3)-C(13)-C(16)-C(21)	-85.0(2)
C(14)-C(13)-C(16)-C(21)	99.3(3)
N(3)-C(13)-C(16)-C(17)	96.9(2)
C(14)-C(13)-C(16)-C(17)	-78.8(3)
C(21)-C(16)-C(17)-C(18)	1.1(3)
C(13)-C(16)-C(17)-C(18)	179.21(18)
C(21)-C(16)-C(17)-C(22)	-179.9(2)
C(13)-C(16)-C(17)-C(22)	-1.8(3)
C(16)-C(17)-C(18)-C(19)	0.2(3)
C(22)-C(17)-C(18)-C(19)	-178.9(2)
C(17)-C(18)-C(19)-C(20)	-1.0(3)
C(17)-C(18)-C(19)-C(23)	178.9(2)
C(18)-C(19)-C(20)-C(21)	0.7(3)
C(23)-C(19)-C(20)-C(21)	-179.3(2)
C(19)-C(20)-C(21)-C(16)	0.5(3)
C(19)-C(20)-C(21)-C(24)	-178.7(2)
C(17)-C(16)-C(21)-C(20)	-1.4(3)
C(13)-C(16)-C(21)-C(20)	-179.51(18)
C(17)-C(16)-C(21)-C(24)	177.8(2)
C(13)-C(16)-C(21)-C(24)	-0.2(3)
N(6)-N(5)-C(25)-C(26)	0.0(2)
Cu(1)-N(5)-C(25)-C(26)	-174.34(16)
N(6)-N(5)-C(25)-C(28)	-178.59(16)
Cu(1)-N(5)-C(25)-C(28)	7.1(3)
N(5)-C(25)-C(26)-C(27)	0.1(2)
C(28)-C(25)-C(26)-C(27)	178.55(19)
N(5)-N(6)-C(27)-C(26)	0.2(2)
B(1)-N(6)-C(27)-C(26)	175.52(19)
C(25)-C(26)-C(27)-N(6)	-0.2(2)
N(5)-C(25)-C(28)-C(29)	72.2(2)
C(26)-C(25)-C(28)-C(29)	-106.1(2)
N(5)-C(25)-C(28)-C(33)	-109.8(2)
C(26)-C(25)-C(28)-C(33)	72.0(3)
C(33)-C(28)-C(29)-C(30)	0.3(3)
C(25)-C(28)-C(29)-C(30)	178.32(18)
C(33)-C(28)-C(29)-C(34)	179.9(2)
C(25)-C(28)-C(29)-C(34)	-2.0(3)
C(28)-C(29)-C(30)-C(31)	-0.1(3)

C(34)-C(29)-C(30)-C(31)	-179.8(2)
C(29)-C(30)-C(31)-C(32)	0.2(3)
C(29)-C(30)-C(31)-C(35)	-179.0(2)
C(30)-C(31)-C(32)-C(33)	-0.5(3)
C(35)-C(31)-C(32)-C(33)	178.7(2)
C(31)-C(32)-C(33)-C(28)	0.6(3)
C(31)-C(32)-C(33)-C(36)	-179.2(2)
C(29)-C(28)-C(33)-C(32)	-0.5(3)
C(25)-C(28)-C(33)-C(32)	-178.55(18)
C(29)-C(28)-C(33)-C(36)	179.4(2)
C(25)-C(28)-C(33)-C(36)	1.3(3)
N(1)-Cu(1)-C(37)-C(38)	-177.74(13)
N(3)-Cu(1)-C(37)-C(38)	-48.5(2)
N(5)-Cu(1)-C(37)-C(38)	80.10(16)
Cu(1)-C(37)-C(38)-C(39)	179.0(7)
N(1)-Cu(1)-C(38)-C(37)	3.7(2)
N(3)-Cu(1)-C(38)-C(37)	150.52(15)
N(5)-Cu(1)-C(38)-C(37)	-115.68(15)
C(37)-Cu(1)-C(38)-C(39)	-179.7(3)
N(1)-Cu(1)-C(38)-C(39)	-175.94(15)
N(3)-Cu(1)-C(38)-C(39)	-29.1(2)
N(5)-Cu(1)-C(38)-C(39)	64.66(19)
C(37)-C(38)-C(39)-C(40)	21.5(9)
Cu(1)-C(38)-C(39)-C(40)	-159.67(15)
C(38)-C(39)-C(40)-C(41)	-176.68(19)
C(39)-C(40)-C(41)-C(42)	-178.9(2)
C(27)-N(6)-B(1)-N(2)	126.6(2)
N(5)-N(6)-B(1)-N(2)	-58.4(2)
C(27)-N(6)-B(1)-N(4)	-114.0(2)
N(5)-N(6)-B(1)-N(4)	61.0(2)
C(3)-N(2)-B(1)-N(6)	-112.7(2)
N(1)-N(2)-B(1)-N(6)	61.4(2)
C(3)-N(2)-B(1)-N(4)	128.67(19)
N(1)-N(2)-B(1)-N(4)	-57.2(2)
C(15)-N(4)-B(1)-N(6)	114.4(2)
N(3)-N(4)-B(1)-N(6)	-56.3(2)
C(15)-N(4)-B(1)-N(2)	-125.91(19)
N(3)-N(4)-B(1)-N(2)	63.4(2)

C(44)#1-Cl(3)-C(44)-Cl(3)#1	0.000(1)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table 1. Crystal data and structure refinement for $Tp^{Ms}Cu$(phenylacetylene), **2**.

Empirical formula	$C_{52}H_{52}BCuN_6$	
	$[C_{44}H_{46}BCuN_6, C_8H_6]$	
Formula weight	835.35	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.1406(6) Å	α= 90°.
	b = 20.6632(15) Å	β= 97.186(2)°.
	c = 23.8733(17) Å	γ = 90°.
Volume	4473.6(5) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.531 mm^{-1}	
F(000)	1760	
Crystal size	0.22 x 0.22 x 0.17 mm^3	
Theta range for data collection	1.31 to 30.53°.	
Index ranges	-12<=h<=8, -29<=k<=20, -34<=l<=31	
Reflections collected	108788	
Independent reflections	13516 [R(int) = 0.0652]	
Completeness to theta = 30.53°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9152 and 0.8922	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13516 / 2 / 556	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1001	
R indices (all data)	R1 = 0.0769, wR2 = 0.1142	
Largest diff. peak and hole	0.335 and -0.664 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cu(1)	7073(1)	1730(1)	1632(1)	27(1)
N(1)	6534(2)	808(1)	1420(1)	23(1)
N(2)	5332(2)	565(1)	1636(1)	22(1)
N(3)	6823(2)	1502(1)	2530(1)	23(1)
N(4)	5562(2)	1158(1)	2568(1)	23(1)
N(5)	4871(2)	2040(1)	1557(1)	23(1)
N(6)	3919(2)	1595(1)	1737(1)	23(1)
C(1)	7031(2)	338(1)	1104(1)	21(1)
C(2)	6132(2)	-210(1)	1113(1)	26(1)
C(3)	5087(2)	-45(1)	1454(1)	25(1)
C(4)	8386(2)	441(1)	833(1)	21(1)
C(5)	9758(2)	256(1)	1123(1)	24(1)
C(6)	11037(2)	427(1)	904(1)	28(1)
C(7)	11012(2)	761(1)	399(1)	29(1)
C(8)	9644(2)	903(1)	100(1)	28(1)
C(9)	8334(2)	751(1)	307(1)	24(1)
C(10)	9852(2)	-135(1)	1662(1)	34(1)
C(11)	12430(3)	966(1)	190(1)	42(1)
C(12)	6871(2)	924(1)	-27(1)	36(1)
C(13)	7425(2)	1617(1)	3066(1)	25(1)
C(14)	6546(2)	1348(1)	3445(1)	32(1)
C(15)	5381(2)	1066(1)	3114(1)	29(1)
C(16)	8824(2)	1985(1)	3191(1)	26(1)
C(17)	8849(2)	2567(1)	3494(1)	30(1)
C(18)	10151(3)	2923(1)	3579(1)	35(1)
C(19)	11425(3)	2718(1)	3374(1)	38(1)
C(20)	11397(2)	2128(1)	3096(1)	37(1)
C(21)	10124(2)	1752(1)	3004(1)	30(1)
C(22)	7487(3)	2834(1)	3710(1)	42(1)
C(23)	12802(3)	3135(2)	3440(1)	58(1)
C(24)	10159(3)	1105(1)	2716(1)	39(1)
C(25)	4046(2)	2555(1)	1377(1)	23(1)

C(26)	2568(2)	2442(1)	1443(1)	30(1)
C(27)	2540(2)	1831(1)	1670(1)	27(1)
C(28)	4705(2)	3152(1)	1169(1)	23(1)
C(29)	5209(2)	3177(1)	642(1)	27(1)
C(30)	5777(2)	3759(1)	463(1)	34(1)
C(31)	5885(2)	4306(1)	798(1)	34(1)
C(32)	5380(2)	4269(1)	1320(1)	33(1)
C(33)	4772(2)	3708(1)	1510(1)	29(1)
C(34)	5154(3)	2591(1)	260(1)	42(1)
C(35)	6546(3)	4928(1)	609(1)	55(1)
C(36)	4216(3)	3703(1)	2080(1)	46(1)
C(37)	8778(2)	1990(1)	1256(1)	30(1)
C(38)	8465(2)	2469(1)	1515(1)	23(1)
C(39)	8533(2)	3122(1)	1736(1)	25(1)
C(40)	7989(3)	3273(1)	2236(1)	34(1)
C(41)	8137(3)	3895(1)	2454(1)	47(1)
C(42)	8816(3)	4369(1)	2171(1)	51(1)
C(43)	9339(3)	4225(1)	1668(1)	46(1)
C(44)	9202(2)	3604(1)	1447(1)	36(1)
C(45)	2268(4)	5152(2)	951(1)	69(1)
C(46)	1635(3)	5594(1)	724(1)	45(1)
C(47)	849(2)	6126(1)	447(1)	36(1)
C(48)	-505(3)	6028(1)	128(1)	45(1)
C(49)	-1261(3)	6558(2)	-132(1)	61(1)
C(50)	-660(4)	7169(2)	-75(1)	73(1)
C(51)	665(4)	7257(1)	233(1)	73(1)
C(52)	1434(3)	6747(1)	498(1)	54(1)
B(1)	4504(2)	974(1)	2038(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for Tp^{Ms}Cu(phenylacetylene), **2**.

Cu(1)-C(37)	1.967(2)	C(11)-H(11A)	0.9800
Cu(1)-N(1)	2.0171(15)	C(11)-H(11B)	0.9800
Cu(1)-C(38)	2.0284(18)	C(11)-H(11C)	0.9800
Cu(1)-N(5)	2.0983(16)	C(12)-H(12A)	0.9800
Cu(1)-N(3)	2.2349(15)	C(12)-H(12B)	0.9800
N(1)-C(1)	1.343(2)	C(12)-H(12C)	0.9800
N(1)-N(2)	1.366(2)	C(13)-C(14)	1.399(3)
N(2)-C(3)	1.343(2)	C(13)-C(16)	1.486(3)
N(2)-B(1)	1.546(3)	C(14)-C(15)	1.374(3)
N(3)-C(13)	1.348(2)	C(14)-H(14)	0.9500
N(3)-N(4)	1.368(2)	C(15)-H(15)	0.9500
N(4)-C(15)	1.347(2)	C(16)-C(17)	1.403(3)
N(4)-B(1)	1.542(2)	C(16)-C(21)	1.404(3)
N(5)-C(25)	1.344(2)	C(17)-C(18)	1.392(3)
N(5)-N(6)	1.371(2)	C(17)-C(22)	1.510(3)
N(6)-C(27)	1.343(2)	C(18)-C(19)	1.384(3)
N(6)-B(1)	1.534(2)	C(18)-H(18)	0.9500
C(1)-C(2)	1.401(2)	C(19)-C(20)	1.388(3)
C(1)-C(4)	1.483(3)	C(19)-C(23)	1.516(3)
C(2)-C(3)	1.373(3)	C(20)-C(21)	1.393(3)
C(2)-H(2)	0.9500	C(20)-H(20)	0.9500
C(3)-H(3)	0.9500	C(21)-C(24)	1.507(3)
C(4)-C(9)	1.405(2)	C(22)-H(22A)	0.9800
C(4)-C(5)	1.407(2)	C(22)-H(22B)	0.9800
C(5)-C(6)	1.385(3)	C(22)-H(22C)	0.9800
C(5)-C(10)	1.515(3)	C(23)-H(23A)	0.9800
C(6)-C(7)	1.386(3)	C(23)-H(23B)	0.9800
C(6)-H(6)	0.9500	C(23)-H(23C)	0.9800
C(7)-C(8)	1.391(3)	C(24)-H(24A)	0.9800
C(7)-C(11)	1.506(3)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.387(3)	C(24)-H(24C)	0.9800
C(8)-H(8)	0.9500	C(25)-C(26)	1.399(3)
C(9)-C(12)	1.511(3)	C(25)-C(28)	1.484(2)
C(10)-H(10A)	0.9800	C(26)-C(27)	1.375(3)
C(10)-H(10B)	0.9800	C(26)-H(26)	0.9500
C(10)-H(10C)	0.9800	C(27)-H(27)	0.9500

C(28)-C(29)	1.394(3)	C(47)-C(52)	1.391(3)
C(28)-C(33)	1.406(3)	C(48)-C(49)	1.398(4)
C(29)-C(30)	1.397(3)	C(48)-H(48)	0.9500
C(29)-C(34)	1.513(3)	C(49)-C(50)	1.377(5)
C(30)-C(31)	1.382(3)	C(49)-H(49)	0.9500
C(30)-H(30)	0.9500	C(50)-C(51)	1.348(5)
C(31)-C(32)	1.384(3)	C(50)-H(50)	0.9500
C(31)-C(35)	1.512(3)	C(51)-C(52)	1.375(4)
C(32)-C(33)	1.386(3)	C(51)-H(51)	0.9500
C(32)-H(32)	0.9500	C(52)-H(52)	0.9500
C(33)-C(36)	1.510(3)	B(1)-H(1)	1.0000
C(34)-H(34A)	0.9800		
C(34)-H(34B)	0.9800	C(37)-Cu(1)-N(1)	109.06(7)
C(34)-H(34C)	0.9800	C(37)-Cu(1)-C(38)	35.46(8)
C(35)-H(35A)	0.9800	N(1)-Cu(1)-C(38)	144.51(7)
C(35)-H(35B)	0.9800	C(37)-Cu(1)-N(5)	133.14(8)
C(35)-H(35C)	0.9800	N(1)-Cu(1)-N(5)	93.73(6)
C(36)-H(36A)	0.9800	C(38)-Cu(1)-N(5)	111.73(7)
C(36)-H(36B)	0.9800	C(37)-Cu(1)-N(3)	132.58(7)
C(36)-H(36C)	0.9800	N(1)-Cu(1)-N(3)	89.46(6)
C(37)-C(38)	1.218(3)	C(38)-Cu(1)-N(3)	115.57(6)
C(37)-H(37)	0.918(15)	N(5)-Cu(1)-N(3)	86.22(6)
C(38)-C(39)	1.448(2)	C(1)-N(1)-N(2)	106.91(14)
C(39)-C(40)	1.384(3)	C(1)-N(1)-Cu(1)	137.27(13)
C(39)-C(44)	1.396(3)	N(2)-N(1)-Cu(1)	115.81(11)
C(40)-C(41)	1.388(3)	C(3)-N(2)-N(1)	109.47(15)
C(40)-H(40)	0.9500	C(3)-N(2)-B(1)	129.65(16)
C(41)-C(42)	1.380(4)	N(1)-N(2)-B(1)	120.85(14)
C(41)-H(41)	0.9500	C(13)-N(3)-N(4)	106.01(15)
C(42)-C(43)	1.378(4)	C(13)-N(3)-Cu(1)	142.59(13)
C(42)-H(42)	0.9500	N(4)-N(3)-Cu(1)	111.22(10)
C(43)-C(44)	1.387(3)	C(15)-N(4)-N(3)	110.16(15)
C(43)-H(43)	0.9500	C(15)-N(4)-B(1)	128.25(17)
C(44)-H(44)	0.9500	N(3)-N(4)-B(1)	121.40(15)
C(45)-C(46)	1.177(4)	C(25)-N(5)-N(6)	106.17(15)
C(45)-H(45)	0.933(17)	C(25)-N(5)-Cu(1)	139.73(13)
C(46)-C(47)	1.428(3)	N(6)-N(5)-Cu(1)	114.10(11)
C(47)-C(48)	1.385(3)	C(27)-N(6)-N(5)	110.02(15)

C(27)-N(6)-B(1)	128.78(16)	C(7)-C(11)-H(11C)	109.5
N(5)-N(6)-B(1)	120.68(15)	H(11A)-C(11)-H(11C)	109.5
N(1)-C(1)-C(2)	109.54(16)	H(11B)-C(11)-H(11C)	109.5
N(1)-C(1)-C(4)	120.08(15)	C(9)-C(12)-H(12A)	109.5
C(2)-C(1)-C(4)	130.32(16)	C(9)-C(12)-H(12B)	109.5
C(3)-C(2)-C(1)	105.25(16)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-H(2)	127.4	C(9)-C(12)-H(12C)	109.5
C(1)-C(2)-H(2)	127.4	H(12A)-C(12)-H(12C)	109.5
N(2)-C(3)-C(2)	108.84(17)	H(12B)-C(12)-H(12C)	109.5
N(2)-C(3)-H(3)	125.6	N(3)-C(13)-C(14)	110.16(17)
C(2)-C(3)-H(3)	125.6	N(3)-C(13)-C(16)	121.29(17)
C(9)-C(4)-C(5)	119.46(18)	C(14)-C(13)-C(16)	128.54(17)
C(9)-C(4)-C(1)	121.25(16)	C(15)-C(14)-C(13)	105.24(17)
C(5)-C(4)-C(1)	119.20(16)	C(15)-C(14)-H(14)	127.4
C(6)-C(5)-C(4)	119.20(17)	C(13)-C(14)-H(14)	127.4
C(6)-C(5)-C(10)	119.76(17)	N(4)-C(15)-C(14)	108.43(18)
C(4)-C(5)-C(10)	121.03(18)	N(4)-C(15)-H(15)	125.8
C(5)-C(6)-C(7)	122.14(18)	C(14)-C(15)-H(15)	125.8
C(5)-C(6)-H(6)	118.9	C(17)-C(16)-C(21)	119.85(19)
C(7)-C(6)-H(6)	118.9	C(17)-C(16)-C(13)	120.02(18)
C(6)-C(7)-C(8)	117.79(19)	C(21)-C(16)-C(13)	120.13(17)
C(6)-C(7)-C(11)	120.5(2)	C(18)-C(17)-C(16)	119.1(2)
C(8)-C(7)-C(11)	121.73(19)	C(18)-C(17)-C(22)	118.88(19)
C(9)-C(8)-C(7)	122.09(18)	C(16)-C(17)-C(22)	121.92(19)
C(9)-C(8)-H(8)	119.0	C(19)-C(18)-C(17)	121.9(2)
C(7)-C(8)-H(8)	119.0	C(19)-C(18)-H(18)	119.1
C(8)-C(9)-C(4)	119.10(17)	C(17)-C(18)-H(18)	119.1
C(8)-C(9)-C(12)	120.40(17)	C(18)-C(19)-C(20)	118.2(2)
C(4)-C(9)-C(12)	120.50(18)	C(18)-C(19)-C(23)	120.9(2)
C(5)-C(10)-H(10A)	109.5	C(20)-C(19)-C(23)	120.8(2)
C(5)-C(10)-H(10B)	109.5	C(19)-C(20)-C(21)	122.0(2)
H(10A)-C(10)-H(10B)	109.5	C(19)-C(20)-H(20)	119.0
C(5)-C(10)-H(10C)	109.5	C(21)-C(20)-H(20)	119.0
H(10A)-C(10)-H(10C)	109.5	C(20)-C(21)-C(16)	118.86(19)
H(10B)-C(10)-H(10C)	109.5	C(20)-C(21)-C(24)	120.1(2)
C(7)-C(11)-H(11A)	109.5	C(16)-C(21)-C(24)	121.05(19)
C(7)-C(11)-H(11B)	109.5	C(17)-C(22)-H(22A)	109.5
H(11A)-C(11)-H(11B)	109.5	C(17)-C(22)-H(22B)	109.5

H(22A)-C(22)-H(22B)	109.5	C(31)-C(32)-H(32)	118.9
C(17)-C(22)-H(22C)	109.5	C(33)-C(32)-H(32)	118.9
H(22A)-C(22)-H(22C)	109.5	C(32)-C(33)-C(28)	118.96(19)
H(22B)-C(22)-H(22C)	109.5	C(32)-C(33)-C(36)	119.65(19)
C(19)-C(23)-H(23A)	109.5	C(28)-C(33)-C(36)	121.39(18)
C(19)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34A)	109.5
H(23A)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34B)	109.5
C(19)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(23A)-C(23)-H(23C)	109.5	C(29)-C(34)-H(34C)	109.5
H(23B)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24A)	109.5	H(34B)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35A)	109.5
H(24A)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35B)	109.5
C(21)-C(24)-H(24C)	109.5	H(35A)-C(35)-H(35B)	109.5
H(24A)-C(24)-H(24C)	109.5	C(31)-C(35)-H(35C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(35A)-C(35)-H(35C)	109.5
N(5)-C(25)-C(26)	110.04(16)	H(35B)-C(35)-H(35C)	109.5
N(5)-C(25)-C(28)	121.98(16)	C(33)-C(36)-H(36A)	109.5
C(26)-C(25)-C(28)	127.92(16)	C(33)-C(36)-H(36B)	109.5
C(27)-C(26)-C(25)	105.30(17)	H(36A)-C(36)-H(36B)	109.5
C(27)-C(26)-H(26)	127.3	C(33)-C(36)-H(36C)	109.5
C(25)-C(26)-H(26)	127.3	H(36A)-C(36)-H(36C)	109.5
N(6)-C(27)-C(26)	108.47(17)	H(36B)-C(36)-H(36C)	109.5
N(6)-C(27)-H(27)	125.8	C(38)-C(37)-Cu(1)	75.01(14)
C(26)-C(27)-H(27)	125.8	C(38)-C(37)-H(37)	161.4(15)
C(29)-C(28)-C(33)	119.77(17)	Cu(1)-C(37)-H(37)	123.6(15)
C(29)-C(28)-C(25)	121.86(16)	C(37)-C(38)-C(39)	159.9(2)
C(33)-C(28)-C(25)	118.33(17)	C(37)-C(38)-Cu(1)	69.53(13)
C(28)-C(29)-C(30)	119.09(18)	C(39)-C(38)-Cu(1)	130.59(15)
C(28)-C(29)-C(34)	121.56(18)	C(40)-C(39)-C(44)	119.48(18)
C(30)-C(29)-C(34)	119.35(19)	C(40)-C(39)-C(38)	121.36(18)
C(31)-C(30)-C(29)	121.9(2)	C(44)-C(39)-C(38)	119.13(19)
C(31)-C(30)-H(30)	119.0	C(39)-C(40)-C(41)	120.3(2)
C(29)-C(30)-H(30)	119.0	C(39)-C(40)-H(40)	119.9
C(30)-C(31)-C(32)	117.93(19)	C(41)-C(40)-H(40)	119.9
C(30)-C(31)-C(35)	121.5(2)	C(42)-C(41)-C(40)	120.1(2)
C(32)-C(31)-C(35)	120.5(2)	C(42)-C(41)-H(41)	120.0
C(31)-C(32)-C(33)	122.27(19)	C(40)-C(41)-H(41)	120.0

C(43)-C(42)-C(41)	120.0(2)
C(43)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0
C(42)-C(43)-C(44)	120.4(2)
C(42)-C(43)-H(43)	119.8
C(44)-C(43)-H(43)	119.8
C(43)-C(44)-C(39)	119.7(2)
C(43)-C(44)-H(44)	120.1
C(39)-C(44)-H(44)	120.1
C(46)-C(45)-H(45)	177(2)
C(45)-C(46)-C(47)	179.2(3)
C(48)-C(47)-C(52)	119.3(2)
C(48)-C(47)-C(46)	120.4(2)
C(52)-C(47)-C(46)	120.3(2)
C(47)-C(48)-C(49)	119.2(3)
C(47)-C(48)-H(48)	120.4
C(49)-C(48)-H(48)	120.4
C(50)-C(49)-C(48)	120.4(3)
C(50)-C(49)-H(49)	119.8
C(48)-C(49)-H(49)	119.8
C(51)-C(50)-C(49)	119.8(3)
C(51)-C(50)-H(50)	120.1
C(49)-C(50)-H(50)	120.1
C(50)-C(51)-C(52)	121.4(3)
C(50)-C(51)-H(51)	119.3
C(52)-C(51)-H(51)	119.3
C(51)-C(52)-C(47)	119.9(3)
C(51)-C(52)-H(52)	120.0
C(47)-C(52)-H(52)	120.0
N(6)-B(1)-N(4)	108.93(14)
N(6)-B(1)-N(2)	109.54(15)
N(4)-B(1)-N(2)	109.85(15)
N(6)-B(1)-H(1)	109.5
N(4)-B(1)-H(1)	109.5
N(2)-B(1)-H(1)	109.5

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	24(1)	18(1)	43(1)	-5(1)	16(1)	-5(1)
N(1)	20(1)	20(1)	29(1)	0(1)	9(1)	-3(1)
N(2)	19(1)	20(1)	28(1)	1(1)	7(1)	-3(1)
N(3)	23(1)	22(1)	25(1)	1(1)	7(1)	-1(1)
N(4)	23(1)	21(1)	27(1)	3(1)	10(1)	-1(1)
N(5)	19(1)	21(1)	29(1)	4(1)	6(1)	-1(1)
N(6)	18(1)	22(1)	31(1)	2(1)	8(1)	-1(1)
C(1)	21(1)	18(1)	24(1)	0(1)	4(1)	0(1)
C(2)	28(1)	18(1)	33(1)	-4(1)	5(1)	-3(1)
C(3)	24(1)	18(1)	32(1)	2(1)	1(1)	-5(1)
C(4)	24(1)	15(1)	24(1)	-4(1)	5(1)	-2(1)
C(5)	26(1)	20(1)	25(1)	-2(1)	5(1)	1(1)
C(6)	24(1)	25(1)	35(1)	-5(1)	5(1)	1(1)
C(7)	32(1)	21(1)	36(1)	-8(1)	15(1)	-4(1)
C(8)	39(1)	21(1)	25(1)	-2(1)	11(1)	-3(1)
C(9)	30(1)	19(1)	24(1)	-4(1)	4(1)	0(1)
C(10)	34(1)	34(1)	33(1)	8(1)	3(1)	4(1)
C(11)	41(2)	36(1)	54(1)	-4(1)	24(1)	-7(1)
C(12)	40(1)	36(1)	31(1)	4(1)	-3(1)	5(1)
C(13)	27(1)	24(1)	24(1)	1(1)	7(1)	3(1)
C(14)	41(1)	33(1)	23(1)	4(1)	10(1)	-1(1)
C(15)	33(1)	27(1)	31(1)	4(1)	15(1)	-1(1)
C(16)	27(1)	29(1)	21(1)	3(1)	3(1)	2(1)
C(17)	32(1)	35(1)	21(1)	-1(1)	3(1)	0(1)
C(18)	43(1)	37(1)	25(1)	-5(1)	2(1)	-7(1)
C(19)	34(1)	52(1)	28(1)	-1(1)	1(1)	-11(1)
C(20)	27(1)	53(1)	33(1)	1(1)	6(1)	2(1)
C(21)	29(1)	35(1)	24(1)	2(1)	3(1)	6(1)
C(22)	48(2)	38(1)	42(1)	-13(1)	14(1)	-3(1)
C(23)	46(2)	79(2)	48(2)	-10(1)	6(1)	-27(1)
C(24)	34(1)	37(1)	46(1)	-2(1)	12(1)	9(1)
C(25)	22(1)	22(1)	25(1)	1(1)	4(1)	3(1)
C(26)	20(1)	32(1)	38(1)	6(1)	7(1)	5(1)

C(27)	17(1)	31(1)	34(1)	2(1)	8(1)	0(1)
C(28)	19(1)	21(1)	28(1)	4(1)	3(1)	3(1)
C(29)	25(1)	28(1)	29(1)	0(1)	6(1)	-2(1)
C(30)	33(1)	37(1)	32(1)	6(1)	8(1)	-7(1)
C(31)	34(1)	26(1)	41(1)	7(1)	3(1)	-5(1)
C(32)	38(1)	22(1)	40(1)	-4(1)	3(1)	3(1)
C(33)	31(1)	26(1)	30(1)	0(1)	4(1)	3(1)
C(34)	50(2)	40(1)	38(1)	-11(1)	16(1)	-10(1)
C(35)	68(2)	40(1)	58(2)	12(1)	5(1)	-22(1)
C(36)	59(2)	46(1)	38(1)	-11(1)	18(1)	-4(1)
C(37)	27(1)	27(1)	38(1)	-6(1)	15(1)	-8(1)
C(38)	18(1)	23(1)	30(1)	3(1)	4(1)	-4(1)
C(39)	22(1)	20(1)	32(1)	-1(1)	-1(1)	-2(1)
C(40)	47(1)	25(1)	29(1)	0(1)	1(1)	-1(1)
C(41)	74(2)	30(1)	33(1)	-9(1)	-3(1)	2(1)
C(42)	71(2)	23(1)	53(1)	-7(1)	-14(1)	-6(1)
C(43)	48(2)	24(1)	66(2)	7(1)	3(1)	-10(1)
C(44)	33(1)	26(1)	49(1)	2(1)	9(1)	-4(1)
C(45)	65(2)	77(2)	64(2)	13(2)	10(2)	34(2)
C(46)	38(1)	57(2)	42(1)	0(1)	10(1)	10(1)
C(47)	33(1)	44(1)	32(1)	-1(1)	14(1)	5(1)
C(48)	38(1)	63(2)	34(1)	3(1)	12(1)	2(1)
C(49)	46(2)	103(3)	34(1)	7(1)	7(1)	27(2)
C(50)	109(3)	66(2)	47(2)	8(1)	23(2)	48(2)
C(51)	119(3)	40(2)	63(2)	-1(1)	26(2)	14(2)
C(52)	59(2)	52(2)	51(1)	-13(1)	11(1)	-2(1)
B(1)	20(1)	20(1)	30(1)	2(1)	8(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Tp^{Ms}Cu(phenylacetylene), **2**.

	x	y	z	U(eq)
H(2)	6225	-609	924	31
H(3)	4316	-319	1547	30
H(6)	11962	310	1105	33
H(8)	9606	1109	-257	33
H(10A)	9609	-588	1571	51
H(10B)	9153	38	1903	51
H(10C)	10854	-109	1862	51
H(11A)	12206	1202	-167	64
H(11B)	13018	581	129	64
H(11C)	12987	1247	470	64
H(12A)	7037	1211	-339	54
H(12B)	6250	1143	220	54
H(12C)	6378	528	-178	54
H(14)	6718	1358	3846	38
H(15)	4583	843	3247	35
H(18)	10165	3318	3784	42
H(20)	12273	1975	2964	44
H(22A)	6650	2808	3411	63
H(22B)	7656	3287	3822	63
H(22C)	7271	2580	4036	63
H(23A)	12773	3432	3119	87
H(23B)	13675	2857	3453	87
H(23C)	12848	3384	3791	87
H(24A)	9590	790	2907	58
H(24B)	11182	957	2732	58
H(24C)	9727	1146	2320	58
H(26)	1757	2726	1350	36
H(27)	1688	1613	1764	32
H(30)	6099	3779	100	41
H(32)	5452	4641	1556	40
H(34A)	5211	2731	-129	63
H(34B)	4227	2358	277	63

H(34C)	5986	2305	385	63
H(35A)	5844	5283	628	83
H(35B)	6765	4879	219	83
H(35C)	7459	5024	856	83
H(36A)	4550	4095	2288	70
H(36B)	4600	3321	2292	70
H(36C)	3135	3690	2027	70
H(37)	9250(20)	1718(10)	1035(9)	36
H(40)	7513	2949	2430	40
H(41)	7771	3995	2799	56
H(42)	8922	4794	2322	61
H(43)	9797	4553	1472	55
H(44)	9563	3508	1100	43
H(45)	2760(30)	4789(12)	1111(13)	82
H(48)	-915	5606	86	53
H(49)	-2195	6496	-348	73
H(50)	-1178	7528	-252	87
H(51)	1077	7679	267	87
H(52)	2363	6820	715	64
H(1)	3660	718	2151	28

Table 6. Torsion angles [°] for $Tp^{Ms}Cu$(phenylacetylene), **2**.

C(37)-Cu(1)-N(1)-C(1)	0.8(2)
C(38)-Cu(1)-N(1)-C(1)	2.3(2)
N(5)-Cu(1)-N(1)-C(1)	139.20(18)
N(3)-Cu(1)-N(1)-C(1)	-134.63(18)
C(37)-Cu(1)-N(1)-N(2)	-177.95(12)
C(38)-Cu(1)-N(1)-N(2)	-176.50(11)
N(5)-Cu(1)-N(1)-N(2)	-39.57(12)
N(3)-Cu(1)-N(1)-N(2)	46.60(12)
C(1)-N(1)-N(2)-C(3)	-0.15(19)
Cu(1)-N(1)-N(2)-C(3)	178.98(11)
C(1)-N(1)-N(2)-B(1)	178.19(14)
Cu(1)-N(1)-N(2)-B(1)	-2.68(19)
C(37)-Cu(1)-N(3)-C(13)	24.8(2)
N(1)-Cu(1)-N(3)-C(13)	140.5(2)
C(38)-Cu(1)-N(3)-C(13)	-13.4(2)
N(5)-Cu(1)-N(3)-C(13)	-125.7(2)
C(37)-Cu(1)-N(3)-N(4)	-161.32(12)
N(1)-Cu(1)-N(3)-N(4)	-45.54(12)
C(38)-Cu(1)-N(3)-N(4)	160.55(11)
N(5)-Cu(1)-N(3)-N(4)	48.24(11)
C(13)-N(3)-N(4)-C(15)	0.5(2)
Cu(1)-N(3)-N(4)-C(15)	-175.70(12)
C(13)-N(3)-N(4)-B(1)	175.88(16)
Cu(1)-N(3)-N(4)-B(1)	-0.29(19)
C(37)-Cu(1)-N(5)-C(25)	-21.5(2)
N(1)-Cu(1)-N(5)-C(25)	-142.18(19)
C(38)-Cu(1)-N(5)-C(25)	12.6(2)
N(3)-Cu(1)-N(5)-C(25)	128.61(19)
C(37)-Cu(1)-N(5)-N(6)	157.76(12)
N(1)-Cu(1)-N(5)-N(6)	37.12(12)
C(38)-Cu(1)-N(5)-N(6)	-168.15(11)
N(3)-Cu(1)-N(5)-N(6)	-52.09(12)
C(25)-N(5)-N(6)-C(27)	-0.1(2)
Cu(1)-N(5)-N(6)-C(27)	-179.62(12)
C(25)-N(5)-N(6)-B(1)	-172.54(15)
Cu(1)-N(5)-N(6)-B(1)	7.9(2)

N(2)-N(1)-C(1)-C(2)	0.43(19)
Cu(1)-N(1)-C(1)-C(2)	-178.41(13)
N(2)-N(1)-C(1)-C(4)	-176.88(14)
Cu(1)-N(1)-C(1)-C(4)	4.3(3)
N(1)-C(1)-C(2)-C(3)	-0.5(2)
C(4)-C(1)-C(2)-C(3)	176.41(17)
N(1)-N(2)-C(3)-C(2)	-0.2(2)
B(1)-N(2)-C(3)-C(2)	-178.34(16)
C(1)-C(2)-C(3)-N(2)	0.4(2)
N(1)-C(1)-C(4)-C(9)	-85.1(2)
C(2)-C(1)-C(4)-C(9)	98.2(2)
N(1)-C(1)-C(4)-C(5)	91.4(2)
C(2)-C(1)-C(4)-C(5)	-85.3(2)
C(9)-C(4)-C(5)-C(6)	4.8(2)
C(1)-C(4)-C(5)-C(6)	-171.80(16)
C(9)-C(4)-C(5)-C(10)	-174.04(17)
C(1)-C(4)-C(5)-C(10)	9.4(2)
C(4)-C(5)-C(6)-C(7)	-1.5(3)
C(10)-C(5)-C(6)-C(7)	177.32(17)
C(5)-C(6)-C(7)-C(8)	-2.6(3)
C(5)-C(6)-C(7)-C(11)	177.02(18)
C(6)-C(7)-C(8)-C(9)	3.6(3)
C(11)-C(7)-C(8)-C(9)	-176.04(18)
C(7)-C(8)-C(9)-C(4)	-0.4(3)
C(7)-C(8)-C(9)-C(12)	178.87(17)
C(5)-C(4)-C(9)-C(8)	-3.8(2)
C(1)-C(4)-C(9)-C(8)	172.67(16)
C(5)-C(4)-C(9)-C(12)	176.88(16)
C(1)-C(4)-C(9)-C(12)	-6.6(2)
N(4)-N(3)-C(13)-C(14)	-0.2(2)
Cu(1)-N(3)-C(13)-C(14)	173.91(16)
N(4)-N(3)-C(13)-C(16)	-179.90(16)
Cu(1)-N(3)-C(13)-C(16)	-5.8(3)
N(3)-C(13)-C(14)-C(15)	-0.1(2)
C(16)-C(13)-C(14)-C(15)	179.55(19)
N(3)-N(4)-C(15)-C(14)	-0.6(2)
B(1)-N(4)-C(15)-C(14)	-175.56(17)
C(13)-C(14)-C(15)-N(4)	0.4(2)

N(3)-C(13)-C(16)-C(17)	119.0(2)
C(14)-C(13)-C(16)-C(17)	-60.7(3)
N(3)-C(13)-C(16)-C(21)	-60.9(2)
C(14)-C(13)-C(16)-C(21)	119.5(2)
C(21)-C(16)-C(17)-C(18)	3.4(3)
C(13)-C(16)-C(17)-C(18)	-176.43(17)
C(21)-C(16)-C(17)-C(22)	-179.21(18)
C(13)-C(16)-C(17)-C(22)	1.0(3)
C(16)-C(17)-C(18)-C(19)	-0.2(3)
C(22)-C(17)-C(18)-C(19)	-177.6(2)
C(17)-C(18)-C(19)-C(20)	-2.5(3)
C(17)-C(18)-C(19)-C(23)	176.1(2)
C(18)-C(19)-C(20)-C(21)	2.0(3)
C(23)-C(19)-C(20)-C(21)	-176.6(2)
C(19)-C(20)-C(21)-C(16)	1.2(3)
C(19)-C(20)-C(21)-C(24)	-178.1(2)
C(17)-C(16)-C(21)-C(20)	-3.9(3)
C(13)-C(16)-C(21)-C(20)	175.92(17)
C(17)-C(16)-C(21)-C(24)	175.40(18)
C(13)-C(16)-C(21)-C(24)	-4.8(3)
N(6)-N(5)-C(25)-C(26)	0.1(2)
Cu(1)-N(5)-C(25)-C(26)	179.44(15)
N(6)-N(5)-C(25)-C(28)	177.70(15)
Cu(1)-N(5)-C(25)-C(28)	-3.0(3)
N(5)-C(25)-C(26)-C(27)	-0.1(2)
C(28)-C(25)-C(26)-C(27)	-177.49(18)
N(5)-N(6)-C(27)-C(26)	0.0(2)
B(1)-N(6)-C(27)-C(26)	171.70(18)
C(25)-C(26)-C(27)-N(6)	0.0(2)
N(5)-C(25)-C(28)-C(29)	74.1(2)
C(26)-C(25)-C(28)-C(29)	-108.8(2)
N(5)-C(25)-C(28)-C(33)	-107.9(2)
C(26)-C(25)-C(28)-C(33)	69.2(3)
C(33)-C(28)-C(29)-C(30)	0.1(3)
C(25)-C(28)-C(29)-C(30)	178.08(18)
C(33)-C(28)-C(29)-C(34)	-179.82(19)
C(25)-C(28)-C(29)-C(34)	-1.9(3)
C(28)-C(29)-C(30)-C(31)	1.5(3)

C(34)-C(29)-C(30)-C(31)	-178.6(2)
C(29)-C(30)-C(31)-C(32)	-1.3(3)
C(29)-C(30)-C(31)-C(35)	178.0(2)
C(30)-C(31)-C(32)-C(33)	-0.4(3)
C(35)-C(31)-C(32)-C(33)	-179.8(2)
C(31)-C(32)-C(33)-C(28)	1.9(3)
C(31)-C(32)-C(33)-C(36)	-178.9(2)
C(29)-C(28)-C(33)-C(32)	-1.8(3)
C(25)-C(28)-C(33)-C(32)	-179.79(17)
C(29)-C(28)-C(33)-C(36)	179.05(19)
C(25)-C(28)-C(33)-C(36)	1.0(3)
N(1)-Cu(1)-C(37)-C(38)	178.55(12)
N(5)-Cu(1)-C(37)-C(38)	63.83(16)
N(3)-Cu(1)-C(37)-C(38)	-73.75(16)
N(1)-Cu(1)-C(38)-C(37)	-2.36(19)
N(5)-Cu(1)-C(38)-C(37)	-135.17(13)
N(3)-Cu(1)-C(38)-C(37)	128.40(13)
C(37)-Cu(1)-C(38)-C(39)	-179.6(2)
N(1)-Cu(1)-C(38)-C(39)	178.07(13)
N(5)-Cu(1)-C(38)-C(39)	45.26(18)
N(3)-Cu(1)-C(38)-C(39)	-51.17(18)
C(37)-C(38)-C(39)-C(40)	-153.6(5)
Cu(1)-C(38)-C(39)-C(40)	25.2(3)
C(37)-C(38)-C(39)-C(44)	24.4(6)
Cu(1)-C(38)-C(39)-C(44)	-156.74(15)
C(44)-C(39)-C(40)-C(41)	-1.4(3)
C(38)-C(39)-C(40)-C(41)	176.62(19)
C(39)-C(40)-C(41)-C(42)	0.6(3)
C(40)-C(41)-C(42)-C(43)	0.4(4)
C(41)-C(42)-C(43)-C(44)	-0.6(4)
C(42)-C(43)-C(44)-C(39)	-0.2(3)
C(40)-C(39)-C(44)-C(43)	1.2(3)
C(38)-C(39)-C(44)-C(43)	-176.90(19)
C(52)-C(47)-C(48)-C(49)	-0.7(4)
C(46)-C(47)-C(48)-C(49)	179.0(2)
C(47)-C(48)-C(49)-C(50)	0.6(4)
C(48)-C(49)-C(50)-C(51)	0.0(4)
C(49)-C(50)-C(51)-C(52)	-0.5(5)

C(50)-C(51)-C(52)-C(47)	0.5(5)
C(48)-C(47)-C(52)-C(51)	0.1(4)
C(46)-C(47)-C(52)-C(51)	-179.6(3)
C(27)-N(6)-B(1)-N(4)	-112.9(2)
N(5)-N(6)-B(1)-N(4)	58.0(2)
C(27)-N(6)-B(1)-N(2)	126.91(19)
N(5)-N(6)-B(1)-N(2)	-62.2(2)
C(15)-N(4)-B(1)-N(6)	113.3(2)
N(3)-N(4)-B(1)-N(6)	-61.2(2)
C(15)-N(4)-B(1)-N(2)	-126.74(19)
N(3)-N(4)-B(1)-N(2)	58.7(2)
C(3)-N(2)-B(1)-N(6)	-122.18(19)
N(1)-N(2)-B(1)-N(6)	59.9(2)
C(3)-N(2)-B(1)-N(4)	118.21(19)
N(1)-N(2)-B(1)-N(4)	-59.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for $Tp^{Ms}Cu$(ethyl propiolate), **3**.

Empirical formula	$C_{165}H_{186}B_4Cl_2Cu_4N_{24}O_8$	
	$[4(C_{41}H_{46}BCuN_6O_2), CH_2Cl_2]$	
Formula weight	3001.68	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.0009(7) Å	α= 97.899(2)°.
	b = 11.2392(9) Å	β= 91.176(2)°.
	c = 38.765(3) Å	γ = 93.499(2)°.
Volume	3875.5(5) $Å^3$	
Z	1	
Density (calculated)	1.286 Mg/m^3	
Absorption coefficient	0.641 mm^{-1}	
F(000)	1578	
Crystal size	0.30 x 0.25 x 0.20 mm^3	
Theta range for data collection	1.59 to 30.72°.	
Index ranges	-12<=h<=12, -16<=k<=16, -55<=l<=55	
Reflections collected	55916	
Independent reflections	23921 [R(int) = 0.0544]	
Completeness to theta = 30.72°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8825 and 0.8309	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23921 / 74 / 1000	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0776, wR2 = 0.1802	
R indices (all data)	R1 = 0.1021, wR2 = 0.1900	
Largest diff. peak and hole	1.059 and -0.935 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cu(1)	1773(1)	6579(1)	1497(1)	20(1)
O(1)	2766(5)	9205(3)	1043(1)	44(1)
N(1)	-340(4)	6942(3)	1411(1)	19(1)
N(2)	-1299(4)	6815(3)	1673(1)	18(1)
N(3)	1219(4)	5127(3)	1725(1)	18(1)
N(4)	-19(4)	5194(3)	1924(1)	18(1)
N(5)	1671(4)	7646(3)	2045(1)	18(1)
N(6)	383(4)	7346(3)	2204(1)	18(1)
C(1)	-1139(5)	7247(4)	1144(1)	20(1)
C(2)	-2626(5)	7310(4)	1236(1)	24(1)
C(3)	-2682(5)	7037(4)	1570(1)	24(1)
C(4)	-462(4)	7426(4)	808(1)	21(1)
C(5)	66(5)	6453(4)	593(1)	26(1)
C(6)	674(6)	6649(4)	276(1)	31(1)
C(7)	723(6)	7772(4)	164(1)	30(1)
C(8)	184(5)	8724(4)	383(1)	28(1)
C(9)	-397(5)	8569(4)	702(1)	24(1)
C(10)	-3(6)	5198(4)	695(1)	33(1)
C(11)	1330(7)	7951(5)	-186(1)	45(1)
C(12)	-898(6)	9642(4)	939(1)	32(1)
C(13)	1685(4)	4021(3)	1722(1)	18(1)
C(14)	735(4)	3361(4)	1917(1)	20(1)
C(15)	-317(5)	4137(4)	2041(1)	20(1)
C(16)	3091(5)	3668(3)	1553(1)	19(1)
C(17)	4457(4)	4115(4)	1717(1)	20(1)
C(18)	5772(5)	3791(4)	1560(1)	24(1)
C(19)	5788(5)	3026(4)	1247(1)	27(1)
C(20)	4416(6)	2583(4)	1091(1)	27(1)
C(21)	3077(5)	2888(4)	1237(1)	24(1)
C(22)	4514(5)	4935(4)	2060(1)	28(1)
C(23)	7230(6)	2674(5)	1087(2)	39(1)
C(24)	1619(5)	2374(4)	1058(1)	32(1)

C(25)	2419(4)	8479(3)	2276(1)	17(1)
C(26)	1615(5)	8731(3)	2580(1)	19(1)
C(27)	333(5)	7981(3)	2522(1)	19(1)
C(28)	3849(5)	9071(3)	2184(1)	18(1)
C(29)	3818(5)	9942(4)	1957(1)	22(1)
C(30)	5153(5)	10533(4)	1880(1)	27(1)
C(31)	6507(5)	10267(4)	2020(1)	28(1)
C(32)	6511(5)	9398(4)	2241(1)	24(1)
C(33)	5208(4)	8791(3)	2329(1)	19(1)
C(34)	2354(5)	10289(4)	1820(1)	28(1)
C(35)	7945(6)	10914(5)	1935(2)	44(1)
C(36)	5282(5)	7887(4)	2581(1)	24(1)
C(37)	3738(5)	6401(4)	1302(1)	28(1)
C(38)	3201(5)	7260(4)	1185(1)	25(1)
C(39)	3306(5)	8256(5)	979(1)	31(1)
O(2A)	4335(11)	8160(9)	746(3)	34(2)
C(40A)	4597(13)	9187(10)	561(3)	39(3)
C(41A)	5627(14)	8715(15)	261(4)	61(4)
O(2B)	3972(12)	7765(9)	666(3)	36(2)
C(40B)	4258(13)	8584(13)	411(3)	45(3)
C(41B)	5728(16)	9290(14)	491(5)	66(4)
B(1)	-753(5)	6400(4)	2013(1)	18(1)
Cu(2)	1734(1)	2062(1)	3708(1)	17(1)
O(3)	1199(4)	5234(3)	3693(1)	25(1)
O(4)	-461(3)	5143(2)	4119(1)	24(1)
N(7)	2064(4)	306(3)	3675(1)	17(1)
N(8)	3313(4)	-57(3)	3508(1)	17(1)
N(9)	2365(4)	2127(3)	3207(1)	17(1)
N(10)	3610(4)	1534(3)	3112(1)	17(1)
N(11)	4054(4)	2537(3)	3868(1)	18(1)
N(12)	5017(4)	1815(3)	3684(1)	16(1)
C(42)	1314(4)	-694(3)	3751(1)	17(1)
C(43)	2090(5)	-1711(3)	3635(1)	20(1)
C(44)	3337(5)	-1258(3)	3481(1)	19(1)
C(45)	-113(4)	-605(3)	3935(1)	16(1)
C(46)	-1462(5)	-935(3)	3752(1)	19(1)
C(47)	-2799(5)	-773(4)	3927(1)	23(1)
C(48)	-2823(5)	-296(4)	4274(1)	25(1)

C(49)	-1471(5)	-2(4)	4453(1)	23(1)
C(50)	-115(5)	-157(3)	4293(1)	19(1)
C(51)	-1499(5)	-1472(4)	3372(1)	28(1)
C(52)	-4273(6)	-139(5)	4451(2)	41(1)
C(53)	1346(5)	159(4)	4494(1)	28(1)
C(54)	1922(4)	2619(3)	2929(1)	18(1)
C(55)	2901(5)	2356(4)	2655(1)	22(1)
C(56)	3930(4)	1662(3)	2780(1)	18(1)
C(57)	533(4)	3266(3)	2938(1)	17(1)
C(58)	567(5)	4511(4)	2921(1)	19(1)
C(59)	-761(5)	5080(4)	2935(1)	23(1)
C(60)	-2124(5)	4461(4)	2963(1)	22(1)
C(61)	-2147(5)	3233(4)	2977(1)	23(1)
C(62)	-846(4)	2619(4)	2962(1)	20(1)
C(63)	2007(5)	5249(4)	2890(1)	25(1)
C(64)	-3555(5)	5100(4)	2982(1)	31(1)
C(65)	-932(5)	1281(4)	2977(1)	27(1)
C(66)	4894(5)	3365(3)	4079(1)	19(1)
C(67)	6403(4)	3184(4)	4033(1)	22(1)
C(68)	6429(4)	2197(3)	3781(1)	19(1)
C(69)	4194(4)	4341(3)	4307(1)	19(1)
C(70)	3636(5)	4159(4)	4628(1)	24(1)
C(71)	2975(6)	5097(4)	4834(1)	28(1)
C(72)	2872(6)	6208(4)	4724(1)	33(1)
C(73)	3479(6)	6391(4)	4405(1)	30(1)
C(74)	4135(5)	5478(4)	4194(1)	23(1)
C(75)	3713(6)	2964(4)	4763(1)	32(1)
C(76)	2174(8)	7218(5)	4952(2)	48(2)
C(77)	4732(6)	5701(4)	3849(1)	33(1)
C(78)	132(5)	2482(4)	4027(1)	25(1)
C(79)	544(4)	3382(4)	3907(1)	19(1)
C(80)	504(5)	4677(4)	3885(1)	20(1)
C(81)	-664(6)	6418(4)	4127(1)	29(1)
C(82)	-1694(6)	6734(4)	4424(1)	33(1)
B(2)	4436(5)	873(4)	3377(1)	16(1)
Cl(1)	5835(3)	4636(3)	441(1)	58(1)
Cl(2)	2973(4)	3414(4)	199(1)	64(1)
C(83)	3990(15)	4601(11)	446(3)	52(3)

Table 3. Bond lengths [Å] and angles [°] for $Tp^{Ms}Cu$(ethyl propiolate), **3**.

Cu(1)-C(37)	1.950(4)	C(10)-H(10C)	0.9800
Cu(1)-C(38)	1.975(4)	C(11)-H(11A)	0.9800
Cu(1)-N(1)	2.000(3)	C(11)-H(11B)	0.9800
Cu(1)-N(3)	2.003(3)	C(11)-H(11C)	0.9800
Cu(1)-N(5)	2.296(3)	C(12)-H(12A)	0.9800
O(1)-C(39)	1.197(6)	C(12)-H(12B)	0.9800
N(1)-C(1)	1.342(5)	C(12)-H(12C)	0.9800
N(1)-N(2)	1.363(5)	C(13)-C(14)	1.399(6)
N(2)-C(3)	1.347(5)	C(13)-C(16)	1.486(6)
N(2)-B(1)	1.539(6)	C(14)-C(15)	1.377(6)
N(3)-C(13)	1.334(5)	C(14)-H(14)	0.9500
N(3)-N(4)	1.367(5)	C(15)-H(15)	0.9500
N(4)-C(15)	1.343(5)	C(16)-C(21)	1.404(6)
N(4)-B(1)	1.543(6)	C(16)-C(17)	1.404(5)
N(5)-C(25)	1.341(5)	C(17)-C(18)	1.387(6)
N(5)-N(6)	1.371(5)	C(17)-C(22)	1.509(6)
N(6)-C(27)	1.339(5)	C(18)-C(19)	1.388(6)
N(6)-B(1)	1.531(5)	C(18)-H(18)	0.9500
C(1)-C(2)	1.396(6)	C(19)-C(20)	1.397(7)
C(1)-C(4)	1.482(6)	C(19)-C(23)	1.501(7)
C(2)-C(3)	1.371(6)	C(20)-C(21)	1.385(7)
C(2)-H(2)	0.9500	C(20)-H(20)	0.9500
C(3)-H(3)	0.9500	C(21)-C(24)	1.516(6)
C(4)-C(5)	1.396(6)	C(22)-H(22A)	0.9800
C(4)-C(9)	1.401(6)	C(22)-H(22B)	0.9800
C(5)-C(6)	1.393(7)	C(22)-H(22C)	0.9800
C(5)-C(10)	1.514(7)	C(23)-H(23A)	0.9800
C(6)-C(7)	1.389(7)	C(23)-H(23B)	0.9800
C(6)-H(6)	0.9500	C(23)-H(23C)	0.9800
C(7)-C(8)	1.390(7)	C(24)-H(24A)	0.9800
C(7)-C(11)	1.507(7)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.379(6)	C(24)-H(24C)	0.9800
C(8)-H(8)	0.9500	C(25)-C(26)	1.402(6)
C(9)-C(12)	1.512(6)	C(25)-C(28)	1.485(6)
C(10)-H(10A)	0.9800	C(26)-C(27)	1.383(6)
C(10)-H(10B)	0.9800	C(26)-H(26)	0.9500

C(27)-H(27)	0.9500	C(41B)-H(41E)	0.9800
C(28)-C(29)	1.403(6)	C(41B)-H(41F)	0.9800
C(28)-C(33)	1.406(6)	B(1)-H(1)	1.0000
C(29)-C(30)	1.395(6)	Cu(2)-C(78)	1.956(4)
C(29)-C(34)	1.504(6)	Cu(2)-C(79)	1.964(4)
C(30)-C(31)	1.389(7)	Cu(2)-N(7)	2.000(3)
C(30)-H(30)	0.9500	Cu(2)-N(9)	2.044(3)
C(31)-C(32)	1.388(7)	Cu(2)-N(11)	2.179(3)
C(31)-C(35)	1.510(6)	O(3)-C(80)	1.197(5)
C(32)-C(33)	1.392(6)	O(4)-C(80)	1.344(5)
C(32)-H(32)	0.9500	O(4)-C(81)	1.451(5)
C(33)-C(36)	1.509(6)	N(7)-C(42)	1.346(5)
C(34)-H(34A)	0.9800	N(7)-N(8)	1.364(5)
C(34)-H(34B)	0.9800	N(8)-C(44)	1.340(5)
C(34)-H(34C)	0.9800	N(8)-B(2)	1.554(5)
C(35)-H(35A)	0.9800	N(9)-C(54)	1.341(5)
C(35)-H(35B)	0.9800	N(9)-N(10)	1.370(5)
C(35)-H(35C)	0.9800	N(10)-C(56)	1.347(5)
C(36)-H(36A)	0.9800	N(10)-B(2)	1.551(6)
C(36)-H(36B)	0.9800	N(11)-C(66)	1.336(5)
C(36)-H(36C)	0.9800	N(11)-N(12)	1.366(5)
C(37)-C(38)	1.240(7)	N(12)-C(68)	1.345(5)
C(37)-H(37)	0.95(4)	N(12)-B(2)	1.542(5)
C(38)-C(39)	1.461(7)	C(42)-C(43)	1.403(5)
C(39)-O(2A)	1.306(11)	C(42)-C(45)	1.484(6)
C(39)-O(2B)	1.422(11)	C(43)-C(44)	1.383(6)
O(2A)-C(40A)	1.451(12)	C(43)-H(43)	0.9500
C(40A)-C(41A)	1.558(14)	C(44)-H(44)	0.9500
C(40A)-H(40A)	0.9900	C(45)-C(46)	1.398(5)
C(40A)-H(40B)	0.9900	C(45)-C(50)	1.408(5)
C(41A)-H(41A)	0.9800	C(46)-C(47)	1.401(6)
C(41A)-H(41B)	0.9800	C(46)-C(51)	1.514(6)
C(41A)-H(41C)	0.9800	C(47)-C(48)	1.379(6)
O(2B)-C(40B)	1.458(12)	C(47)-H(47)	0.9500
C(40B)-C(41B)	1.505(13)	C(48)-C(49)	1.389(6)
C(40B)-H(40C)	0.9900	C(48)-C(52)	1.497(7)
C(40B)-H(40D)	0.9900	C(49)-C(50)	1.391(6)
C(41B)-H(41D)	0.9800	C(49)-H(49)	0.9500

C(50)-C(53)	1.513(6)	C(67)-H(67)	0.9500
C(51)-H(51A)	0.9800	C(68)-H(68)	0.9500
C(51)-H(51B)	0.9800	C(69)-C(70)	1.386(6)
C(51)-H(51C)	0.9800	C(69)-C(74)	1.411(6)
C(52)-H(52A)	0.9800	C(70)-C(71)	1.403(6)
C(52)-H(52B)	0.9800	C(70)-C(75)	1.512(6)
C(52)-H(52C)	0.9800	C(71)-C(72)	1.383(7)
C(53)-H(53A)	0.9800	C(71)-H(71)	0.9500
C(53)-H(53B)	0.9800	C(72)-C(73)	1.397(7)
C(53)-H(53C)	0.9800	C(72)-C(76)	1.517(6)
C(54)-C(55)	1.407(6)	C(73)-C(74)	1.389(6)
C(54)-C(57)	1.483(6)	C(73)-H(73)	0.9500
C(55)-C(56)	1.370(6)	C(74)-C(77)	1.498(7)
C(55)-H(55)	0.9500	C(75)-H(75A)	0.9800
C(56)-H(56)	0.9500	C(75)-H(75B)	0.9800
C(57)-C(58)	1.408(6)	C(75)-H(75C)	0.9800
C(57)-C(62)	1.411(6)	C(76)-H(76A)	0.9800
C(58)-C(59)	1.389(6)	C(76)-H(76B)	0.9800
C(58)-C(63)	1.511(6)	C(76)-H(76C)	0.9800
C(59)-C(60)	1.387(6)	C(77)-H(77A)	0.9800
C(59)-H(59)	0.9500	C(77)-H(77B)	0.9800
C(60)-C(61)	1.387(6)	C(77)-H(77C)	0.9800
C(60)-C(64)	1.511(6)	C(78)-C(79)	1.212(6)
C(61)-C(62)	1.394(6)	C(78)-H(78)	0.96(4)
C(61)-H(61)	0.9500	C(79)-C(80)	1.473(6)
C(62)-C(65)	1.510(6)	C(81)-C(82)	1.513(7)
C(63)-H(63A)	0.9800	C(81)-H(81A)	0.9900
C(63)-H(63B)	0.9800	C(81)-H(81B)	0.9900
C(63)-H(63C)	0.9800	C(82)-H(82A)	0.9800
C(64)-H(64A)	0.9800	C(82)-H(82B)	0.9800
C(64)-H(64B)	0.9800	C(82)-H(82C)	0.9800
C(64)-H(64C)	0.9800	B(2)-H(2A)	1.0000
C(65)-H(65A)	0.9800	Cl(1)-C(83)	1.659(14)
C(65)-H(65B)	0.9800	Cl(2)-C(83)	1.732(13)
C(65)-H(65C)	0.9800	C(83)-H(83A)	0.9900
C(66)-C(67)	1.396(6)	C(83)-H(83B)	0.9900
C(66)-C(69)	1.492(6)		
C(67)-C(68)	1.378(5)	C(37)-Cu(1)-C(38)	36.84(19)

C(37)-Cu(1)-N(1)	146.29(18)	C(9)-C(4)-C(1)	119.8(4)
C(38)-Cu(1)-N(1)	114.01(17)	C(6)-C(5)-C(4)	118.8(4)
C(37)-Cu(1)-N(3)	108.51(17)	C(6)-C(5)-C(10)	119.5(4)
C(38)-Cu(1)-N(3)	144.21(17)	C(4)-C(5)-C(10)	121.7(4)
N(1)-Cu(1)-N(3)	94.07(14)	C(7)-C(6)-C(5)	122.0(5)
C(37)-Cu(1)-N(5)	117.05(17)	C(7)-C(6)-H(6)	119.0
C(38)-Cu(1)-N(5)	115.32(15)	C(5)-C(6)-H(6)	119.0
N(1)-Cu(1)-N(5)	88.62(13)	C(6)-C(7)-C(8)	118.0(4)
N(3)-Cu(1)-N(5)	85.67(13)	C(6)-C(7)-C(11)	121.0(5)
C(1)-N(1)-N(2)	107.1(3)	C(8)-C(7)-C(11)	121.0(4)
C(1)-N(1)-Cu(1)	136.3(3)	C(9)-C(8)-C(7)	121.7(4)
N(2)-N(1)-Cu(1)	116.5(3)	C(9)-C(8)-H(8)	119.2
C(3)-N(2)-N(1)	109.4(3)	C(7)-C(8)-H(8)	119.2
C(3)-N(2)-B(1)	129.9(4)	C(8)-C(9)-C(4)	119.6(4)
N(1)-N(2)-B(1)	120.5(3)	C(8)-C(9)-C(12)	119.8(4)
C(13)-N(3)-N(4)	107.1(3)	C(4)-C(9)-C(12)	120.5(4)
C(13)-N(3)-Cu(1)	136.9(3)	C(5)-C(10)-H(10A)	109.5
N(4)-N(3)-Cu(1)	115.9(2)	C(5)-C(10)-H(10B)	109.5
C(15)-N(4)-N(3)	109.6(3)	H(10A)-C(10)-H(10B)	109.5
C(15)-N(4)-B(1)	129.6(4)	C(5)-C(10)-H(10C)	109.5
N(3)-N(4)-B(1)	120.5(3)	H(10A)-C(10)-H(10C)	109.5
C(25)-N(5)-N(6)	105.4(3)	H(10B)-C(10)-H(10C)	109.5
C(25)-N(5)-Cu(1)	143.3(3)	C(7)-C(11)-H(11A)	109.5
N(6)-N(5)-Cu(1)	111.3(2)	C(7)-C(11)-H(11B)	109.5
C(27)-N(6)-N(5)	110.7(3)	H(11A)-C(11)-H(11B)	109.5
C(27)-N(6)-B(1)	129.5(3)	C(7)-C(11)-H(11C)	109.5
N(5)-N(6)-B(1)	119.7(3)	H(11A)-C(11)-H(11C)	109.5
N(1)-C(1)-C(2)	109.3(4)	H(11B)-C(11)-H(11C)	109.5
N(1)-C(1)-C(4)	122.1(4)	C(9)-C(12)-H(12A)	109.5
C(2)-C(1)-C(4)	128.6(4)	C(9)-C(12)-H(12B)	109.5
C(3)-C(2)-C(1)	105.8(4)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-H(2)	127.1	C(9)-C(12)-H(12C)	109.5
C(1)-C(2)-H(2)	127.1	H(12A)-C(12)-H(12C)	109.5
N(2)-C(3)-C(2)	108.4(4)	H(12B)-C(12)-H(12C)	109.5
N(2)-C(3)-H(3)	125.8	N(3)-C(13)-C(14)	109.6(3)
C(2)-C(3)-H(3)	125.8	N(3)-C(13)-C(16)	121.5(4)
C(5)-C(4)-C(9)	119.9(4)	C(14)-C(13)-C(16)	128.7(4)
C(5)-C(4)-C(1)	120.3(4)	C(15)-C(14)-C(13)	105.4(4)

C(15)-C(14)-H(14)	127.3	C(21)-C(24)-H(24C)	109.5
C(13)-C(14)-H(14)	127.3	H(24A)-C(24)-H(24C)	109.5
N(4)-C(15)-C(14)	108.3(4)	H(24B)-C(24)-H(24C)	109.5
N(4)-C(15)-H(15)	125.8	N(5)-C(25)-C(26)	111.0(4)
C(14)-C(15)-H(15)	125.8	N(5)-C(25)-C(28)	120.6(3)
C(21)-C(16)-C(17)	119.6(4)	C(26)-C(25)-C(28)	128.2(3)
C(21)-C(16)-C(13)	121.4(4)	C(27)-C(26)-C(25)	104.4(3)
C(17)-C(16)-C(13)	119.1(4)	C(27)-C(26)-H(26)	127.8
C(18)-C(17)-C(16)	119.3(4)	C(25)-C(26)-H(26)	127.8
C(18)-C(17)-C(22)	119.6(4)	N(6)-C(27)-C(26)	108.5(4)
C(16)-C(17)-C(22)	121.0(4)	N(6)-C(27)-H(27)	125.8
C(17)-C(18)-C(19)	122.2(4)	C(26)-C(27)-H(27)	125.8
C(17)-C(18)-H(18)	118.9	C(29)-C(28)-C(33)	120.4(4)
C(19)-C(18)-H(18)	118.9	C(29)-C(28)-C(25)	118.8(4)
C(18)-C(19)-C(20)	117.5(4)	C(33)-C(28)-C(25)	120.7(4)
C(18)-C(19)-C(23)	121.0(4)	C(30)-C(29)-C(28)	119.1(4)
C(20)-C(19)-C(23)	121.5(5)	C(30)-C(29)-C(34)	120.6(4)
C(21)-C(20)-C(19)	122.2(4)	C(28)-C(29)-C(34)	120.2(4)
C(21)-C(20)-H(20)	118.9	C(31)-C(30)-C(29)	121.3(4)
C(19)-C(20)-H(20)	118.9	C(31)-C(30)-H(30)	119.3
C(20)-C(21)-C(16)	119.2(4)	C(29)-C(30)-H(30)	119.3
C(20)-C(21)-C(24)	120.0(4)	C(32)-C(31)-C(30)	118.6(4)
C(16)-C(21)-C(24)	120.8(4)	C(32)-C(31)-C(35)	120.5(5)
C(17)-C(22)-H(22A)	109.5	C(30)-C(31)-C(35)	121.0(5)
C(17)-C(22)-H(22B)	109.5	C(31)-C(32)-C(33)	122.2(4)
H(22A)-C(22)-H(22B)	109.5	C(31)-C(32)-H(32)	118.9
C(17)-C(22)-H(22C)	109.5	C(33)-C(32)-H(32)	118.9
H(22A)-C(22)-H(22C)	109.5	C(32)-C(33)-C(28)	118.4(4)
H(22B)-C(22)-H(22C)	109.5	C(32)-C(33)-C(36)	119.6(4)
C(19)-C(23)-H(23A)	109.5	C(28)-C(33)-C(36)	122.0(4)
C(19)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34A)	109.5
H(23A)-C(23)-H(23B)	109.5	C(29)-C(34)-H(34B)	109.5
C(19)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(23A)-C(23)-H(23C)	109.5	C(29)-C(34)-H(34C)	109.5
H(23B)-C(23)-H(23C)	109.5	H(34A)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24A)	109.5	H(34B)-C(34)-H(34C)	109.5
C(21)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35A)	109.5
H(24A)-C(24)-H(24B)	109.5	C(31)-C(35)-H(35B)	109.5

H(35A)-C(35)-H(35B)	109.5	C(40B)-C(41B)-H(41F)	109.5
C(31)-C(35)-H(35C)	109.5	H(41D)-C(41B)-H(41F)	109.5
H(35A)-C(35)-H(35C)	109.5	H(41E)-C(41B)-H(41F)	109.5
H(35B)-C(35)-H(35C)	109.5	N(6)-B(1)-N(2)	109.8(3)
C(33)-C(36)-H(36A)	109.5	N(6)-B(1)-N(4)	109.7(3)
C(33)-C(36)-H(36B)	109.5	N(2)-B(1)-N(4)	108.9(3)
H(36A)-C(36)-H(36B)	109.5	N(6)-B(1)-H(1)	109.5
C(33)-C(36)-H(36C)	109.5	N(2)-B(1)-H(1)	109.5
H(36A)-C(36)-H(36C)	109.5	N(4)-B(1)-H(1)	109.5
H(36B)-C(36)-H(36C)	109.5	C(78)-Cu(2)-C(79)	36.02(18)
C(38)-C(37)-Cu(1)	72.7(3)	C(78)-Cu(2)-N(7)	110.51(17)
C(38)-C(37)-H(37)	153(3)	C(79)-Cu(2)-N(7)	146.47(16)
Cu(1)-C(37)-H(37)	134(3)	C(78)-Cu(2)-N(9)	142.06(17)
C(37)-C(38)-C(39)	151.4(5)	C(79)-Cu(2)-N(9)	115.16(16)
C(37)-C(38)-Cu(1)	70.5(3)	N(7)-Cu(2)-N(9)	92.35(13)
C(39)-C(38)-Cu(1)	138.0(3)	C(78)-Cu(2)-N(11)	120.66(17)
O(1)-C(39)-O(2A)	117.8(6)	C(79)-Cu(2)-N(11)	108.00(14)
O(1)-C(39)-O(2B)	128.2(6)	N(7)-Cu(2)-N(11)	91.24(13)
O(1)-C(39)-C(38)	126.9(5)	N(9)-Cu(2)-N(11)	87.30(13)
O(2A)-C(39)-C(38)	113.8(6)	C(80)-O(4)-C(81)	115.6(3)
O(2B)-C(39)-C(38)	104.2(6)	C(42)-N(7)-N(8)	106.8(3)
C(39)-O(2A)-C(40A)	116.0(10)	C(42)-N(7)-Cu(2)	137.1(3)
O(2A)-C(40A)-C(41A)	103.7(10)	N(8)-N(7)-Cu(2)	115.9(2)
O(2A)-C(40A)-H(40A)	111.0	C(44)-N(8)-N(7)	109.6(3)
C(41A)-C(40A)-H(40A)	111.0	C(44)-N(8)-B(2)	129.7(3)
O(2A)-C(40A)-H(40B)	111.0	N(7)-N(8)-B(2)	120.7(3)
C(41A)-C(40A)-H(40B)	111.0	C(54)-N(9)-N(10)	106.4(3)
H(40A)-C(40A)-H(40B)	109.0	C(54)-N(9)-Cu(2)	138.2(3)
C(39)-O(2B)-C(40B)	116.3(10)	N(10)-N(9)-Cu(2)	115.4(3)
O(2B)-C(40B)-C(41B)	110.5(9)	C(56)-N(10)-N(9)	109.8(3)
O(2B)-C(40B)-H(40C)	109.5	C(56)-N(10)-B(2)	130.0(3)
C(41B)-C(40B)-H(40C)	109.5	N(9)-N(10)-B(2)	120.1(3)
O(2B)-C(40B)-H(40D)	109.5	C(66)-N(11)-N(12)	106.4(3)
C(41B)-C(40B)-H(40D)	109.5	C(66)-N(11)-Cu(2)	140.7(3)
H(40C)-C(40B)-H(40D)	108.1	N(12)-N(11)-Cu(2)	112.8(2)
C(40B)-C(41B)-H(41D)	109.5	C(68)-N(12)-N(11)	109.9(3)
C(40B)-C(41B)-H(41E)	109.5	C(68)-N(12)-B(2)	129.1(3)
H(41D)-C(41B)-H(41E)	109.5	N(11)-N(12)-B(2)	120.3(3)

N(7)-C(42)-C(43)	110.0(4)	H(52B)-C(52)-H(52C)	109.5
N(7)-C(42)-C(45)	120.2(3)	C(50)-C(53)-H(53A)	109.5
C(43)-C(42)-C(45)	129.7(3)	C(50)-C(53)-H(53B)	109.5
C(44)-C(43)-C(42)	104.4(3)	H(53A)-C(53)-H(53B)	109.5
C(44)-C(43)-H(43)	127.8	C(50)-C(53)-H(53C)	109.5
C(42)-C(43)-H(43)	127.8	H(53A)-C(53)-H(53C)	109.5
N(8)-C(44)-C(43)	109.2(3)	H(53B)-C(53)-H(53C)	109.5
N(8)-C(44)-H(44)	125.4	N(9)-C(54)-C(55)	109.9(4)
C(43)-C(44)-H(44)	125.4	N(9)-C(54)-C(57)	120.3(4)
C(46)-C(45)-C(50)	119.7(4)	C(55)-C(54)-C(57)	129.7(4)
C(46)-C(45)-C(42)	120.1(4)	C(56)-C(55)-C(54)	105.1(4)
C(50)-C(45)-C(42)	120.2(3)	C(56)-C(55)-H(55)	127.4
C(45)-C(46)-C(47)	119.1(4)	C(54)-C(55)-H(55)	127.4
C(45)-C(46)-C(51)	121.1(4)	N(10)-C(56)-C(55)	108.7(4)
C(47)-C(46)-C(51)	119.8(4)	N(10)-C(56)-H(56)	125.7
C(48)-C(47)-C(46)	121.9(4)	C(55)-C(56)-H(56)	125.7
C(48)-C(47)-H(47)	119.0	C(58)-C(57)-C(62)	119.6(4)
C(46)-C(47)-H(47)	119.0	C(58)-C(57)-C(54)	121.2(4)
C(47)-C(48)-C(49)	118.2(4)	C(62)-C(57)-C(54)	119.2(4)
C(47)-C(48)-C(52)	120.4(4)	C(59)-C(58)-C(57)	119.1(4)
C(49)-C(48)-C(52)	121.4(4)	C(59)-C(58)-C(63)	118.9(4)
C(48)-C(49)-C(50)	122.0(4)	C(57)-C(58)-C(63)	122.0(4)
C(48)-C(49)-H(49)	119.0	C(60)-C(59)-C(58)	122.1(4)
C(50)-C(49)-H(49)	119.0	C(60)-C(59)-H(59)	118.9
C(49)-C(50)-C(45)	119.0(4)	C(58)-C(59)-H(59)	118.9
C(49)-C(50)-C(53)	121.2(4)	C(59)-C(60)-C(61)	118.4(4)
C(45)-C(50)-C(53)	119.8(4)	C(59)-C(60)-C(64)	121.2(4)
C(46)-C(51)-H(51A)	109.5	C(61)-C(60)-C(64)	120.3(4)
C(46)-C(51)-H(51B)	109.5	C(60)-C(61)-C(62)	121.7(4)
H(51A)-C(51)-H(51B)	109.5	C(60)-C(61)-H(61)	119.1
C(46)-C(51)-H(51C)	109.5	C(62)-C(61)-H(61)	119.1
H(51A)-C(51)-H(51C)	109.5	C(61)-C(62)-C(57)	119.1(4)
H(51B)-C(51)-H(51C)	109.5	C(61)-C(62)-C(65)	119.6(4)
C(48)-C(52)-H(52A)	109.5	C(57)-C(62)-C(65)	121.3(4)
C(48)-C(52)-H(52B)	109.5	C(58)-C(63)-H(63A)	109.5
H(52A)-C(52)-H(52B)	109.5	C(58)-C(63)-H(63B)	109.5
C(48)-C(52)-H(52C)	109.5	H(63A)-C(63)-H(63B)	109.5
H(52A)-C(52)-H(52C)	109.5	C(58)-C(63)-H(63C)	109.5

H(63A)-C(63)-H(63C)	109.5	C(73)-C(74)-C(69)	118.9(4)
H(63B)-C(63)-H(63C)	109.5	C(73)-C(74)-C(77)	120.0(4)
C(60)-C(64)-H(64A)	109.5	C(69)-C(74)-C(77)	121.1(4)
C(60)-C(64)-H(64B)	109.5	C(70)-C(75)-H(75A)	109.5
H(64A)-C(64)-H(64B)	109.5	C(70)-C(75)-H(75B)	109.5
C(60)-C(64)-H(64C)	109.5	H(75A)-C(75)-H(75B)	109.5
H(64A)-C(64)-H(64C)	109.5	C(70)-C(75)-H(75C)	109.5
H(64B)-C(64)-H(64C)	109.5	H(75A)-C(75)-H(75C)	109.5
C(62)-C(65)-H(65A)	109.5	H(75B)-C(75)-H(75C)	109.5
C(62)-C(65)-H(65B)	109.5	C(72)-C(76)-H(76A)	109.5
H(65A)-C(65)-H(65B)	109.5	C(72)-C(76)-H(76B)	109.5
C(62)-C(65)-H(65C)	109.5	H(76A)-C(76)-H(76B)	109.5
H(65A)-C(65)-H(65C)	109.5	C(72)-C(76)-H(76C)	109.5
H(65B)-C(65)-H(65C)	109.5	H(76A)-C(76)-H(76C)	109.5
N(11)-C(66)-C(67)	110.5(3)	H(76B)-C(76)-H(76C)	109.5
N(11)-C(66)-C(69)	120.6(4)	C(74)-C(77)-H(77A)	109.5
C(67)-C(66)-C(69)	128.9(3)	C(74)-C(77)-H(77B)	109.5
C(68)-C(67)-C(66)	104.9(3)	H(77A)-C(77)-H(77B)	109.5
C(68)-C(67)-H(67)	127.6	C(74)-C(77)-H(77C)	109.5
C(66)-C(67)-H(67)	127.6	H(77A)-C(77)-H(77C)	109.5
N(12)-C(68)-C(67)	108.4(4)	H(77B)-C(77)-H(77C)	109.5
N(12)-C(68)-H(68)	125.8	C(79)-C(78)-Cu(2)	72.3(3)
C(67)-C(68)-H(68)	125.8	C(79)-C(78)-H(78)	166(3)
C(70)-C(69)-C(74)	119.9(4)	Cu(2)-C(78)-H(78)	121(3)
C(70)-C(69)-C(66)	121.6(4)	C(78)-C(79)-C(80)	151.9(4)
C(74)-C(69)-C(66)	118.5(4)	C(78)-C(79)-Cu(2)	71.6(3)
C(69)-C(70)-C(71)	119.8(4)	C(80)-C(79)-Cu(2)	136.3(3)
C(69)-C(70)-C(75)	121.6(4)	O(3)-C(80)-O(4)	125.1(4)
C(71)-C(70)-C(75)	118.6(4)	O(3)-C(80)-C(79)	126.8(4)
C(72)-C(71)-C(70)	121.1(5)	O(4)-C(80)-C(79)	108.2(4)
C(72)-C(71)-H(71)	119.4	O(4)-C(81)-C(82)	105.2(4)
C(70)-C(71)-H(71)	119.4	O(4)-C(81)-H(81A)	110.7
C(71)-C(72)-C(73)	118.5(4)	C(82)-C(81)-H(81A)	110.7
C(71)-C(72)-C(76)	120.4(5)	O(4)-C(81)-H(81B)	110.7
C(73)-C(72)-C(76)	121.1(5)	C(82)-C(81)-H(81B)	110.7
C(74)-C(73)-C(72)	121.8(4)	H(81A)-C(81)-H(81B)	108.8
C(74)-C(73)-H(73)	119.1	C(81)-C(82)-H(82A)	109.5
C(72)-C(73)-H(73)	119.1	C(81)-C(82)-H(82B)	109.5

H(82A)-C(82)-H(82B)	109.5
C(81)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
N(12)-B(2)-N(10)	108.2(3)
N(12)-B(2)-N(8)	109.8(3)
N(10)-B(2)-N(8)	108.5(3)
N(12)-B(2)-H(2A)	110.1
N(10)-B(2)-H(2A)	110.1
N(8)-B(2)-H(2A)	110.1
Cl(1)-C(83)-Cl(2)	118.7(7)
Cl(1)-C(83)-H(83A)	107.6
Cl(2)-C(83)-H(83A)	107.6
Cl(1)-C(83)-H(83B)	107.6
Cl(2)-C(83)-H(83B)	107.6
H(83A)-C(83)-H(83B)	107.1

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Tp^{Ms}Cu$(ethyl propiolate), **3**. 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}
Cu(1)	14(1)	21(1)	26(1)	7(1)	4(1)	2(1)
O(1)	44(2)	27(2)	62(3)	16(2)	-10(2)	2(2)
N(1)	14(2)	20(2)	21(2)	3(1)	1(1)	1(1)
N(2)	11(2)	21(2)	22(2)	5(1)	0(1)	2(1)
N(3)	14(2)	16(2)	24(2)	6(1)	2(1)	4(1)
N(4)	12(2)	20(2)	21(2)	3(1)	2(1)	-1(1)
N(5)	14(2)	19(2)	21(2)	2(1)	1(1)	1(1)
N(6)	14(2)	18(2)	20(2)	1(1)	2(1)	2(1)
C(1)	15(2)	20(2)	25(2)	3(2)	1(2)	1(2)
C(2)	14(2)	30(2)	30(2)	11(2)	-1(2)	1(2)
C(3)	14(2)	25(2)	34(2)	7(2)	-1(2)	3(2)
C(4)	14(2)	28(2)	22(2)	9(2)	-3(2)	-1(2)
C(5)	25(2)	29(2)	23(2)	6(2)	-3(2)	0(2)
C(6)	34(3)	34(2)	25(2)	5(2)	3(2)	6(2)
C(7)	30(2)	37(3)	23(2)	10(2)	0(2)	3(2)
C(8)	27(2)	25(2)	33(2)	11(2)	0(2)	1(2)
C(9)	21(2)	26(2)	27(2)	7(2)	-2(2)	1(2)
C(10)	42(3)	24(2)	33(3)	4(2)	3(2)	4(2)
C(11)	60(4)	44(3)	34(3)	16(2)	15(3)	10(3)
C(12)	41(3)	24(2)	34(3)	10(2)	6(2)	5(2)
C(13)	12(2)	18(2)	23(2)	2(1)	-1(2)	1(1)
C(14)	15(2)	15(2)	31(2)	5(2)	0(2)	2(2)
C(15)	16(2)	21(2)	24(2)	6(2)	1(2)	-4(2)
C(16)	17(2)	15(2)	26(2)	5(1)	2(2)	5(2)
C(17)	14(2)	20(2)	26(2)	6(2)	0(2)	2(2)
C(18)	15(2)	26(2)	34(2)	11(2)	3(2)	7(2)
C(19)	26(2)	26(2)	33(2)	11(2)	7(2)	8(2)
C(20)	33(2)	20(2)	31(2)	2(2)	8(2)	12(2)
C(21)	21(2)	20(2)	31(2)	5(2)	-2(2)	2(2)
C(22)	17(2)	34(2)	32(2)	0(2)	-1(2)	1(2)
C(23)	33(3)	44(3)	44(3)	10(2)	15(2)	20(2)
C(24)	27(2)	29(2)	36(3)	-1(2)	-5(2)	1(2)

C(25)	14(2)	13(2)	24(2)	4(1)	-1(2)	1(1)
C(26)	20(2)	16(2)	21(2)	3(1)	0(2)	3(2)
C(27)	16(2)	20(2)	22(2)	4(1)	4(2)	6(2)
C(28)	19(2)	16(2)	19(2)	0(1)	1(2)	4(2)
C(29)	24(2)	17(2)	23(2)	2(2)	-2(2)	-1(2)
C(30)	30(2)	25(2)	28(2)	8(2)	3(2)	-2(2)
C(31)	22(2)	30(2)	30(2)	3(2)	3(2)	-8(2)
C(32)	18(2)	26(2)	29(2)	1(2)	0(2)	0(2)
C(33)	15(2)	17(2)	23(2)	-1(1)	-1(2)	3(2)
C(34)	30(2)	23(2)	33(2)	10(2)	-8(2)	4(2)
C(35)	30(3)	53(3)	48(3)	13(3)	4(2)	-18(2)
C(36)	21(2)	23(2)	30(2)	6(2)	-1(2)	5(2)
C(37)	12(2)	32(2)	43(3)	13(2)	5(2)	1(2)
C(38)	15(2)	30(2)	29(2)	6(2)	3(2)	0(2)
C(39)	16(2)	39(3)	43(3)	19(2)	1(2)	-2(2)
O(2A)	16(5)	43(6)	47(5)	26(4)	4(4)	-3(4)
C(40A)	26(5)	43(6)	53(7)	31(5)	-7(5)	-15(5)
C(41A)	27(6)	109(13)	55(8)	46(7)	-4(5)	-7(7)
O(2B)	18(5)	51(6)	45(6)	32(4)	2(4)	-5(4)
C(40B)	27(5)	74(9)	44(7)	41(6)	1(5)	5(5)
C(41B)	46(8)	74(10)	87(11)	58(8)	-22(8)	-27(7)
B(1)	15(2)	19(2)	20(2)	4(2)	1(2)	0(2)
Cu(2)	15(1)	12(1)	25(1)	3(1)	5(1)	4(1)
O(3)	26(2)	16(1)	32(2)	4(1)	8(1)	1(1)
O(4)	25(2)	12(1)	37(2)	5(1)	14(1)	7(1)
N(7)	14(2)	16(2)	22(2)	2(1)	4(1)	4(1)
N(8)	14(2)	16(2)	22(2)	2(1)	3(1)	5(1)
N(9)	13(2)	16(2)	23(2)	3(1)	0(1)	5(1)
N(10)	12(2)	14(2)	24(2)	2(1)	2(1)	3(1)
N(11)	16(2)	15(2)	23(2)	-1(1)	0(1)	2(1)
N(12)	10(1)	16(2)	23(2)	1(1)	1(1)	4(1)
C(42)	18(2)	13(2)	20(2)	5(1)	1(2)	2(1)
C(43)	21(2)	10(2)	30(2)	4(1)	4(2)	3(2)
C(44)	18(2)	14(2)	26(2)	4(1)	0(2)	8(2)
C(45)	18(2)	8(2)	22(2)	6(1)	4(2)	3(1)
C(46)	19(2)	15(2)	23(2)	4(1)	0(2)	4(2)
C(47)	15(2)	17(2)	37(2)	6(2)	-2(2)	1(2)
C(48)	22(2)	16(2)	38(2)	7(2)	10(2)	9(2)

C(49)	29(2)	14(2)	25(2)	2(2)	10(2)	4(2)
C(50)	20(2)	13(2)	24(2)	5(1)	2(2)	2(2)
C(51)	29(2)	28(2)	27(2)	3(2)	-7(2)	-1(2)
C(52)	29(3)	34(3)	59(3)	1(2)	19(2)	9(2)
C(53)	30(2)	27(2)	26(2)	6(2)	-3(2)	2(2)
C(54)	16(2)	16(2)	21(2)	2(1)	0(2)	3(2)
C(55)	20(2)	23(2)	23(2)	5(2)	-1(2)	2(2)
C(56)	16(2)	18(2)	21(2)	1(1)	2(2)	2(2)
C(57)	16(2)	20(2)	17(2)	4(1)	0(2)	4(2)
C(58)	19(2)	23(2)	17(2)	5(1)	1(2)	2(2)
C(59)	24(2)	23(2)	22(2)	3(2)	2(2)	9(2)
C(60)	22(2)	27(2)	17(2)	6(2)	0(2)	10(2)
C(61)	14(2)	28(2)	28(2)	5(2)	2(2)	3(2)
C(62)	14(2)	21(2)	25(2)	4(2)	-3(2)	1(2)
C(63)	23(2)	19(2)	34(2)	6(2)	8(2)	2(2)
C(64)	25(2)	35(2)	35(3)	7(2)	-1(2)	16(2)
C(65)	23(2)	19(2)	40(3)	6(2)	-2(2)	-2(2)
C(66)	16(2)	18(2)	23(2)	-1(1)	1(2)	2(2)
C(67)	11(2)	21(2)	33(2)	-1(2)	-3(2)	2(2)
C(68)	11(2)	17(2)	29(2)	3(2)	1(2)	0(2)
C(69)	15(2)	17(2)	25(2)	-2(2)	0(2)	3(2)
C(70)	22(2)	19(2)	29(2)	-1(2)	-1(2)	2(2)
C(71)	34(3)	24(2)	26(2)	-2(2)	2(2)	9(2)
C(72)	42(3)	22(2)	32(2)	-5(2)	-2(2)	11(2)
C(73)	41(3)	17(2)	33(2)	1(2)	-6(2)	8(2)
C(74)	22(2)	21(2)	27(2)	2(2)	-3(2)	4(2)
C(75)	42(3)	19(2)	37(3)	6(2)	12(2)	5(2)
C(76)	72(4)	28(2)	43(3)	-8(2)	5(3)	25(3)
C(77)	36(3)	29(2)	34(3)	8(2)	0(2)	9(2)
C(78)	20(2)	22(2)	36(2)	5(2)	15(2)	11(2)
C(79)	13(2)	19(2)	25(2)	2(2)	4(2)	5(2)
C(80)	17(2)	17(2)	25(2)	2(2)	2(2)	3(2)
C(81)	40(3)	12(2)	38(3)	7(2)	14(2)	7(2)
C(82)	40(3)	17(2)	44(3)	4(2)	16(2)	11(2)
B(2)	14(2)	15(2)	20(2)	2(2)	3(2)	4(2)
Cl(1)	33(1)	86(2)	63(2)	33(2)	-5(1)	11(2)
Cl(2)	59(2)	85(2)	45(2)	9(2)	-3(2)	-9(2)
C(83)	61(8)	48(7)	49(7)	7(5)	-17(6)	27(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ea07210a.

	x	y	z	U(eq)
H(2)	-3434	7501	1097	29
H(3)	-3547	7010	1706	28
H(6)	1066	5994	133	37
H(8)	218	9500	312	33
H(10A)	176	4613	490	49
H(10B)	-990	5012	784	49
H(10C)	759	5156	876	49
H(11A)	2093	7380	-248	67
H(11B)	1772	8775	-175	67
H(11C)	521	7817	-363	67
H(12A)	-221	9818	1144	48
H(12B)	-1910	9462	1015	48
H(12C)	-889	10342	814	48
H(14)	801	2548	1955	24
H(15)	-1117	3957	2185	24
H(18)	6693	4104	1671	29
H(20)	4401	2054	877	33
H(22A)	5555	5144	2135	42
H(22B)	4006	4523	2235	42
H(22C)	4020	5670	2032	42
H(23A)	8064	3070	1234	58
H(23B)	7285	2923	855	58
H(23C)	7281	1799	1068	58
H(24A)	1147	3004	951	48
H(24B)	956	2080	1229	48
H(24C)	1812	1707	877	48
H(26)	1889	9292	2781	23
H(27)	-451	7925	2681	23
H(30)	5135	11129	1728	33
H(32)	7435	9211	2337	29
H(34A)	2529	10963	1687	42
H(34B)	1713	10530	2015	42

H(34C)	1867	9601	1668	42
H(35A)	8444	11310	2152	66
H(35B)	7731	11519	1785	66
H(35C)	8594	10332	1815	66
H(36A)	6208	7474	2550	36
H(36B)	4429	7297	2537	36
H(36C)	5257	8304	2820	36
H(37)	4540(40)	5910(40)	1337(13)	34
H(40A)	5095	9878	715	47
H(40B)	3652	9437	467	47
H(41A)	6262	8121	340	91
H(41B)	6252	9389	196	91
H(41C)	5015	8338	59	91
H(40C)	3450	9145	414	54
H(40D)	4269	8119	175	54
H(41D)	5671	9830	711	99
H(41E)	5957	9765	303	99
H(41F)	6512	8734	512	99
H(1)	-1618	6286	2166	22
H(43)	1821	-2527	3656	24
H(44)	4090	-1723	3374	23
H(47)	-3716	-999	3802	28
H(49)	-1472	316	4693	27
H(51A)	-669	-1107	3255	42
H(51B)	-2443	-1315	3262	42
H(51C)	-1407	-2343	3353	42
H(52A)	-4083	201	4696	61
H(52B)	-4828	-923	4439	61
H(52C)	-4858	406	4335	61
H(53A)	1150	499	4734	41
H(53B)	1941	752	4383	41
H(53C)	1893	-568	4495	41
H(55)	2857	2606	2431	26
H(56)	4735	1327	2655	22
H(59)	-736	5921	2925	27
H(61)	-3074	2799	2997	28
H(63A)	2257	5208	2644	38
H(63B)	2807	4930	3019	38

H(63C)	1889	6089	2988	38
H(64A)	-3451	5800	3163	46
H(64B)	-4373	4548	3037	46
H(64C)	-3768	5366	2756	46
H(65A)	-565	1132	3206	41
H(65B)	-319	883	2796	41
H(65C)	-1969	960	2940	41
H(67)	7230	3642	4151	26
H(68)	7297	1844	3690	23
H(71)	2592	4966	5053	34
H(73)	3443	7159	4330	36
H(75A)	2713	2564	4756	48
H(75B)	4111	3099	5003	48
H(75C)	4366	2455	4616	48
H(76A)	2516	7234	5194	72
H(76B)	1087	7083	4936	72
H(76C)	2466	7988	4873	72
H(77A)	4739	6563	3831	49
H(77B)	4098	5248	3661	49
H(77C)	5749	5439	3829	49
H(78)	-390(50)	1880(30)	4139(12)	30
H(81A)	-1116	6577	3904	35
H(81B)	301	6893	4168	35
H(82A)	-2643	6256	4378	50
H(82B)	-1872	7592	4446	50
H(82C)	-1235	6558	4641	50
H(2A)	5286	456	3263	19
H(83A)	3678	5356	370	62
H(83B)	3695	4613	691	62

Table 6. Torsion angles [°] for $Tp^{Ms}Cu$(ethyl propiolate), **3**.

C(37)-Cu(1)-N(1)-C(1)	-2.2(6)
C(38)-Cu(1)-N(1)-C(1)	22.2(4)
N(3)-Cu(1)-N(1)-C(1)	-135.1(4)
N(5)-Cu(1)-N(1)-C(1)	139.4(4)
C(37)-Cu(1)-N(1)-N(2)	174.2(3)
C(38)-Cu(1)-N(1)-N(2)	-161.4(3)
N(3)-Cu(1)-N(1)-N(2)	41.4(3)
N(5)-Cu(1)-N(1)-N(2)	-44.2(3)
C(1)-N(1)-N(2)-C(3)	0.1(4)
Cu(1)-N(1)-N(2)-C(3)	-177.3(3)
C(1)-N(1)-N(2)-B(1)	176.8(3)
Cu(1)-N(1)-N(2)-B(1)	-0.6(4)
C(37)-Cu(1)-N(3)-C(13)	-15.8(5)
C(38)-Cu(1)-N(3)-C(13)	-3.9(6)
N(1)-Cu(1)-N(3)-C(13)	138.8(4)
N(5)-Cu(1)-N(3)-C(13)	-132.9(4)
C(37)-Cu(1)-N(3)-N(4)	169.9(3)
C(38)-Cu(1)-N(3)-N(4)	-178.3(3)
N(1)-Cu(1)-N(3)-N(4)	-35.5(3)
N(5)-Cu(1)-N(3)-N(4)	52.8(3)
C(13)-N(3)-N(4)-C(15)	-0.1(4)
Cu(1)-N(3)-N(4)-C(15)	175.9(3)
C(13)-N(3)-N(4)-B(1)	173.8(3)
Cu(1)-N(3)-N(4)-B(1)	-10.2(4)
C(37)-Cu(1)-N(5)-C(25)	22.6(5)
C(38)-Cu(1)-N(5)-C(25)	-18.6(5)
N(1)-Cu(1)-N(5)-C(25)	-134.7(5)
N(3)-Cu(1)-N(5)-C(25)	131.2(5)
C(37)-Cu(1)-N(5)-N(6)	-157.3(3)
C(38)-Cu(1)-N(5)-N(6)	161.5(3)
N(1)-Cu(1)-N(5)-N(6)	45.4(3)
N(3)-Cu(1)-N(5)-N(6)	-48.8(3)
C(25)-N(5)-N(6)-C(27)	0.5(4)
Cu(1)-N(5)-N(6)-C(27)	-179.5(3)
C(25)-N(5)-N(6)-B(1)	-179.7(3)
Cu(1)-N(5)-N(6)-B(1)	0.2(4)

N(2)-N(1)-C(1)-C(2)	-0.4(4)
Cu(1)-N(1)-C(1)-C(2)	176.3(3)
N(2)-N(1)-C(1)-C(4)	-178.2(4)
Cu(1)-N(1)-C(1)-C(4)	-1.5(6)
N(1)-C(1)-C(2)-C(3)	0.4(5)
C(4)-C(1)-C(2)-C(3)	178.1(4)
N(1)-N(2)-C(3)-C(2)	0.2(5)
B(1)-N(2)-C(3)-C(2)	-176.1(4)
C(1)-C(2)-C(3)-N(2)	-0.4(5)
N(1)-C(1)-C(4)-C(5)	67.2(5)
C(2)-C(1)-C(4)-C(5)	-110.2(5)
N(1)-C(1)-C(4)-C(9)	-115.0(5)
C(2)-C(1)-C(4)-C(9)	67.7(6)
C(9)-C(4)-C(5)-C(6)	1.1(6)
C(1)-C(4)-C(5)-C(6)	179.0(4)
C(9)-C(4)-C(5)-C(10)	-179.1(4)
C(1)-C(4)-C(5)-C(10)	-1.2(6)
C(4)-C(5)-C(6)-C(7)	-2.2(7)
C(10)-C(5)-C(6)-C(7)	177.9(5)
C(5)-C(6)-C(7)-C(8)	2.0(7)
C(5)-C(6)-C(7)-C(11)	-177.5(5)
C(6)-C(7)-C(8)-C(9)	-0.6(7)
C(11)-C(7)-C(8)-C(9)	178.9(5)
C(7)-C(8)-C(9)-C(4)	-0.4(7)
C(7)-C(8)-C(9)-C(12)	176.9(4)
C(5)-C(4)-C(9)-C(8)	0.2(6)
C(1)-C(4)-C(9)-C(8)	-177.7(4)
C(5)-C(4)-C(9)-C(12)	-177.1(4)
C(1)-C(4)-C(9)-C(12)	5.0(6)
N(4)-N(3)-C(13)-C(14)	0.5(4)
Cu(1)-N(3)-C(13)-C(14)	-174.2(3)
N(4)-N(3)-C(13)-C(16)	-174.8(3)
Cu(1)-N(3)-C(13)-C(16)	10.5(6)
N(3)-C(13)-C(14)-C(15)	-0.7(5)
C(16)-C(13)-C(14)-C(15)	174.2(4)
N(3)-N(4)-C(15)-C(14)	-0.4(5)
B(1)-N(4)-C(15)-C(14)	-173.5(4)
C(13)-C(14)-C(15)-N(4)	0.6(5)

N(3)-C(13)-C(16)-C(21)	-107.7(5)
C(14)-C(13)-C(16)-C(21)	77.9(6)
N(3)-C(13)-C(16)-C(17)	73.0(5)
C(14)-C(13)-C(16)-C(17)	-101.4(5)
C(21)-C(16)-C(17)-C(18)	0.9(6)
C(13)-C(16)-C(17)-C(18)	-179.8(4)
C(21)-C(16)-C(17)-C(22)	-178.8(4)
C(13)-C(16)-C(17)-C(22)	0.5(6)
C(16)-C(17)-C(18)-C(19)	-0.6(7)
C(22)-C(17)-C(18)-C(19)	179.1(4)
C(17)-C(18)-C(19)-C(20)	0.0(7)
C(17)-C(18)-C(19)-C(23)	-178.9(4)
C(18)-C(19)-C(20)-C(21)	0.3(7)
C(23)-C(19)-C(20)-C(21)	179.3(5)
C(19)-C(20)-C(21)-C(16)	-0.1(7)
C(19)-C(20)-C(21)-C(24)	-179.6(4)
C(17)-C(16)-C(21)-C(20)	-0.5(6)
C(13)-C(16)-C(21)-C(20)	-179.9(4)
C(17)-C(16)-C(21)-C(24)	179.0(4)
C(13)-C(16)-C(21)-C(24)	-0.3(6)
N(6)-N(5)-C(25)-C(26)	-0.9(4)
Cu(1)-N(5)-C(25)-C(26)	179.2(3)
N(6)-N(5)-C(25)-C(28)	-176.5(3)
Cu(1)-N(5)-C(25)-C(28)	3.6(7)
N(5)-C(25)-C(26)-C(27)	0.9(5)
C(28)-C(25)-C(26)-C(27)	176.1(4)
N(5)-N(6)-C(27)-C(26)	0.0(5)
B(1)-N(6)-C(27)-C(26)	-179.6(4)
C(25)-C(26)-C(27)-N(6)	-0.6(4)
N(5)-C(25)-C(28)-C(29)	74.3(5)
C(26)-C(25)-C(28)-C(29)	-100.4(5)
N(5)-C(25)-C(28)-C(33)	-107.5(4)
C(26)-C(25)-C(28)-C(33)	77.7(5)
C(33)-C(28)-C(29)-C(30)	-0.4(6)
C(25)-C(28)-C(29)-C(30)	177.7(4)
C(33)-C(28)-C(29)-C(34)	-176.4(4)
C(25)-C(28)-C(29)-C(34)	1.8(5)
C(28)-C(29)-C(30)-C(31)	0.6(6)

C(34)-C(29)-C(30)-C(31)	176.5(4)
C(29)-C(30)-C(31)-C(32)	-0.3(7)
C(29)-C(30)-C(31)-C(35)	-179.8(4)
C(30)-C(31)-C(32)-C(33)	-0.2(6)
C(35)-C(31)-C(32)-C(33)	179.3(4)
C(31)-C(32)-C(33)-C(28)	0.4(6)
C(31)-C(32)-C(33)-C(36)	-177.8(4)
C(29)-C(28)-C(33)-C(32)	0.0(6)
C(25)-C(28)-C(33)-C(32)	-178.2(4)
C(29)-C(28)-C(33)-C(36)	178.1(4)
C(25)-C(28)-C(33)-C(36)	0.0(5)
N(1)-Cu(1)-C(37)-C(38)	38.9(5)
N(3)-Cu(1)-C(37)-C(38)	168.5(3)
N(5)-Cu(1)-C(37)-C(38)	-96.8(3)
Cu(1)-C(37)-C(38)-C(39)	176.7(10)
N(1)-Cu(1)-C(38)-C(37)	-157.6(3)
N(3)-Cu(1)-C(38)-C(37)	-18.9(5)
N(5)-Cu(1)-C(38)-C(37)	102.0(3)
C(37)-Cu(1)-C(38)-C(39)	-177.6(7)
N(1)-Cu(1)-C(38)-C(39)	24.8(5)
N(3)-Cu(1)-C(38)-C(39)	163.5(4)
N(5)-Cu(1)-C(38)-C(39)	-75.6(5)
C(37)-C(38)-C(39)-O(1)	-144.8(9)
Cu(1)-C(38)-C(39)-O(1)	30.5(8)
C(37)-C(38)-C(39)-O(2A)	20.8(13)
Cu(1)-C(38)-C(39)-O(2A)	-164.0(6)
C(37)-C(38)-C(39)-O(2B)	44.3(11)
Cu(1)-C(38)-C(39)-O(2B)	-140.4(6)
O(1)-C(39)-O(2A)-C(40A)	-6.5(12)
O(2B)-C(39)-O(2A)-C(40A)	116(2)
C(38)-C(39)-O(2A)-C(40A)	-173.5(7)
C(39)-O(2A)-C(40A)-C(41A)	-169.5(9)
O(1)-C(39)-O(2B)-C(40B)	11.1(12)
O(2A)-C(39)-O(2B)-C(40B)	-61.3(19)
C(38)-C(39)-O(2B)-C(40B)	-178.2(8)
C(39)-O(2B)-C(40B)-C(41B)	85.1(15)
C(27)-N(6)-B(1)-N(2)	119.6(4)
N(5)-N(6)-B(1)-N(2)	-60.0(5)

C(27)-N(6)-B(1)-N(4)	-120.8(4)
N(5)-N(6)-B(1)-N(4)	59.6(5)
C(3)-N(2)-B(1)-N(6)	-119.3(4)
N(1)-N(2)-B(1)-N(6)	64.8(4)
C(3)-N(2)-B(1)-N(4)	120.7(4)
N(1)-N(2)-B(1)-N(4)	-55.2(4)
C(15)-N(4)-B(1)-N(6)	114.5(4)
N(3)-N(4)-B(1)-N(6)	-58.0(5)
C(15)-N(4)-B(1)-N(2)	-125.3(4)
N(3)-N(4)-B(1)-N(2)	62.2(4)
C(78)-Cu(2)-N(7)-C(42)	17.2(5)
C(79)-Cu(2)-N(7)-C(42)	14.4(6)
N(9)-Cu(2)-N(7)-C(42)	-131.9(4)
N(11)-Cu(2)-N(7)-C(42)	140.8(4)
C(78)-Cu(2)-N(7)-N(8)	-169.2(3)
C(79)-Cu(2)-N(7)-N(8)	-171.9(3)
N(9)-Cu(2)-N(7)-N(8)	41.7(3)
N(11)-Cu(2)-N(7)-N(8)	-45.6(3)
C(42)-N(7)-N(8)-C(44)	0.1(4)
Cu(2)-N(7)-N(8)-C(44)	-175.3(3)
C(42)-N(7)-N(8)-B(2)	179.1(3)
Cu(2)-N(7)-N(8)-B(2)	3.6(4)
C(78)-Cu(2)-N(9)-C(54)	9.2(5)
C(79)-Cu(2)-N(9)-C(54)	-22.5(4)
N(7)-Cu(2)-N(9)-C(54)	137.7(4)
N(11)-Cu(2)-N(9)-C(54)	-131.1(4)
C(78)-Cu(2)-N(9)-N(10)	-172.4(3)
C(79)-Cu(2)-N(9)-N(10)	155.9(2)
N(7)-Cu(2)-N(9)-N(10)	-43.9(3)
N(11)-Cu(2)-N(9)-N(10)	47.3(3)
C(54)-N(9)-N(10)-C(56)	0.1(4)
Cu(2)-N(9)-N(10)-C(56)	-178.7(2)
C(54)-N(9)-N(10)-B(2)	179.0(3)
Cu(2)-N(9)-N(10)-B(2)	0.1(4)
C(78)-Cu(2)-N(11)-C(66)	-28.9(5)
C(79)-Cu(2)-N(11)-C(66)	8.4(5)
N(7)-Cu(2)-N(11)-C(66)	-143.7(5)
N(9)-Cu(2)-N(11)-C(66)	124.0(5)

C(78)-Cu(2)-N(11)-N(12)	156.1(3)
C(79)-Cu(2)-N(11)-N(12)	-166.6(3)
N(7)-Cu(2)-N(11)-N(12)	41.3(3)
N(9)-Cu(2)-N(11)-N(12)	-51.0(3)
C(66)-N(11)-N(12)-C(68)	-0.2(5)
Cu(2)-N(11)-N(12)-C(68)	176.5(3)
C(66)-N(11)-N(12)-B(2)	-170.9(3)
Cu(2)-N(11)-N(12)-B(2)	5.8(4)
N(8)-N(7)-C(42)-C(43)	0.3(4)
Cu(2)-N(7)-C(42)-C(43)	174.3(3)
N(8)-N(7)-C(42)-C(45)	179.9(3)
Cu(2)-N(7)-C(42)-C(45)	-6.0(6)
N(7)-C(42)-C(43)-C(44)	-0.6(5)
C(45)-C(42)-C(43)-C(44)	179.8(4)
N(7)-N(8)-C(44)-C(43)	-0.5(5)
B(2)-N(8)-C(44)-C(43)	-179.4(4)
C(42)-C(43)-C(44)-N(8)	0.7(5)
N(7)-C(42)-C(45)-C(46)	104.6(4)
C(43)-C(42)-C(45)-C(46)	-75.8(6)
N(7)-C(42)-C(45)-C(50)	-73.6(5)
C(43)-C(42)-C(45)-C(50)	105.9(5)
C(50)-C(45)-C(46)-C(47)	2.2(6)
C(42)-C(45)-C(46)-C(47)	-176.0(3)
C(50)-C(45)-C(46)-C(51)	-177.2(4)
C(42)-C(45)-C(46)-C(51)	4.5(6)
C(45)-C(46)-C(47)-C(48)	0.1(6)
C(51)-C(46)-C(47)-C(48)	179.5(4)
C(46)-C(47)-C(48)-C(49)	-1.7(6)
C(46)-C(47)-C(48)-C(52)	-179.9(4)
C(47)-C(48)-C(49)-C(50)	1.0(6)
C(52)-C(48)-C(49)-C(50)	179.2(4)
C(48)-C(49)-C(50)-C(45)	1.3(6)
C(48)-C(49)-C(50)-C(53)	-179.5(4)
C(46)-C(45)-C(50)-C(49)	-2.9(5)
C(42)-C(45)-C(50)-C(49)	175.4(4)
C(46)-C(45)-C(50)-C(53)	177.9(4)
C(42)-C(45)-C(50)-C(53)	-3.9(5)
N(10)-N(9)-C(54)-C(55)	-0.9(4)

Cu(2)-N(9)-C(54)-C(55)	177.6(3)
N(10)-N(9)-C(54)-C(57)	176.1(3)
Cu(2)-N(9)-C(54)-C(57)	-5.4(6)
N(9)-C(54)-C(55)-C(56)	1.3(4)
C(57)-C(54)-C(55)-C(56)	-175.4(4)
N(9)-N(10)-C(56)-C(55)	0.6(4)
B(2)-N(10)-C(56)-C(55)	-178.0(3)
C(54)-C(55)-C(56)-N(10)	-1.1(4)
N(9)-C(54)-C(57)-C(58)	114.8(4)
C(55)-C(54)-C(57)-C(58)	-68.9(6)
N(9)-C(54)-C(57)-C(62)	-65.5(5)
C(55)-C(54)-C(57)-C(62)	110.8(5)
C(62)-C(57)-C(58)-C(59)	1.2(6)
C(54)-C(57)-C(58)-C(59)	-179.1(4)
C(62)-C(57)-C(58)-C(63)	-179.2(4)
C(54)-C(57)-C(58)-C(63)	0.5(6)
C(57)-C(58)-C(59)-C(60)	-0.4(6)
C(63)-C(58)-C(59)-C(60)	-180.0(4)
C(58)-C(59)-C(60)-C(61)	-0.2(6)
C(58)-C(59)-C(60)-C(64)	179.4(4)
C(59)-C(60)-C(61)-C(62)	-0.2(7)
C(64)-C(60)-C(61)-C(62)	-179.8(4)
C(60)-C(61)-C(62)-C(57)	1.0(7)
C(60)-C(61)-C(62)-C(65)	-179.9(4)
C(58)-C(57)-C(62)-C(61)	-1.5(6)
C(54)-C(57)-C(62)-C(61)	178.8(4)
C(58)-C(57)-C(62)-C(65)	179.4(4)
C(54)-C(57)-C(62)-C(65)	-0.4(6)
N(12)-N(11)-C(66)-C(67)	0.0(5)
Cu(2)-N(11)-C(66)-C(67)	-175.2(4)
N(12)-N(11)-C(66)-C(69)	177.4(4)
Cu(2)-N(11)-C(66)-C(69)	2.2(7)
N(11)-C(66)-C(67)-C(68)	0.2(5)
C(69)-C(66)-C(67)-C(68)	-176.9(4)
N(11)-N(12)-C(68)-C(67)	0.3(5)
B(2)-N(12)-C(68)-C(67)	169.9(4)
C(66)-C(67)-C(68)-N(12)	-0.3(5)
N(11)-C(66)-C(69)-C(70)	83.4(5)

C(67)-C(66)-C(69)-C(70)	-99.8(6)
N(11)-C(66)-C(69)-C(74)	-97.9(5)
C(67)-C(66)-C(69)-C(74)	78.9(6)
C(74)-C(69)-C(70)-C(71)	1.8(6)
C(66)-C(69)-C(70)-C(71)	-179.5(4)
C(74)-C(69)-C(70)-C(75)	-178.4(4)
C(66)-C(69)-C(70)-C(75)	0.3(6)
C(69)-C(70)-C(71)-C(72)	-0.2(7)
C(75)-C(70)-C(71)-C(72)	-179.9(5)
C(70)-C(71)-C(72)-C(73)	-1.7(7)
C(70)-C(71)-C(72)-C(76)	-179.2(5)
C(71)-C(72)-C(73)-C(74)	2.0(7)
C(76)-C(72)-C(73)-C(74)	179.4(5)
C(72)-C(73)-C(74)-C(69)	-0.4(7)
C(72)-C(73)-C(74)-C(77)	178.2(5)
C(70)-C(69)-C(74)-C(73)	-1.5(6)
C(66)-C(69)-C(74)-C(73)	179.7(4)
C(70)-C(69)-C(74)-C(77)	179.9(4)
C(66)-C(69)-C(74)-C(77)	1.2(6)
N(7)-Cu(2)-C(78)-C(79)	-177.4(3)
N(9)-Cu(2)-C(78)-C(79)	-54.0(4)
N(11)-Cu(2)-C(78)-C(79)	78.2(3)
Cu(2)-C(78)-C(79)-C(80)	-175.9(9)
N(7)-Cu(2)-C(79)-C(78)	4.4(5)
N(9)-Cu(2)-C(79)-C(78)	146.7(3)
N(11)-Cu(2)-C(79)-C(78)	-117.7(3)
C(78)-Cu(2)-C(79)-C(80)	177.2(6)
N(7)-Cu(2)-C(79)-C(80)	-178.4(3)
N(9)-Cu(2)-C(79)-C(80)	-36.1(5)
N(11)-Cu(2)-C(79)-C(80)	59.5(5)
C(81)-O(4)-C(80)-O(3)	1.2(6)
C(81)-O(4)-C(80)-C(79)	-178.7(4)
C(78)-C(79)-C(80)-O(3)	-177.9(8)
Cu(2)-C(79)-C(80)-O(3)	7.8(7)
C(78)-C(79)-C(80)-O(4)	1.9(11)
Cu(2)-C(79)-C(80)-O(4)	-172.4(3)
C(80)-O(4)-C(81)-C(82)	-175.9(4)
C(68)-N(12)-B(2)-N(10)	-112.3(4)

N(11)-N(12)-B(2)-N(10)	56.4(4)
C(68)-N(12)-B(2)-N(8)	129.5(4)
N(11)-N(12)-B(2)-N(8)	-61.8(5)
C(56)-N(10)-B(2)-N(12)	116.2(4)
N(9)-N(10)-B(2)-N(12)	-62.4(4)
C(56)-N(10)-B(2)-N(8)	-124.8(4)
N(9)-N(10)-B(2)-N(8)	56.7(4)
C(44)-N(8)-B(2)-N(12)	-123.1(4)
N(7)-N(8)-B(2)-N(12)	58.2(5)
C(44)-N(8)-B(2)-N(10)	118.9(4)
N(7)-N(8)-B(2)-N(10)	-59.9(4)

Symmetry transformations used to generate equivalent atoms: