A Novel Example of Chiral Counteranion Induced Enantioselective Metal Catalysis: The Importance of Ion-Pairing in Copper Catalyzed Olefin Aziridination and Cyclopropanation

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Supporting Information

General Procedures

Unless otherwise noted, all manipulations were performed under an inert atmosphere in a vacuum atmosphere 553-2 dry box or by using standard Schlenk or vacuum line techniques. All other reagents were purchased from Aldrich® and used as received. Benzene was distilled from sodium/benzophenone ketyl under nitrogen. Acetonitrile and methylene chloride were distilled from CaH_2 under nitrogen. Deuterated solvents were dried as their protonoted analogues, but were transferred under vacuum from the drying agent, and stored over 3Å molecular sieves. ^1H and ^{13}C NMR were recorded on JEOL-270, Varian 400, and Unity500 spectrometers. Infrared spectra were recorded on a Bruker IFS-48 spectrometer.

Synthesis of Cu^+ (R)-3^-

To a solution of (R)-(+)-1,1'-bi-2-naphthol (570 mg, 2.0 mmol) in 25 ml CH_2Cl_2 was added $H_2BBr{\cdot}SMe_2$ (1.0 ml, 1.0 M in CH_2Cl_2). The solution was stirred for 1 h at -10°C, followed by 2 h at 25°C. The solvent was evaporated, CH_3CN added, and the suspension added dropwise to a CH_3CN suspension of Ag_2CO_3 (1.1 g, 4.0 mmol). The mixture was filtered through celite, concentrated to 3 ml, and precipitated with Et_2O to yield Ag^+ **(R)-3**$^-$ • 4 CH_3CN (670 mg, 79%). A 5 ml CH_3CN solution of Ag^+ **(R)-3**$^-$ (600 mg, 0.71 mmol) was added to CuCl (70 mg, 0.70 mmol) in 5 ml CH_3CN. The reaction was stirred for 5 minutes, filtered, condensed to 2 ml, and Et_2O added until white crystals formed. The precipitate was recrystallized from CH_3CN/Et_2O, affording Cu^+ **(R)-3**$^-$ • 4 CH_3CN (450 mg, 79%).

^1H NMR (CD_2Cl_2): δ 7.96 (d, 4H), δ 7.90 (d, 4H), δ 7.49 (d, 4H), δ 7.30 (m, 8H), δ 7.15 (ddd, 4H), δ 1.48 (s, 12H).

^{13}C NMR (CD_2Cl_2): δ 154.6, 133.4, 129.9, 128,8, 128.0, 126.9, 124.4, 123.1, 122.4, 115.2, 1.0.

^{11}B NMR (CD_2Cl_2): δ 8.59.

Elemental Analysis: Calc. for $C_{48}H_{36}N_4O_4BCu$: C, 71.42; H, 4.49; N, 6.93. Found: C, 71.11; H, 4.56; N, 6.71.

Synthesis of (bipy)Cu(CH_2CHPh)$^+$ (R)-3$^-$ (8)

To a 1 ml CH_2Cl_2 solution of Cu^+ (**R**)-**3**$^-$ (50 mg, 0.062 mmol) was added styrene (32 mg, 0.31 mmol) and bypridine (9.7 mg, 0.062 mmol). The solution was stirred for 5 minutes, pentane was layered on top, and let stand for 2 days to yield yellow crystals of **8** (48 mg, 85 %).

^{1}H NMR (CH_2Cl_2): δ 7.83 (m, 8H), δ 7.60 (d, 2H), δ 7.30 (m, 14H), δ 7.05 (m, 9H), δ 6.95 (m, 2H), δ 6.78 (m, 4H), δ 5.20 (dd, 1H), δ 4.22 (d, 1H), δ 4.00 (d, 1H).

Table 1. Crystal data and structure refinement for C96 H72 B2 Cu2 N8 O8.

Crystal data		
Chemical formula, sum	C96 H72 B2 Cu2 N8 O8	
Chemical formula, moiety	Cu(CH3CN)3(BO4C40H24). Cu(CH3CN)4.BO4C40H24.CH3CN	
Chemical formula weight, Mr	1614.40	
Cell setting	Monoclinic	
Space group	P2(1)	
Unit cell dimensions (A, deg)	a = 11.113(4) b = 25.109(7) c = 14.869(3)	alpha = 90 beta = 104.84(3) gamma = 90
Volume of unit cell, V (A^3)	4011(2)	
Formula units per cell, Z	2	
Density calculated from formula and cell, Dx (Mg/m^3)	1.337	
F(000)	1672	
Radiation type	Cu k/alpha	
Wavelength, lambda (A)	1.54178	
No. of reflections for cell measurement	24	
Theta range (deg)	20 to 25	
Linear absorption coefficient, mu (mm^-1)	1.173	
Measurement temperature (K)	293(2)	
Crystal shape	prism	
Colour	colourless	
Size (mm)	0.73 x 0.50 x 0.44	
Data collection		
Diffractometer type	Enraf Nonius CAD4	
Data-collection method	omega/2theta scans	
Absorption correction type	Analytical	
Maximum and minimum transmission values, Tmax and Tmin	0.74 and 0.58	

No. of reflections measured	52945
No. of independent reflections	15245
No. of observed reflections	14208
Criterion for observed reflections	>2\s(I)
Rint	.125
Minimum and maximum values of theta (deg)	3.07 to 70.01
Ranges of h,k,l	-13<=h<=13, -30<=k<=30, -18<=l<=18
No. of standard reflections	5
Interval, time (min)	60
Intensity decay (%)	5.1
Refinement	
Refinement method	Full-matrix on F^2
Final R indices, I>2sigma(I)	R1 = 0.0716, wR2 = 0.1866
R indices, all data	R1 = 0.0732, wR2 = 0.1887
Goodness-of-fit on F^2, S	1.022

R1 = sum (absabs Foabs -abs Fcabsabs)/sum (abs Foabs),
wR2 = [sum [w(Fo^2^-Fc^2^)^2^]/sum [w(Fo^2^)^2^]]^1*2^ and
GoF = [sum [w(Fo^2^-Fc^2^)^2^]/(No. of reflns - No. of params.)]^1*2^

No. of reflections used in refinement	15245
No. of parameters refined	1054
No. of restraints	1
Method of refining and locating H atoms	constrained
Weighting scheme	based on measured e.s.d's
Function minimized	sum w(Fo^2^-Fc^2^)

w=1/[\s^2^(Fo^2^)+(0.1622P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Maximum shift/sigma	0.023
DELTA rho max (e A ^-3^)	0.467
DELTA rho min (e A ^-3^)	-0.517
Extinction correction method	SHELXL-93 (1995)

Secondary extinction value	0.0017(2)
Absolute structure method	Flack, H.D. (1983)
Absolute structure parameter	0.04(2)

Discussion of structure determination and refinement procedure

Space group confirmed by PLATON program (Speck, 1995). Data reduction performed using a locally modified version of the NRC-2 program (Ahmed et al, 1973). The structure was solved by direct method using SHELXS96 (Sheldrick, 1990) and difmap synthesis using NRCVAX (Gabe et al (1989) and SHELXL96 (Sheldrick, 1996). All non-hydrogen atoms anisotropic, hydrogen atoms isotropic. Hydrogen atoms constrained to the parent site using a riding model; SHELXL96 defaults, C-H 0.93 to 0.98,\%A. The isotropic factors, Uiso, were adjusted to 50% higher value of the parent site (methyl) and 20% higher (others). A final verification of possible voids was performed using the VOID routine of the PLATON program (Speck, 1995).

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (A^2^ x 10 ^2^) for C96 H72 B2 Cu2 N8 O8.

U~eq~ = (1/3)sum~i~sum~j~U~ij~a^*^~i~a^*^~j~a~i~.a~j~.

	x	y	z	U~eq~
Cu(1)	-0.03904(6)	0.22804(2)	-0.08280(5)	5.77(2)
B(1)	0.1965(3)	0.16626(14)	-0.0967(3)	3.90(7)
O(1)	0.1903(2)	0.18145(10)	-0.0024(2)	4.61(5)
O(2)	0.3104(2)	0.18396(9)	-0.1205(2)	3.87(5)
O(3)	0.0841(2)	0.19217(10)	-0.1573(2)	4.43(5)
O(4)	0.1927(2)	0.10856(9)	-0.1095(2)	3.87(4)
C(1)	0.2968(3)	0.17748(13)	0.0670(2)	4.21(7)
C(2)	0.3026(4)	0.1398(2)	0.1398(3)	5.37(9)
C(3)	0.4079(5)	0.1347(2)	0.2090(3)	5.65(10)
C(4)	0.5152(5)	0.1646(2)	0.2091(2)	5.38(9)
C(5)	0.6305(6)	0.1572(2)	0.2766(3)	6.86(12)
C(6)	0.7339(6)	0.1843(2)	0.2751(3)	7.54(14)
C(7)	0.7289(5)	0.2225(2)	0.2043(3)	6.85(11)
C(8)	0.6194(4)	0.2314(2)	0.1376(3)	5.22(8)
C(9)	0.5094(3)	0.20346(14)	0.1379(2)	4.35(7)
C(10)	0.3949(3)	0.21092(13)	0.0676(2)	3.95(6)
C(11)	0.3423(3)	0.23552(13)	-0.0992(2)	3.77(6)
C(12)	0.3410(3)	0.2718(2)	-0.1716(2)	4.31(7)
C(13)	0.3698(3)	0.3242(2)	-0.1535(2)	4.53(7)
C(14)	0.3989(3)	0.34346(14)	-0.0609(3)	4.24(7)
C(15)	0.4279(4)	0.3977(2)	-0.0403(3)	4.92(8)
C(16)	0.4588(4)	0.41574(14)	0.0502(3)	5.12(8)
C(17)	0.4572(4)	0.3801(2)	0.1237(3)	5.10(8)
C(18)	0.4288(4)	0.32782(14)	0.1054(2)	4.49(7)
C(19)	0.4034(3)	0.30668(13)	0.0130(2)	3.90(6)
C(20)	0.3814(3)	0.25182(13)	-0.0065(2)	3.70(6)
C(21)	0.0525(3)	0.17558(13)	-0.2472(3)	4.22(7)
C(22)	0.0695(3)	0.2115(2)	-0.3160(3)	5.31(9)
C(23)	0.0480(3)	0.1949(2)	-0.4070(3)	5.99(11)
C(24)	0.0108(3)	0.1420(2)	-0.4330(2)	5.17(9)
C(25)	-0.0037(4)	0.1234(3)	-0.5247(3)	6.81(13)
C(26)	-0.0384(5)	0.0727(3)	-0.5486(3)	7.5(2)
C(27)	-0.0590(4)	0.0360(2)	-0.4800(3)	6.55(11)
C(28)	-0.0449(3)	0.0532(2)	-0.3904(3)	4.84(8)
C(29)	-0.0121(3)	0.1061(2)	-0.3640(2)	4.17(7)
C(30)	0.0056(3)	0.12448(13)	-0.2704(2)	3.73(6)
C(31)	0.0808(3)	0.08532(12)	-0.1148(2)	3.54(6)
C(32)	0.0654(3)	0.05490(13)	-0.0377(2)	4.04(6)
C(33)	-0.0448(3)	0.03070(13)	-0.0409(2)	4.05(6)
C(34)	-0.1479(3)	0.03598(12)	-0.1193(2)	3.75(6)
C(35)	-0.2642(3)	0.01235(14)	-0.1223(2)	4.32(7)
C(36)	-0.3648(3)	0.0188(2)	-0.1979(3)	4.53(7)
C(37)	-0.3523(3)	0.0505(2)	-0.2726(3)	4.68(7)
C(38)	-0.2408(3)	0.07421(14)	-0.2718(2)	4.00(6)
C(39)	-0.1341(3)	0.06710(12)	-0.1963(2)	3.46(6)
C(40)	-0.0160(3)	0.09080(12)	-0.1941(2)	3.49(6)
N(1)	-0.0890(5)	0.1804(3)	0.0165(4)	9.4(2)
C(41)	-0.1564(6)	0.1534(2)	0.0362(4)	7.9(2)

C(42)	-0.2570(11)	0.1190(3)	0.0468(9)	14.7(5)
N(2)	0.0314(3)	0.29462(14)	-0.0322(3)	5.64(8)
C(43)	0.0705(4)	0.3344(2)	-0.0022(3)	5.72(9)
C(44)	0.1173(6)	0.3859(3)	0.0331(6)	9.1(2)
N(3)	-0.2007(4)	0.2156(2)	-0.1732(3)	7.11(11)
C(45)	-0.3024(4)	0.2072(2)	-0.2090(3)	5.99(10)
C(46)	-0.4315(4)	0.1970(2)	-0.2525(3)	6.03(10)
Cu(2)	0.13861(7)	0.92623(3)	0.78597(5)	6.61(2)
N(4)	0.2251(4)	0.8741(2)	0.7162(3)	6.28(9)
C(91)	0.2923(5)	0.8474(2)	0.6901(3)	6.20(11)
C(92)	0.3762(7)	0.8149(3)	0.6549(4)	8.5(2)
N(5)	0.1869(4)	0.8902(2)	0.9110(3)	7.19(11)
C(95)	0.2305(4)	0.8644(2)	0.9735(3)	5.91(10)
C(96)	0.2835(5)	0.8317(2)	1.0532(3)	6.91(12)
N(6)	0.2173(4)	0.9948(2)	0.7713(3)	5.92(8)
C(97)	0.2602(4)	1.0331(2)	0.7512(3)	5.23(8)
C(98)	0.3128(4)	1.0810(2)	0.7239(4)	6.09(10)
N(7)	-0.0456(4)	0.9258(2)	0.7305(3)	6.63(9)
C(99)	-0.1477(5)	0.9202(2)	0.6997(4)	6.59(11)
C(100)	-0.2800(5)	0.9122(3)	0.6572(5)	9.1(2)
N(8)	0.5767(5)	0.4587(3)	0.3746(4)	9.0(2)
C(101)	0.6600(5)	0.4495(2)	0.4322(3)	6.47(11)
C(102)	0.7697(6)	0.4370(4)	0.5063(4)	9.4(2)
B(2)	0.4557(4)	0.8344(2)	0.3801(3)	4.34(8)
O(5)	0.3635(2)	0.82915(11)	0.2891(2)	4.71(5)
O(6)	0.4761(2)	0.89017(11)	0.4100(2)	4.70(5)
O(7)	0.5667(2)	0.80817(11)	0.3650(2)	4.57(5)
O(8)	0.4104(2)	0.80988(11)	0.4555(2)	4.77(5)
C(51)	0.2625(3)	0.8609(2)	0.2735(2)	4.62(7)
C(52)	0.1443(4)	0.8372(2)	0.2663(3)	5.95(10)
C(53)	0.0395(4)	0.8673(2)	0.2482(3)	6.39(11)
C(54)	0.0447(3)	0.9232(2)	0.2372(3)	5.84(10)
C(55)	-0.0643(4)	0.9558(3)	0.2207(3)	7.31(14)
C(56)	-0.0564(4)	1.0095(3)	0.2158(3)	7.39(14)
C(57)	0.0592(4)	1.0337(2)	0.2278(3)	6.50(12)
C(58)	0.1662(4)	1.0042(2)	0.2420(3)	5.27(9)
C(59)	0.1625(3)	0.9478(2)	0.2454(2)	4.94(8)
C(60)	0.2725(3)	0.9153(2)	0.2607(2)	4.36(7)
C(61)	0.4930(3)	0.9256(2)	0.3463(2)	4.17(6)
C(62)	0.6098(3)	0.9522(2)	0.3636(3)	4.74(8)
C(63)	0.6324(3)	0.9882(2)	0.3022(3)	4.93(8)
C(64)	0.5434(3)	0.99846(14)	0.2171(3)	4.40(7)
C(65)	0.5702(4)	1.0319(2)	0.1481(3)	5.28(8)
C(66)	0.4861(4)	1.0383(2)	0.0635(3)	5.56(9)
C(67)	0.3723(4)	1.0115(2)	0.0447(3)	5.08(8)
C(68)	0.3413(3)	0.9802(2)	0.1102(2)	4.43(7)
C(69)	0.4253(3)	0.97269(14)	0.1999(2)	4.06(6)
C(70)	0.3979(3)	0.93866(14)	0.2686(2)	4.17(7)
C(71)	0.6625(3)	0.80093(14)	0.4418(2)	4.10(7)
C(72)	0.7757(4)	0.8278(2)	0.4456(3)	4.81(8)
C(73)	0.8734(3)	0.8238(2)	0.5221(3)	4.90(8)
C(74)	0.8623(3)	0.79448(14)	0.6015(3)	4.56(7)
C(75)	0.9568(4)	0.7947(2)	0.6856(3)	5.57(9)
C(76)	0.9394(4)	0.7706(2)	0.7639(3)	6.14(10)
C(77)	0.8283(4)	0.7439(2)	0.7612(3)	6.01(10)
C(78)	0.7353(4)	0.7415(2)	0.6791(3)	5.08(8)
C(79)	0.7493(3)	0.76640(13)	0.5970(2)	4.14(6)
C(80)	0.6522(3)	0.76710(13)	0.5122(2)	3.99(6)
C(81)	0.4222(3)	0.75665(14)	0.4689(2)	4.21(7)
C(82)	0.3123(3)	0.7257(2)	0.4582(2)	4.88(8)

C(83)	0.3194(3)	0.6727(2)	0.4761(3)	5.04(8)
C(84)	0.4351(3)	0.6461(2)	0.5017(2)	4.42(7)
C(85)	0.4439(4)	0.5904(2)	0.5179(3)	5.34(9)
C(86)	0.5560(5)	0.5650(2)	0.5414(3)	5.81(10)
C(87)	0.6653(4)	0.5942(2)	0.5456(3)	5.56(9)
C(88)	0.6617(4)	0.6477(2)	0.5313(3)	4.69(7)
C(89)	0.5467(3)	0.67650(14)	0.5109(2)	4.17(7)
C(90)	0.5389(3)	0.73310(14)	0.4987(2)	3.96(6)

Table 3. Bond lengths (A) and angles (deg) for C96 H72 B2 Cu2 N8 O8.

Cu(1)-N(2)	1.916(4)	Cu(1)-N(3)	1.973(4)
Cu(1)-N(1)	2.083(6)	Cu(1)-O(3)	2.165(2)
B(1)-O(4)	1.461(4)	B(1)-O(2)	1.467(4)
B(1)-O(1)	1.472(4)	B(1)-O(3)	1.489(4)
O(1)-C(1)	1.361(5)	O(2)-C(11)	1.358(4)
O(3)-C(21)	1.358(4)	O(4)-C(31)	1.357(4)
C(1)-C(10)	1.374(5)	C(1)-C(2)	1.426(5)
C(2)-C(3)	1.353(7)	C(3)-C(4)	1.409(7)
C(4)-C(5)	1.424(7)	C(4)-C(9)	1.428(5)
C(5)-C(6)	1.342(9)	C(6)-C(7)	1.413(8)
C(7)-C(8)	1.377(6)	C(8)-C(9)	1.410(6)
C(9)-C(10)	1.438(5)	C(10)-C(20)	1.485(4)
C(11)-C(20)	1.397(4)	C(11)-C(12)	1.408(5)
C(12)-C(13)	1.362(5)	C(13)-C(14)	1.418(5)
C(14)-C(15)	1.414(5)	C(14)-C(19)	1.427(5)
C(15)-C(16)	1.378(6)	C(16)-C(17)	1.416(6)
C(17)-C(18)	1.362(5)	C(18)-C(19)	1.432(5)
C(19)-C(20)	1.416(5)	C(21)-C(30)	1.394(5)
C(21)-C(22)	1.412(5)	C(22)-C(23)	1.377(7)
C(23)-C(24)	1.414(7)	C(24)-C(25)	1.410(6)
C(24)-C(29)	1.438(5)	C(25)-C(26)	1.350(9)
C(26)-C(27)	1.436(8)	C(27)-C(28)	1.371(5)
C(28)-C(29)	1.407(6)	C(29)-C(30)	1.432(5)
C(30)-C(40)	1.483(4)	C(31)-C(40)	1.385(4)
C(31)-C(32)	1.424(4)	C(32)-C(33)	1.357(5)
C(33)-C(34)	1.415(5)	C(34)-C(35)	1.412(5)
C(34)-C(39)	1.427(4)	C(35)-C(36)	1.377(5)
C(36)-C(37)	1.401(5)	C(37)-C(38)	1.373(5)
C(38)-C(39)	1.420(4)	C(39)-C(40)	1.434(4)
N(1)-C(41)	1.104(8)	C(41)-C(42)	1.453(9)
N(2)-C(43)	1.134(6)	C(43)-C(44)	1.441(7)
N(3)-C(45)	1.139(6)	C(45)-C(46)	1.438(6)
Cu(2)-N(6)	1.969(4)	Cu(2)-N(7)	2.001(4)
Cu(2)-N(5)	2.013(5)	Cu(2)-N(4)	2.054(4)
N(4)-C(91)	1.144(7)	C(91)-C(92)	1.436(7)
N(5)-C(95)	1.134(7)	C(95)-C(96)	1.438(7)
N(6)-C(97)	1.146(6)	C(97)-C(98)	1.440(6)
N(7)-C(99)	1.119(6)	C(99)-C(100)	1.458(8)
N(8)-C(101)	1.113(7)	C(101)-C(102)	1.453(8)
B(2)-O(7)	1.466(5)	B(2)-O(6)	1.468(5)
B(2)-O(8)	1.476(4)	B(2)-O(5)	1.479(5)
O(5)-C(51)	1.347(5)	O(6)-C(61)	1.347(4)
O(7)-C(71)	1.359(4)	O(8)-C(81)	1.353(4)
C(51)-C(60)	1.388(6)	C(51)-C(52)	1.421(5)
C(52)-C(53)	1.357(7)	C(53)-C(54)	1.415(8)
C(54)-C(59)	1.425(6)	C(54)-C(55)	1.429(7)
C(55)-C(56)	1.355(9)	C(56)-C(57)	1.391(8)
C(57)-C(58)	1.372(6)	C(58)-C(59)	1.416(6)
C(59)-C(60)	1.440(5)	C(60)-C(70)	1.488(5)
C(61)-C(70)	1.391(5)	C(61)-C(62)	1.423(5)
C(62)-C(63)	1.353(6)	C(63)-C(64)	1.415(5)
C(64)-C(65)	1.415(5)	C(64)-C(69)	1.426(5)
C(65)-C(66)	1.371(6)	C(66)-C(67)	1.397(6)
C(67)-C(68)	1.362(5)	C(68)-C(69)	1.431(5)
C(69)-C(70)	1.424(5)	C(71)-C(80)	1.376(5)
C(71)-C(72)	1.416(5)	C(72)-C(73)	1.361(6)

C(73)-C(74)	1.423(5)	C(74)-C(75)	1.412(6)
C(74)-C(79)	1.426(5)	C(75)-C(76)	1.369(7)
C(76)-C(77)	1.397(6)	C(77)-C(78)	1.383(6)
C(78)-C(79)	1.415(5)	C(79)-C(80)	1.434(5)
C(80)-C(90)	1.491(4)	C(81)-C(90)	1.391(5)
C(81)-C(82)	1.421(5)	C(82)-C(83)	1.357(6)
C(83)-C(84)	1.411(6)	C(84)-C(85)	1.420(6)
C(84)-C(89)	1.432(5)	C(85)-C(86)	1.362(7)
C(86)-C(87)	1.407(6)	C(87)-C(88)	1.358(6)
C(88)-C(89)	1.432(5)	C(89)-C(90)	1.433(5)

N(2)-Cu(1)-N(3)	127.9(2)	N(2)-Cu(1)-N(1)	112.3(2)
N(3)-Cu(1)-N(1)	91.7(2)	N(2)-Cu(1)-O(3)	108.40(12)
N(3)-Cu(1)-O(3)	99.81(14)	N(1)-Cu(1)-O(3)	116.2(2)
O(4)-B(1)-O(2)	105.5(3)	O(4)-B(1)-O(1)	112.0(3)
O(2)-B(1)-O(1)	113.9(3)	O(4)-B(1)-O(3)	111.3(3)
O(2)-B(1)-O(3)	111.3(3)	O(1)-B(1)-O(3)	103.1(3)
C(1)-O(1)-B(1)	117.4(3)	C(11)-O(2)-B(1)	115.0(2)
C(21)-O(3)-B(1)	115.2(2)	C(21)-O(3)-Cu(1)	126.4(2)
B(1)-O(3)-Cu(1)	114.5(2)	C(31)-O(4)-B(1)	115.4(2)
O(1)-C(1)-C(10)	119.6(3)	O(1)-C(1)-C(2)	119.1(3)
C(10)-C(1)-C(2)	121.3(3)	C(3)-C(2)-C(1)	120.2(4)
C(2)-C(3)-C(4)	121.1(3)	C(3)-C(4)-C(5)	122.6(4)
C(3)-C(4)-C(9)	119.1(4)	C(5)-C(4)-C(9)	118.3(4)
C(6)-C(5)-C(4)	122.8(4)	C(5)-C(6)-C(7)	119.1(5)
C(8)-C(7)-C(6)	120.4(5)	C(7)-C(8)-C(9)	121.5(4)
C(8)-C(9)-C(4)	117.9(4)	C(8)-C(9)-C(10)	122.6(3)
C(4)-C(9)-C(10)	119.4(3)	C(1)-C(10)-C(9)	118.5(3)
C(1)-C(10)-C(20)	119.3(3)	C(9)-C(10)-C(20)	122.1(3)
O(2)-C(11)-C(20)	120.4(3)	O(2)-C(11)-C(12)	119.3(3)
C(20)-C(11)-C(12)	120.3(3)	C(13)-C(12)-C(11)	121.2(3)
C(12)-C(13)-C(14)	120.3(3)	C(15)-C(14)-C(13)	121.5(3)
C(15)-C(14)-C(19)	119.7(3)	C(13)-C(14)-C(19)	118.8(3)
C(16)-C(15)-C(14)	121.0(3)	C(15)-C(16)-C(17)	119.8(3)
C(18)-C(17)-C(16)	120.2(3)	C(17)-C(18)-C(19)	121.8(3)
C(20)-C(19)-C(14)	120.1(3)	C(20)-C(19)-C(18)	122.6(3)
C(14)-C(19)-C(18)	117.3(3)	C(11)-C(20)-C(19)	118.8(3)
C(11)-C(20)-C(10)	118.5(3)	C(19)-C(20)-C(10)	122.7(3)
O(3)-C(21)-C(30)	120.7(3)	O(3)-C(21)-C(22)	117.9(3)
C(30)-C(21)-C(22)	121.3(3)	C(23)-C(22)-C(21)	119.8(4)
C(22)-C(23)-C(24)	121.2(3)	C(25)-C(24)-C(23)	122.0(4)
C(25)-C(24)-C(29)	118.9(4)	C(23)-C(24)-C(29)	119.1(4)
C(26)-C(25)-C(24)	121.5(4)	C(25)-C(26)-C(27)	120.3(4)
C(28)-C(27)-C(26)	119.3(5)	C(27)-C(28)-C(29)	121.7(4)
C(28)-C(29)-C(30)	122.5(3)	C(28)-C(29)-C(24)	118.3(3)
C(30)-C(29)-C(24)	119.1(3)	C(21)-C(30)-C(29)	119.1(3)
C(21)-C(30)-C(40)	117.4(3)	C(29)-C(30)-C(40)	123.4(3)
O(4)-C(31)-C(40)	120.5(3)	O(4)-C(31)-C(32)	118.8(3)
C(40)-C(31)-C(32)	120.7(3)	C(33)-C(32)-C(31)	120.4(3)
C(32)-C(33)-C(34)	121.3(3)	C(35)-C(34)-C(33)	121.9(3)
C(35)-C(34)-C(39)	119.3(3)	C(33)-C(34)-C(39)	118.8(3)
C(36)-C(35)-C(34)	121.5(3)	C(35)-C(36)-C(37)	119.3(3)
C(38)-C(37)-C(36)	120.8(3)	C(37)-C(38)-C(39)	121.5(3)
C(38)-C(39)-C(34)	117.6(3)	C(38)-C(39)-C(40)	122.7(3)
C(34)-C(39)-C(40)	119.7(3)	C(31)-C(40)-C(39)	119.1(3)
C(31)-C(40)-C(30)	117.7(3)	C(39)-C(40)-C(30)	123.1(3)
C(41)-N(1)-Cu(1)	149.7(6)	N(1)-C(41)-C(42)	170.7(9)
C(43)-N(2)-Cu(1)	178.5(3)	N(2)-C(43)-C(44)	178.0(6)
C(45)-N(3)-Cu(1)	165.7(5)	N(3)-C(45)-C(46)	178.8(5)
N(6)-Cu(2)-N(7)	113.3(2)	N(6)-Cu(2)-N(5)	118.4(2)

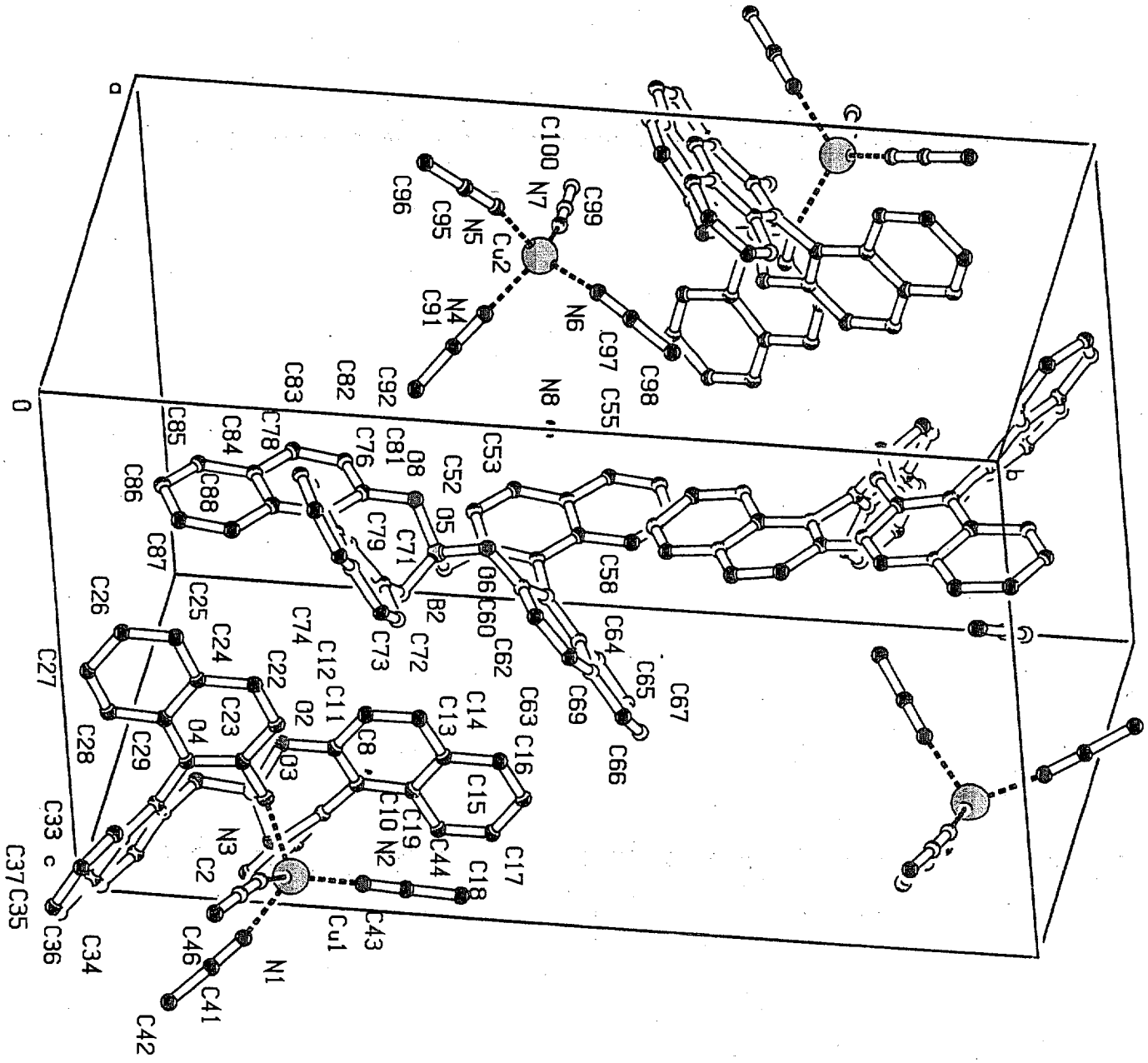
N(7)-Cu(2)-N(5)	112.4(2)	N(6)-Cu(2)-N(4)	102.8(2)
N(7)-Cu(2)-N(4)	110.4(2)	N(5)-Cu(2)-N(4)	97.5(2)
C(91)-N(4)-Cu(2)	167.4(4)	N(4)-C(91)-C(92)	178.3(5)
C(95)-N(5)-Cu(2)	165.9(4)	N(5)-C(95)-C(96)	178.9(5)
C(97)-N(6)-Cu(2)	171.5(4)	N(6)-C(97)-C(98)	178.8(5)
C(99)-N(7)-Cu(2)	173.2(4)	N(7)-C(99)-C(100)	178.3(5)
N(8)-C(101)-C(102)	179.1(6)	O(7)-B(2)-O(6)	113.8(3)
O(7)-B(2)-O(8)	113.1(3)	O(6)-B(2)-O(8)	103.0(3)
O(7)-B(2)-O(5)	103.4(3)	O(6)-B(2)-O(5)	112.3(3)
O(8)-B(2)-O(5)	111.5(3)	C(51)-O(5)-B(2)	117.1(3)
C(61)-O(6)-B(2)	117.1(3)	C(71)-O(7)-B(2)	116.1(3)
C(81)-O(8)-B(2)	119.1(3)	O(5)-C(51)-C(60)	120.8(3)
O(5)-C(51)-C(52)	118.7(4)	C(60)-C(51)-C(52)	120.4(4)
C(53)-C(52)-C(51)	120.8(5)	C(52)-C(53)-C(54)	121.1(4)
C(53)-C(54)-C(59)	119.0(4)	C(53)-C(54)-C(55)	121.9(4)
C(59)-C(54)-C(55)	119.1(5)	C(56)-C(55)-C(54)	121.0(5)
C(55)-C(56)-C(57)	119.9(4)	C(58)-C(57)-C(56)	121.2(5)
C(57)-C(58)-C(59)	120.9(4)	C(58)-C(59)-C(54)	117.7(4)
C(58)-C(59)-C(60)	122.7(3)	C(54)-C(59)-C(60)	119.5(4)
C(51)-C(60)-C(59)	119.0(3)	C(51)-C(60)-C(70)	118.9(3)
C(59)-C(60)-C(70)	121.9(3)	O(6)-C(61)-C(70)	121.7(3)
O(6)-C(61)-C(62)	117.9(3)	C(70)-C(61)-C(62)	120.2(3)
C(63)-C(62)-C(61)	120.7(3)	C(62)-C(63)-C(64)	121.0(3)
C(65)-C(64)-C(63)	121.8(3)	C(65)-C(64)-C(69)	119.6(3)
C(63)-C(64)-C(69)	118.6(3)	C(66)-C(65)-C(64)	121.0(4)
C(65)-C(66)-C(67)	119.7(4)	C(68)-C(67)-C(66)	121.1(4)
C(67)-C(68)-C(69)	121.2(4)	C(70)-C(69)-C(64)	120.0(3)
C(70)-C(69)-C(68)	122.6(3)	C(64)-C(69)-C(68)	117.3(3)
C(61)-C(70)-C(69)	118.7(3)	C(61)-C(70)-C(60)	118.0(3)
C(69)-C(70)-C(60)	123.2(3)	O(7)-C(71)-C(80)	121.5(3)
O(7)-C(71)-C(72)	117.8(3)	C(80)-C(71)-C(72)	120.7(3)
C(73)-C(72)-C(71)	120.5(3)	C(72)-C(73)-C(74)	120.9(3)
C(75)-C(74)-C(73)	122.0(3)	C(75)-C(74)-C(79)	119.4(3)
C(73)-C(74)-C(79)	118.6(3)	C(76)-C(75)-C(74)	121.0(4)
C(75)-C(76)-C(77)	120.3(4)	C(78)-C(77)-C(76)	120.1(4)
C(77)-C(78)-C(79)	121.3(4)	C(78)-C(79)-C(74)	117.8(3)
C(78)-C(79)-C(80)	122.7(3)	C(74)-C(79)-C(80)	119.4(3)
C(71)-C(80)-C(79)	119.1(3)	C(71)-C(80)-C(90)	118.9(3)
C(79)-C(80)-C(90)	122.0(3)	O(8)-C(81)-C(90)	120.9(3)
O(8)-C(81)-C(82)	118.4(3)	C(90)-C(81)-C(82)	120.5(3)
C(83)-C(82)-C(81)	120.6(3)	C(82)-C(83)-C(84)	121.4(3)
C(83)-C(84)-C(85)	122.0(3)	C(83)-C(84)-C(89)	118.7(3)
C(85)-C(84)-C(89)	119.2(4)	C(86)-C(85)-C(84)	121.5(3)
C(85)-C(86)-C(87)	119.3(4)	C(88)-C(87)-C(86)	121.2(4)
C(87)-C(88)-C(89)	121.4(4)	C(88)-C(89)-C(84)	117.1(3)
C(88)-C(89)-C(90)	123.3(3)	C(84)-C(89)-C(90)	119.6(3)
C(81)-C(90)-C(89)	118.9(3)	C(81)-C(90)-C(80)	119.1(3)
C(89)-C(90)-C(80)	122.0(3)		

Table 4. Torsion angles (deg) for C96 H72 B2 Cu2 N8 O8.

O(4)-B(1)-O(1)-C(1)	79.1(4)	O(2)-B(1)-O(1)-C(1)	-40.4(4)
O(3)-B(1)-O(1)-C(1)	-161.2(3)	O(4)-B(1)-O(2)-C(11)	-170.1(3)
O(1)-B(1)-O(2)-C(11)	-46.9(4)	O(3)-B(1)-O(2)-C(11)	69.1(3)
O(4)-B(1)-O(3)-C(21)	-46.6(4)	O(2)-B(1)-O(3)-C(21)	70.7(3)
O(1)-B(1)-O(3)-C(21)	-166.8(2)	O(4)-B(1)-O(3)-Cu(1)	112.8(2)
O(2)-B(1)-O(3)-Cu(1)	-129.9(2)	O(1)-B(1)-O(3)-Cu(1)	-7.4(3)
N(2)-Cu(1)-O(3)-C(21)	-125.5(3)	N(3)-Cu(1)-O(3)-C(21)	10.1(3)
N(1)-Cu(1)-O(3)-C(21)	107.0(3)	N(2)-Cu(1)-O(3)-B(1)	77.8(2)
N(3)-Cu(1)-O(3)-B(1)	-146.6(2)	N(1)-Cu(1)-O(3)-B(1)	-49.7(3)
O(2)-B(1)-O(4)-C(31)	-163.7(2)	O(1)-B(1)-O(4)-C(31)	71.9(4)
O(3)-B(1)-O(4)-C(31)	-42.9(4)	B(1)-O(1)-C(1)-C(10)	67.6(4)
B(1)-O(1)-C(1)-C(2)	-114.7(3)	O(1)-C(1)-C(2)-C(3)	179.3(3)
C(10)-C(1)-C(2)-C(3)	-3.0(5)	C(1)-C(2)-C(3)-C(4)	-2.5(6)
C(2)-C(3)-C(4)-C(5)	-174.8(4)	C(2)-C(3)-C(4)-C(9)	4.2(6)
C(3)-C(4)-C(5)-C(6)	177.7(5)	C(9)-C(4)-C(5)-C(6)	-1.2(7)
C(4)-C(5)-C(6)-C(7)	0.7(8)	C(5)-C(6)-C(7)-C(8)	-0.3(8)
C(6)-C(7)-C(8)-C(9)	0.5(7)	C(7)-C(8)-C(9)-C(4)	-1.0(6)
C(7)-C(8)-C(9)-C(10)	-178.1(4)	C(3)-C(4)-C(9)-C(8)	-177.7(3)
C(5)-C(4)-C(9)-C(8)	1.3(5)	C(3)-C(4)-C(9)-C(10)	-0.4(5)
C(5)-C(4)-C(9)-C(10)	178.5(3)	O(1)-C(1)-C(10)-C(9)	-175.7(3)
C(2)-C(1)-C(10)-C(9)	6.6(5)	O(1)-C(1)-C(10)-C(20)	1.6(4)
C(2)-C(1)-C(10)-C(20)	-176.1(3)	C(8)-C(9)-C(10)-C(1)	172.2(3)
C(4)-C(9)-C(10)-C(1)	-4.9(5)	C(8)-C(9)-C(10)-C(20)	-4.9(5)
C(4)-C(9)-C(10)-C(20)	178.0(3)	B(1)-O(2)-C(11)-C(20)	68.0(4)
B(1)-O(2)-C(11)-C(12)	-114.9(3)	O(2)-C(11)-C(12)-C(13)	178.6(3)
C(20)-C(11)-C(12)-C(13)	-4.3(5)	C(11)-C(12)-C(13)-C(14)	-1.6(5)
C(12)-C(13)-C(14)-C(15)	-179.3(3)	C(12)-C(13)-C(14)-C(19)	3.0(5)
C(13)-C(14)-C(15)-C(16)	-178.5(3)	C(19)-C(14)-C(15)-C(16)	-0.9(5)
C(14)-C(15)-C(16)-C(17)	-2.4(6)	C(15)-C(16)-C(17)-C(18)	1.9(6)
C(16)-C(17)-C(18)-C(19)	1.8(6)	C(15)-C(14)-C(19)-C(20)	-176.4(3)
C(13)-C(14)-C(19)-C(20)	1.3(5)	C(15)-C(14)-C(19)-C(18)	4.4(5)
C(13)-C(14)-C(19)-C(18)	-177.9(3)	C(17)-C(18)-C(19)-C(20)	175.9(3)
C(17)-C(18)-C(19)-C(14)	-4.9(5)	O(2)-C(11)-C(20)-C(19)	-174.5(3)
C(12)-C(11)-C(20)-C(19)	8.4(4)	O(2)-C(11)-C(20)-C(10)	3.9(4)
C(12)-C(11)-C(20)-C(10)	-173.2(3)	C(14)-C(19)-C(20)-C(11)	-6.9(4)
C(18)-C(19)-C(20)-C(11)	172.2(3)	C(14)-C(19)-C(20)-C(10)	174.8(3)
C(18)-C(19)-C(20)-C(10)	-6.1(5)	C(1)-C(10)-C(20)-C(11)	-52.8(4)
C(9)-C(10)-C(20)-C(11)	124.4(3)	C(1)-C(10)-C(20)-C(19)	125.5(3)
C(9)-C(10)-C(20)-C(19)	-57.3(4)	B(1)-O(3)-C(21)-C(30)	69.9(4)
Cu(1)-O(3)-C(21)-C(30)	-86.7(3)	B(1)-O(3)-C(21)-C(22)	-109.8(3)
Cu(1)-O(3)-C(21)-C(22)	93.7(3)	O(3)-C(21)-C(22)-C(23)	174.9(3)
C(30)-C(21)-C(22)-C(23)	-4.7(5)	C(21)-C(22)-C(23)-C(24)	-1.0(6)
C(22)-C(23)-C(24)-C(25)	-175.7(4)	C(22)-C(23)-C(24)-C(29)	3.8(5)
C(23)-C(24)-C(25)-C(26)	179.5(4)	C(29)-C(24)-C(25)-C(26)	0.1(6)
C(24)-C(25)-C(26)-C(27)	-1.4(7)	C(25)-C(26)-C(27)-C(28)	1.0(7)
C(26)-C(27)-C(28)-C(29)	0.7(6)	C(27)-C(28)-C(29)-C(30)	-178.7(3)
C(27)-C(28)-C(29)-C(24)	-2.0(5)	C(25)-C(24)-C(29)-C(28)	1.6(5)
C(23)-C(24)-C(29)-C(28)	-177.9(3)	C(25)-C(24)-C(29)-C(30)	178.4(3)
C(23)-C(24)-C(29)-C(30)	-1.1(5)	O(3)-C(21)-C(30)-C(29)	-172.3(3)
C(22)-C(21)-C(30)-C(29)	7.3(5)	O(3)-C(21)-C(30)-C(40)	4.0(4)
C(22)-C(21)-C(30)-C(40)	-176.4(3)	C(28)-C(29)-C(30)-C(21)	172.3(3)
C(24)-C(29)-C(30)-C(21)	-4.4(4)	C(28)-C(29)-C(30)-C(40)	-3.7(5)
C(24)-C(29)-C(30)-C(40)	179.6(3)	B(1)-O(4)-C(31)-C(40)	74.0(4)
B(1)-O(4)-C(31)-C(32)	-106.6(3)	O(4)-C(31)-C(32)-C(33)	-179.4(3)
C(40)-C(31)-C(32)-C(33)	0.1(5)	C(31)-C(32)-C(33)-C(34)	-1.6(5)
C(32)-C(33)-C(34)-C(35)	-178.0(3)	C(32)-C(33)-C(34)-C(39)	0.5(5)

C(33)-C(34)-C(35)-C(36)	178.4(3)	C(39)-C(34)-C(35)-C(36)	-0.1(5)
C(34)-C(35)-C(36)-C(37)	-1.5(6)	C(35)-C(36)-C(37)-C(38)	1.2(6)
C(36)-C(37)-C(38)-C(39)	0.8(6)	C(37)-C(38)-C(39)-C(34)	-2.4(5)
C(37)-C(38)-C(39)-C(40)	179.1(3)	C(35)-C(34)-C(39)-C(38)	2.1(4)
C(33)-C(34)-C(39)-C(38)	-176.5(3)	C(35)-C(34)-C(39)-C(40)	-179.4(3)
C(33)-C(34)-C(39)-C(40)	2.0(4)	O(4)-C(31)-C(40)-C(39)	-178.2(3)
C(32)-C(31)-C(40)-C(39)	2.4(4)	O(4)-C(31)-C(40)-C(30)	-2.5(4)
C(32)-C(31)-C(40)-C(30)	178.1(3)	C(38)-C(39)-C(40)-C(31)	175.0(3)
C(34)-C(39)-C(40)-C(31)	-3.4(4)	C(38)-C(39)-C(40)-C(30)	-0.4(5)
C(34)-C(39)-C(40)-C(30)	-178.8(3)	C(21)-C(30)-C(40)-C(31)	-51.2(4)
C(29)-C(30)-C(40)-C(31)	124.9(3)	C(21)-C(30)-C(40)-C(39)	124.3(3)
C(29)-C(30)-C(40)-C(39)	-59.6(4)	N(2)-Cu(1)-N(1)-C(41)	136.8(11)
N(3)-Cu(1)-N(1)-C(41)	4.2(11)	O(3)-Cu(1)-N(1)-C(41)	-97.6(11)
Cu(1)-N(1)-C(41)-C(42)	1(5)	N(3)-Cu(1)-N(2)-C(43)	35(15)
N(1)-Cu(1)-N(2)-C(43)	-76(15)	O(3)-Cu(1)-N(2)-C(43)	154(15)
Cu(1)-N(2)-C(43)-C(44)	-55(25)	N(2)-Cu(1)-N(3)-C(45)	-92(2)
N(1)-Cu(1)-N(3)-C(45)	29(2)	O(3)-Cu(1)-N(3)-C(45)	146(2)
Cu(1)-N(3)-C(45)-C(46)	18(27)	N(6)-Cu(2)-N(4)-C(91)	65(2)
N(7)-Cu(2)-N(4)-C(91)	-173(2)	N(5)-Cu(2)-N(4)-C(91)	-56(2)
Cu(2)-N(4)-C(91)-C(92)	-111(20)	N(6)-Cu(2)-N(5)-C(95)	-96(2)
N(7)-Cu(2)-N(5)-C(95)	129(2)	N(4)-Cu(2)-N(5)-C(95)	14(2)
Cu(2)-N(5)-C(95)-C(96)	-148(26)	N(7)-Cu(2)-N(6)-C(97)	-71(2)
N(5)-Cu(2)-N(6)-C(97)	154(2)	N(4)-Cu(2)-N(6)-C(97)	48(2)
Cu(2)-N(6)-C(97)-C(98)	13(22)	N(6)-Cu(2)-N(7)-C(99)	162(4)
N(5)-Cu(2)-N(7)-C(99)	-61(4)	N(4)-Cu(2)-N(7)-C(99)	47(4)
Cu(2)-N(7)-C(99)-C(100)	-59(22)	O(7)-B(2)-O(5)-C(51)	-163.6(3)
O(6)-B(2)-O(5)-C(51)	-40.4(4)	O(8)-B(2)-O(5)-C(51)	74.6(4)
O(7)-B(2)-O(6)-C(61)	70.7(4)	O(8)-B(2)-O(6)-C(61)	-166.5(3)
O(5)-B(2)-O(6)-C(61)	-46.4(4)	O(6)-B(2)-O(7)-C(71)	66.2(4)
O(8)-B(2)-O(7)-C(71)	-50.9(4)	O(5)-B(2)-O(7)-C(71)	-171.7(3)
O(7)-B(2)-O(8)-C(81)	-34.1(4)	O(6)-B(2)-O(8)-C(81)	-157.4(3)
O(5)-B(2)-O(8)-C(81)	81.9(4)	B(2)-O(5)-C(51)-C(60)	70.3(4)
B(2)-O(5)-C(51)-C(52)	-112.4(4)	O(5)-C(51)-C(52)-C(53)	-178.3(4)
C(60)-C(51)-C(52)-C(53)	-0.9(6)	C(51)-C(52)-C(53)-C(54)	-0.9(6)
C(52)-C(53)-C(54)-C(59)	0.0(6)	C(52)-C(53)-C(54)-C(55)	-178.2(4)
C(53)-C(54)-C(55)-C(56)	176.1(4)	C(59)-C(54)-C(55)-C(56)	-2.2(7)
C(54)-C(55)-C(56)-C(57)	-0.6(7)	C(55)-C(56)-C(57)-C(58)	1.9(7)
C(56)-C(57)-C(58)-C(59)	-0.3(6)	C(57)-C(58)-C(59)-C(54)	-2.4(5)
C(57)-C(58)-C(59)-C(60)	-179.6(3)	C(53)-C(54)-C(59)-C(58)	-174.7(4)
C(55)-C(54)-C(59)-C(58)	3.6(5)	C(53)-C(54)-C(59)-C(60)	2.6(5)
C(55)-C(54)-C(59)-C(60)	-179.1(3)	O(5)-C(51)-C(60)-C(59)	-179.2(3)
C(52)-C(51)-C(60)-C(59)	3.5(5)	O(5)-C(51)-C(60)-C(70)	-2.6(5)
C(52)-C(51)-C(60)-C(70)	-179.9(3)	C(58)-C(59)-C(60)-C(51)	172.8(3)
C(54)-C(59)-C(60)-C(51)	-4.3(5)	C(58)-C(59)-C(60)-C(70)	-3.6(5)
C(54)-C(59)-C(60)-C(70)	179.2(3)	B(2)-O(6)-C(61)-C(70)	67.3(4)
B(2)-O(6)-C(61)-C(62)	-116.5(4)	O(6)-C(61)-C(62)-C(63)	179.9(3)
C(70)-C(61)-C(62)-C(63)	-3.8(5)	C(61)-C(62)-C(63)-C(64)	-3.3(6)
C(62)-C(63)-C(64)-C(65)	-173.5(4)	C(62)-C(63)-C(64)-C(69)	4.2(5)
C(63)-C(64)-C(65)-C(66)	175.3(4)	C(69)-C(64)-C(65)-C(66)	-2.4(5)
C(64)-C(65)-C(66)-C(67)	-0.2(6)	C(65)-C(66)-C(67)-C(68)	2.1(6)
C(66)-C(67)-C(68)-C(69)	-1.4(5)	C(65)-C(64)-C(69)-C(70)	179.5(3)
C(63)-C(64)-C(69)-C(70)	1.7(5)	C(65)-C(64)-C(69)-C(68)	3.1(5)
C(63)-C(64)-C(69)-C(68)	-174.7(3)	C(67)-C(68)-C(69)-C(70)	-177.6(3)
C(67)-C(68)-C(69)-C(64)	-1.2(5)	O(6)-C(61)-C(70)-C(69)	-174.3(3)
C(62)-C(61)-C(70)-C(69)	9.6(5)	O(6)-C(61)-C(70)-C(60)	4.5(5)
C(62)-C(61)-C(70)-C(60)	-171.7(3)	C(64)-C(69)-C(70)-C(61)	-8.5(5)
C(68)-C(69)-C(70)-C(61)	167.7(3)	C(64)-C(69)-C(70)-C(60)	172.8(3)
C(68)-C(69)-C(70)-C(60)	-11.0(5)	C(51)-C(60)-C(70)-C(61)	-49.5(4)
C(59)-C(60)-C(70)-C(61)	127.0(3)	C(51)-C(60)-C(70)-C(69)	129.3(3)
C(59)-C(60)-C(70)-C(69)	-54.3(5)	B(2)-O(7)-C(71)-C(80)	66.4(4)

B(2)-O(7)-C(71)-C(72)	-116.0(3)	O(7)-C(71)-C(72)-C(73)	177.5(3)
C(80)-C(71)-C(72)-C(73)	-4.9(5)	C(71)-C(72)-C(73)-C(74)	-2.9(5)
C(72)-C(73)-C(74)-C(75)	-172.5(4)	C(72)-C(73)-C(74)-C(79)	4.2(5)
C(73)-C(74)-C(75)-C(76)	173.5(4)	C(79)-C(74)-C(75)-C(76)	-3.2(6)
C(74)-C(75)-C(76)-C(77)	1.7(7)	C(75)-C(76)-C(77)-C(78)	0.3(8)
C(76)-C(77)-C(78)-C(79)	-0.9(7)	C(77)-C(78)-C(79)-C(74)	-0.5(6)
C(77)-C(78)-C(79)-C(80)	-176.6(4)	C(75)-C(74)-C(79)-C(78)	2.5(5)
C(73)-C(74)-C(79)-C(78)	-174.3(3)	C(75)-C(74)-C(79)-C(80)	178.7(3)
C(73)-C(74)-C(79)-C(80)	1.9(5)	O(7)-C(71)-C(80)-C(79)	-171.6(3)
C(72)-C(71)-C(80)-C(79)	10.9(5)	O(7)-C(71)-C(80)-C(90)	7.1(5)
C(72)-C(71)-C(80)-C(90)	-170.4(3)	C(78)-C(79)-C(80)-C(71)	166.7(3)
C(74)-C(79)-C(80)-C(71)	-9.4(5)	C(78)-C(79)-C(80)-C(90)	-12.0(5)
C(74)-C(79)-C(80)-C(90)	172.0(3)	B(2)-O(8)-C(81)-C(90)	66.3(4)
B(2)-O(8)-C(81)-C(82)	-118.1(3)	O(8)-C(81)-C(82)-C(83)	-176.2(3)
C(90)-C(81)-C(82)-C(83)	-0.5(5)	C(81)-C(82)-C(83)-C(84)	-2.9(5)
C(82)-C(83)-C(84)-C(85)	-178.1(3)	C(82)-C(83)-C(84)-C(89)	1.6(5)
C(83)-C(84)-C(85)-C(86)	179.2(3)	C(89)-C(84)-C(85)-C(86)	-0.5(5)
C(84)-C(85)-C(86)-C(87)	-3.0(6)	C(85)-C(86)-C(87)-C(88)	3.5(6)
C(86)-C(87)-C(88)-C(89)	-0.4(6)	C(87)-C(88)-C(89)-C(84)	-3.0(5)
C(87)-C(88)-C(89)-C(90)	177.7(3)	C(83)-C(84)-C(89)-C(88)	-176.3(3)
C(85)-C(84)-C(89)-C(88)	3.4(5)	C(83)-C(84)-C(89)-C(90)	3.0(5)
C(85)-C(84)-C(89)-C(90)	-177.3(3)	O(8)-C(81)-C(90)-C(89)	-179.4(3)
C(82)-C(81)-C(90)-C(89)	5.1(4)	O(8)-C(81)-C(90)-C(80)	-2.4(4)
C(82)-C(81)-C(90)-C(80)	-177.9(3)	C(88)-C(89)-C(90)-C(81)	172.9(3)
C(84)-C(89)-C(90)-C(81)	-6.3(4)	C(88)-C(89)-C(90)-C(80)	-3.9(5)
C(84)-C(89)-C(90)-C(80)	176.8(3)	C(71)-C(80)-C(90)-C(81)	-50.6(4)
C(79)-C(80)-C(90)-C(81)	128.1(3)	C(71)-C(80)-C(90)-C(89)	126.3(3)
C(79)-C(80)-C(90)-C(89)	-55.0(4)		


a
0
b
c
C100
N7
C99
C96
C95
N5
Cu2
N4
C91
N6
C97
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C98
C92
C83
C82
N8
C85
C84
C78
C76
O8
C81
C53
C52
O5
C86
C88
C87
C79
C71
O6
C60
C62
C58
C64
C65
C67
C69
C66
C63
C16
C26
C25
C24
C74
C12
C11
C73
C72
B2
C14
C13
C27
C22
O2
C8
C15
C28
C23
O4
O3
C19
C10
N2
C44
C17
C18
C29
C33
N3
C2
C43
Cu1
C37
C35
C36
C34
C46
N1
C41
C42

Table 1. Crystal data and structure refinement for C58 H40 B Cu N2 O4.

Crystal data		
Chemical formula, sum	C58 H40 B Cu N2 O4	
Chemical formula, moiety	C58 H40 B Cu N2 O4	
Chemical formula weight, Mr	1023.52	
Cell setting	Monoclinic	
Space group	P2(1)	
Unit cell dimensions (A, deg)	a = 12.7853(3)	alpha = 90.0000(10)
	b = 15.7945(3)	beta = 101.9080(10)
	c = 13.2045(2)	gamma = 90.0000(10)
Volume of unit cell, V (A^3)	2609.10(9)	
Formula units per cell, Z	2	
Formula units per assymetric unit, Z'	1	
Density calculated from formula and cell, Dx (Mg/m^3)	1.303	
F(000)	1057	
Radiation type	CuK\a	
Wavelength, lambda (A)	1.54178	
No. of reflections for cell measurement	2475	
Theta range (deg)	3.5 to 53	
Linear absorption coefficient, mu (mm^-1)	2.164	
Measurement temperature (K)	293(2)	
Crystal shape	plate	
Colour	colourless	
Size (mm)	0.54 x 0.34 x 0.09	
Data collection		
Diffractometer type	Bruker Smart-2000	
Data-collection method	omega scans	
Absorption correction type	multi scan	
Maximum and minimum transmission		

values, Tmax and Tmin	1.00 and 0.48
No. of reflections measured	22205
No. of independent reflections	8336
Completeness of data to Theta max	97.7
No. of observed reflections	5114
Criterion for observed reflections	>2\s(I)
Rint	0.1000
Minimum and maximum values of theta (deg)	3.42 to 73.05
Ranges of h,k,l	-15<=h<=15, -15<=k<=18, -16<=l<=16
Refinement	
Refinement method	Full-matrix on F^2
Final R indices, I>2sigma(I)	R1 = 0.0968, wR2 = 0.2291
R indices, all data	R1 = 0.1149, wR2 = 0.2461
Goodness-of-fit on F^2, S	0.950

R1 = sum (absabs Foabs -abs Fcabsabs)/sum (abs Foabs),
wR2 = [sum [w(Fo^2^-Fc^2^)^2^]/sum [w(Fo^2^)^2^]]^1*2^ and
GoF = [sum [w(Fo^2^-Fc^2^)^2^]/(No. of reflns - No. of params.)]^1*2^

No. of reflections used in refinement	8336
No. of parameters refined	596
No. of restraints	12
Method of refining and locating H atoms	constrained
Weighting scheme	based on measured s.u.'s
Function minimized	sum w(Fo^2^-Fc^2^)

w=1/[\s^2^(Fo^2^)+(0.1309P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Maximum shift/sigma	0.004
DELTA rho max (e A ^-3^)	0.400
DELTA rho min (e A ^-3^)	-0.433
Extinction correction method	SHELXL-93 (1993)
Secondary extinction value	0.0004(2)

Absolute structure method	Flack, H.D. (1983)
Absolute structure parameter	0.11(6)

Discussion data collection, structure determination and refinement procedure

Data was collected on Bruker SMART-2000 Charge-coupled Device (CCD) Area Detector
Crystal to detector distance was 4.908 cm, data collection was carried out in 512 x 512 pixel mode, utilizing 4 x 4 pixel binning.
The initial unit cell parameters were determined by a least-squares fit of the angular setting of strong reflections, collected by a .3 degree scan in omega in 30 frames at four different phi settings (120) frames total).
One complete hemisphere of data was collected to better than 0.82 A resolution.
Data was collected at 2 different detector 2theta settings: -38 and -110 deg.
At the -38 degree setting, 606 frames were collected for each of 4 phi positions. At the -110 degree setting, data was collected at 8 different phi positions for 606 frames each.

Data reduction processing was carried out by the use of the program SAINT (Siemens, 1999), which applied Lorentz and polarization corrections to three-dimensionally integrated diffraction spots.
The program SADABS (Sheldrick, 1996) was utilized for the scaling of diffraction data, the application of a decay correction, and an empirical absorption correction based on redundant reflections.
The space group was confirmed by XPREP routine in SHELXTL program (Sheldrick, 1998).
The structure was solved by direct method using SHELXS96 (Sheldrick, 1996) and difmap synthesis using SHELXL96 (Sheldrick, 1996). All non-hydrogen atoms anisotropic, hydrogen atoms are isotropic. Hydrogen atoms are constrained to the parent site using a riding model; SHELXL96 defaults, C-H 0.93 to 0.98%A.
The isotropic factors, Uiso, were adjusted to a value 20% higher then Ueq of the parent site.
The program PLATON (Spek, 1990) was used to verify for possible voids.
The structure has a void of 550 cubic A which contains 190 electrons.
This corresponds to 2.25 dichloromethane molecules per cation and anion.
This corresponds to the elemental analysis results and was considered in calculating Fw, density, absorption coefficient and F(000).
Contribution of this disordered solvent area to the overall diffraction was dealt with using option SQUEEZE in PLATON which subtracts the solvent contribution from the structure factors. Final agreement factors are calculated against these modified structures factors.

The phenyl group of the styrene ligand shows large thermal motion.

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (A^2^ x 10 ^2^) for C58 H40 B Cu N2 O4.

U~eq~ = (1/3)sum~i~sum~j~U~ij~a^*^~i~a^*^~j~a~i~.a~j~.

	x	y	z	U~eq~
Cu	0.52347(7)	0.10675(8)	0.33933(8)	6.33(3)
N(1)	0.6551(5)	0.1362(4)	0.4380(5)	6.07(14)
N(2)	0.6258(5)	0.0404(5)	0.2742(5)	6.30(14)
C(1)	0.6651(8)	0.1861(6)	0.5242(7)	8.1(2)
C(2)	0.7641(9)	0.1913(6)	0.5950(8)	8.5(2)
C(3)	0.8501(7)	0.1519(7)	0.5764(9)	9.0(3)
C(4)	0.8439(6)	0.1068(7)	0.4889(6)	7.7(2)
C(5)	0.7434(5)	0.0969(5)	0.4197(5)	5.59(13)
C(6)	0.7250(5)	0.0457(5)	0.3236(5)	5.8(2)
C(7)	0.8079(7)	0.0054(6)	0.2910(6)	7.7(2)
C(8)	0.7858(8)	-0.0413(7)	0.1997(7)	8.4(3)
C(9)	0.6843(10)	-0.0464(7)	0.1493(8)	9.8(3)
C(10)	0.5996(8)	-0.0039(7)	0.1840(7)	8.1(2)
C(11)	0.3965(8)	0.1820(8)	0.3434(8)	9.1(3)
C(12)	0.3739(6)	0.1319(6)	0.2601(7)	7.7(2)
C(13)	0.3805(7)	0.1574(6)	0.1519(6)	7.6(2)
C(14)	0.4246(12)	0.2359(9)	0.1314(8)	11.7(5)
C(15)	0.4322(13)	0.2567(11)	0.0294(9)	13.0(6)
C(16)	0.385(2)	0.2058(14)	-0.0522(12)	20.3(12)
C(17)	0.346(2)	0.127(2)	-0.0319(11)	22.0(14)
C(18)	0.3419(11)	0.1012(12)	0.0699(8)	13.0(5)
B	0.4428(5)	-0.0870(5)	0.4221(5)	4.65(13)
O(1)	0.4238(3)	-0.0699(3)	0.3115(3)	5.43(10)
O(2)	0.3464(3)	-0.0945(3)	0.4643(3)	5.54(10)
O(3)	0.5125(3)	-0.0130(3)	0.4658(3)	5.34(9)
O(4)	0.4971(3)	-0.1680(3)	0.4531(4)	5.69(10)
C(19)	0.3453(5)	-0.1179(4)	0.2508(5)	4.98(13)
C(20)	0.2387(4)	-0.1054(4)	0.2547(4)	4.52(11)
C(21)	0.1609(5)	-0.1607(4)	0.1946(4)	4.97(13)
C(22)	0.0547(5)	-0.1625(5)	0.2044(5)	5.58(14)
C(23)	-0.0176(6)	-0.2194(6)	0.1445(6)	7.3(2)
C(24)	0.0129(8)	-0.2737(9)	0.0748(8)	9.7(3)
C(25)	0.1157(8)	-0.2714(7)	0.0613(7)	8.6(3)
C(26)	0.1946(6)	-0.2164(6)	0.1205(6)	6.7(2)
C(27)	0.3007(7)	-0.2194(6)	0.1132(6)	7.3(2)
C(28)	0.3746(6)	-0.1746(5)	0.1785(6)	6.4(2)
C(29)	0.2679(5)	-0.0384(4)	0.4287(4)	5.15(13)
C(30)	0.2108(4)	-0.0423(4)	0.3258(4)	4.56(11)
C(31)	0.1334(5)	0.0254(4)	0.2921(5)	5.21(13)
C(32)	0.0822(6)	0.0316(5)	0.1872(6)	6.5(2)
C(33)	0.0120(8)	0.0991(9)	0.1555(9)	10.4(4)
C(34)	-0.0116(8)	0.1572(7)	0.2248(8)	9.1(3)
C(35)	0.0384(7)	0.1533(6)	0.3253(8)	8.5(3)
C(36)	0.1118(6)	0.0870(4)	0.3621(6)	6.1(2)
C(37)	0.1669(6)	0.0832(5)	0.4665(7)	7.4(2)
C(38)	0.2416(6)	0.0213(6)	0.4982(6)	6.7(2)
C(39)	0.5702(5)	-0.0187(4)	0.5628(5)	5.19(13)
C(40)	0.6528(4)	-0.0772(4)	0.5913(5)	4.98(12)

C(41)	0.7045(5)	-0.0828(5)	0.6988(5)	5.7(2)
C(42)	0.7774(6)	-0.1472(6)	0.7373(6)	6.4(2)
C(43)	0.8279(8)	-0.1501(8)	0.8405(6)	8.5(3)
C(44)	0.8135(10)	-0.0824(10)	0.9086(7)	10.8(4)
C(45)	0.7330(8)	-0.0244(7)	0.8748(5)	8.5(3)
C(46)	0.6785(6)	-0.0205(6)	0.7687(5)	6.6(2)
C(47)	0.6031(7)	0.0395(6)	0.7359(6)	7.6(2)
C(48)	0.5442(6)	0.0407(5)	0.6345(6)	6.6(2)
C(49)	0.6019(4)	-0.1755(4)	0.4450(4)	4.53(11)
C(50)	0.6818(5)	-0.1332(4)	0.5124(4)	4.77(12)
C(51)	0.7896(5)	-0.1399(4)	0.4967(5)	5.12(13)
C(52)	0.8763(5)	-0.0926(5)	0.5541(5)	5.83(14)
C(53)	0.9764(6)	-0.1013(6)	0.5380(6)	6.4(2)
C(54)	1.0000(6)	-0.1575(7)	0.4630(7)	7.8(2)
C(55)	0.9189(6)	-0.2047(6)	0.4074(6)	7.3(2)
C(56)	0.8115(5)	-0.1982(5)	0.4214(5)	5.51(14)
C(57)	0.7290(6)	-0.2423(5)	0.3586(5)	6.4(2)
C(58)	0.6248(6)	-0.2324(5)	0.3704(5)	6.0(2)

Table 3. Bond lengths (A) and angles (deg) for C58 H40 B Cu N2 O4.

Cu-N(1)	1.960(7)	Cu-N(2)	2.003(6)
Cu-C(12)	2.021(9)	Cu-C(11)	2.022(10)
Cu-O(3)	2.546(5)	N(1)-C(5)	1.353(8)
N(1)-C(1)	1.367(10)	N(2)-C(6)	1.304(10)
N(2)-C(10)	1.362(10)	C(1)-C(2)	1.412(14)
C(1)-H(1)	0.9300	C(2)-C(3)	1.33(2)
C(2)-H(2)	0.9300	C(3)-C(4)	1.35(2)
C(3)-H(3)	0.9300	C(4)-C(5)	1.424(10)
C(4)-H(4)	0.9300	C(5)-C(6)	1.482(10)
C(6)-C(7)	1.379(9)	C(7)-C(8)	1.391(13)
C(7)-H(7)	0.9300	C(8)-C(9)	1.33(2)
C(8)-H(8)	0.9300	C(9)-C(10)	1.428(13)
C(9)-H(9)	0.9300	C(10)-H(10)	0.9300
C(11)-C(12)	1.34(2)	C(11)-H(11A)	0.9300
C(11)-H(11B)	0.9300	C(12)-C(13)	1.503(11)
C(12)-H(12)	0.9300	C(13)-C(18)	1.409(13)
C(13)-C(14)	1.411(12)	C(14)-C(15)	1.409(13)
C(14)-H(14)	0.9300	C(15)-C(16)	1.38(2)
C(15)-H(15)	0.9300	C(16)-C(17)	1.39(2)
C(16)-H(16)	0.9300	C(17)-C(18)	1.42(2)
C(17)-H(17)	0.9300	C(18)-H(18)	0.9300
B-O(1)	1.455(7)	B-O(2)	1.459(7)
B-O(4)	1.473(8)	B-O(3)	1.510(8)
O(1)-C(19)	1.376(7)	O(2)-C(29)	1.349(7)
O(3)-C(39)	1.342(7)	O(4)-C(49)	1.371(7)
C(19)-C(20)	1.388(8)	C(19)-C(28)	1.414(9)
C(20)-C(21)	1.433(8)	C(20)-C(30)	1.463(8)
C(21)-C(22)	1.390(9)	C(21)-C(26)	1.447(9)
C(22)-C(23)	1.410(10)	C(22)-H(22)	0.9300
C(23)-C(24)	1.373(14)	C(23)-H(23)	0.9300
C(24)-C(25)	1.362(13)	C(24)-H(24)	0.9300
C(25)-C(26)	1.435(12)	C(25)-H(25)	0.9300
C(26)-C(27)	1.380(11)	C(27)-C(28)	1.342(11)
C(27)-H(27)	0.9300	C(28)-H(28)	0.9300
C(29)-C(38)	1.404(9)	C(29)-C(30)	1.405(8)
C(30)-C(31)	1.463(8)	C(31)-C(32)	1.408(10)
C(31)-C(36)	1.409(9)	C(32)-C(33)	1.400(12)
C(32)-H(32)	0.9300	C(33)-C(34)	1.37(2)
C(33)-H(33)	0.9300	C(34)-C(35)	1.35(2)
C(34)-H(34)	0.9300	C(35)-C(36)	1.423(10)
C(35)-H(35)	0.9300	C(36)-C(37)	1.414(12)
C(37)-C(38)	1.370(12)	C(37)-H(37)	0.9300
C(38)-H(38)	0.9300	C(39)-C(40)	1.395(9)
C(39)-C(48)	1.421(9)	C(40)-C(41)	1.439(9)
C(40)-C(50)	1.470(8)	C(41)-C(42)	1.402(11)
C(41)-C(46)	1.435(11)	C(42)-C(43)	1.383(11)
C(42)-H(42)	0.9300	C(43)-C(44)	1.43(2)
C(43)-H(43)	0.9300	C(44)-C(45)	1.38(2)
C(44)-H(44)	0.9300	C(45)-C(46)	1.431(10)
C(45)-H(45)	0.9300	C(46)-C(47)	1.358(12)
C(47)-C(48)	1.395(12)	C(47)-H(47)	0.9300
C(48)-H(48)	0.9300	C(49)-C(50)	1.381(8)
C(49)-C(58)	1.408(9)	C(50)-C(51)	1.439(8)
C(51)-C(52)	1.420(9)	C(51)-C(56)	1.425(9)
C(52)-C(53)	1.346(10)	C(52)-H(52)	0.9300
C(53)-C(54)	1.409(12)	C(53)-H(53)	0.9300

C(54)-C(55)	1.362(13)	C(54)-H(54)	0.9300
C(55)-C(56)	1.426(9)	C(55)-H(55)	0.9300
C(56)-C(57)	1.387(10)	C(57)-C(58)	1.382(11)
C(57)-H(57)	0.9300	C(58)-H(58)	0.9300

N(1)-Cu-N(2)	82.1(2)	N(1)-Cu-C(12)	152.7(3)
N(2)-Cu-C(12)	120.8(3)	N(1)-Cu-C(11)	115.3(4)
N(2)-Cu-C(11)	156.6(3)	C(12)-Cu-C(11)	38.6(4)
N(1)-Cu-O(3)	84.0(2)	N(2)-Cu-O(3)	91.3(2)
C(12)-Cu-O(3)	108.2(3)	C(11)-Cu-O(3)	105.5(3)
C(5)-N(1)-C(1)	118.4(7)	C(5)-N(1)-Cu	113.9(5)
C(1)-N(1)-Cu	127.6(6)	C(6)-N(2)-C(10)	120.6(7)
C(6)-N(2)-Cu	113.9(5)	C(10)-N(2)-Cu	125.4(6)
N(1)-C(1)-C(2)	120.1(8)	N(1)-C(1)-H(1)	120.0
C(2)-C(1)-H(1)	120.0	C(3)-C(2)-C(1)	120.8(9)
C(3)-C(2)-H(2)	119.6	C(1)-C(2)-H(2)	119.6
C(2)-C(3)-C(4)	120.1(9)	C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9	C(3)-C(4)-C(5)	119.7(8)
C(3)-C(4)-H(4)	120.2	C(5)-C(4)-H(4)	120.2
N(1)-C(5)-C(4)	120.7(7)	N(1)-C(5)-C(6)	114.4(6)
C(4)-C(5)-C(6)	125.0(7)	N(2)-C(6)-C(7)	123.0(8)
N(2)-C(6)-C(5)	115.5(6)	C(7)-C(6)-C(5)	121.5(7)
C(6)-C(7)-C(8)	118.9(8)	C(6)-C(7)-H(7)	120.6
C(8)-C(7)-H(7)	120.6	C(9)-C(8)-C(7)	117.9(8)
C(9)-C(8)-H(8)	121.0	C(7)-C(8)-H(8)	121.0
C(8)-C(9)-C(10)	122.4(10)	C(8)-C(9)-H(9)	118.8
C(10)-C(9)-H(9)	118.8	N(2)-C(10)-C(9)	117.1(9)
N(2)-C(10)-H(10)	121.4	C(9)-C(10)-H(10)	121.4
C(12)-C(11)-Cu	70.7(6)	C(12)-C(11)-H(11A)	120.0
Cu-C(11)-H(11A)	107.0	C(12)-C(11)-H(11B)	120.0
Cu-C(11)-H(11B)	92.2	H(11A)-C(11)-H(11B)	120.0
C(11)-C(12)-C(13)	125.3(9)	C(11)-C(12)-Cu	70.7(6)
C(13)-C(12)-Cu	108.1(5)	C(11)-C(12)-H(12)	117.4
C(13)-C(12)-H(12)	117.4	Cu-C(12)-H(12)	91.2
C(18)-C(13)-C(14)	119.8(10)	C(18)-C(13)-C(12)	118.8(9)
C(14)-C(13)-C(12)	121.4(8)	C(15)-C(14)-C(13)	119.8(11)
C(15)-C(14)-H(14)	120.1	C(13)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	120.4(13)	C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8	C(15)-C(16)-C(17)	119(2)
C(15)-C(16)-H(16)	120.4	C(17)-C(16)-H(16)	120.4
C(16)-C(17)-C(18)	122(2)	C(16)-C(17)-H(17)	119.1
C(18)-C(17)-H(17)	119.1	C(13)-C(18)-C(17)	118(2)
C(13)-C(18)-H(18)	120.9	C(17)-C(18)-H(18)	120.9
O(1)-B-O(2)	114.8(5)	O(1)-B-O(4)	114.3(5)
O(2)-B-O(4)	102.1(5)	O(1)-B-O(3)	101.7(5)
O(2)-B-O(3)	113.3(5)	O(4)-B-O(3)	111.0(5)
C(19)-O(1)-B	115.6(5)	C(29)-O(2)-B	116.1(5)
C(39)-O(3)-B	118.5(5)	C(39)-O(3)-Cu	125.6(4)
B-O(3)-Cu	115.6(3)	C(49)-O(4)-B	117.8(5)
O(1)-C(19)-C(20)	120.2(5)	O(1)-C(19)-C(28)	118.6(5)
C(20)-C(19)-C(28)	120.9(6)	C(19)-C(20)-C(21)	117.9(5)
C(19)-C(20)-C(30)	119.4(5)	C(21)-C(20)-C(30)	122.5(5)
C(22)-C(21)-C(20)	122.7(6)	C(22)-C(21)-C(26)	119.0(6)
C(20)-C(21)-C(26)	118.4(6)	C(21)-C(22)-C(23)	120.0(7)
C(21)-C(22)-H(22)	120.0	C(23)-C(22)-H(22)	120.0
C(24)-C(23)-C(22)	122.0(7)	C(24)-C(23)-H(23)	119.0
C(22)-C(23)-H(23)	119.0	C(25)-C(24)-C(23)	119.1(9)
C(25)-C(24)-H(24)	120.4	C(23)-C(24)-H(24)	120.4
C(24)-C(25)-C(26)	122.2(9)	C(24)-C(25)-H(25)	118.9
C(26)-C(25)-H(25)	118.9	C(27)-C(26)-C(25)	122.2(7)

C(27)-C(26)-C(21)	120.2(7)	C(25)-C(26)-C(21)	117.5(7)
C(28)-C(27)-C(26)	120.6(7)	C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7	C(27)-C(28)-C(19)	121.2(6)
C(27)-C(28)-H(28)	119.4	C(19)-C(28)-H(28)	119.4
O(2)-C(29)-C(38)	118.4(6)	O(2)-C(29)-C(30)	120.6(5)
C(38)-C(29)-C(30)	121.0(6)	C(29)-C(30)-C(31)	116.5(5)
C(29)-C(30)-C(20)	120.3(5)	C(31)-C(30)-C(20)	122.8(5)
C(32)-C(31)-C(36)	118.9(6)	C(32)-C(31)-C(30)	119.9(6)
C(36)-C(31)-C(30)	121.2(6)	C(33)-C(32)-C(31)	119.1(8)
C(33)-C(32)-H(32)	120.4	C(31)-C(32)-H(32)	120.4
C(34)-C(33)-C(32)	121.6(9)	C(34)-C(33)-H(33)	119.2
C(32)-C(33)-H(33)	119.2	C(35)-C(34)-C(33)	120.0(8)
C(35)-C(34)-H(34)	120.0	C(33)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	121.0(8)	C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5	C(31)-C(36)-C(37)	119.0(6)
C(31)-C(36)-C(35)	119.3(7)	C(37)-C(36)-C(35)	121.7(7)
C(38)-C(37)-C(36)	120.3(6)	C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9	C(37)-C(38)-C(29)	121.7(7)
C(37)-C(38)-H(38)	119.2	C(29)-C(38)-H(38)	119.2
O(3)-C(39)-C(40)	122.6(6)	O(3)-C(39)-C(48)	115.6(6)
C(40)-C(39)-C(48)	121.7(6)	C(39)-C(40)-C(41)	118.4(6)
C(39)-C(40)-C(50)	119.6(5)	C(41)-C(40)-C(50)	122.0(6)
C(42)-C(41)-C(46)	119.2(6)	C(42)-C(41)-C(40)	122.6(7)
C(46)-C(41)-C(40)	118.2(7)	C(43)-C(42)-C(41)	121.5(8)
C(43)-C(42)-H(42)	119.3	C(41)-C(42)-H(42)	119.3
C(42)-C(43)-C(44)	119.9(10)	C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0	C(45)-C(44)-C(43)	118.4(9)
C(45)-C(44)-H(44)	120.8	C(43)-C(44)-H(44)	120.8
C(44)-C(45)-C(46)	121.7(9)	C(44)-C(45)-H(45)	119.2
C(46)-C(45)-H(45)	119.2	C(47)-C(46)-C(45)	120.8(8)
C(47)-C(46)-C(41)	121.2(7)	C(45)-C(46)-C(41)	118.0(8)
C(46)-C(47)-C(48)	121.5(7)	C(46)-C(47)-H(47)	119.2
C(48)-C(47)-H(47)	119.2	C(47)-C(48)-C(39)	118.5(7)
C(47)-C(48)-H(48)	120.8	C(39)-C(48)-H(48)	120.8
O(4)-C(49)-C(50)	120.8(5)	O(4)-C(49)-C(58)	117.2(5)
C(50)-C(49)-C(58)	121.8(5)	C(49)-C(50)-C(51)	118.3(5)
C(49)-C(50)-C(40)	119.2(5)	C(51)-C(50)-C(40)	122.3(5)
C(52)-C(51)-C(56)	117.9(6)	C(52)-C(51)-C(50)	123.4(6)
C(56)-C(51)-C(50)	118.7(6)	C(53)-C(52)-C(51)	121.7(7)
C(53)-C(52)-H(52)	119.2	C(51)-C(52)-H(52)	119.2
C(52)-C(53)-C(54)	121.7(7)	C(52)-C(53)-H(53)	119.2
C(54)-C(53)-H(53)	119.2	C(55)-C(54)-C(53)	118.2(6)
C(55)-C(54)-H(54)	120.9	C(53)-C(54)-H(54)	120.9
C(54)-C(55)-C(56)	122.6(8)	C(54)-C(55)-H(55)	118.7
C(56)-C(55)-H(55)	118.7	C(57)-C(56)-C(51)	120.5(6)
C(57)-C(56)-C(55)	121.3(7)	C(51)-C(56)-C(55)	118.0(7)
C(58)-C(57)-C(56)	120.5(7)	C(58)-C(57)-H(57)	119.8
C(56)-C(57)-H(57)	119.8	C(57)-C(58)-C(49)	119.7(6)
C(57)-C(58)-H(58)	120.1	C(49)-C(58)-H(58)	120.1

Table 4. Torsion angles (deg) for C58 H40 B Cu N2 O4.

N(2)-Cu-N(1)-C(5)	-3.4(5)	C(12)-Cu-N(1)-C(5)	-152.6(6)
C(11)-Cu-N(1)-C(5)	-167.0(5)	O(3)-Cu-N(1)-C(5)	88.7(5)
N(2)-Cu-N(1)-C(1)	-178.8(8)	C(12)-Cu-N(1)-C(1)	32.0(11)
C(11)-Cu-N(1)-C(1)	17.6(8)	O(3)-Cu-N(1)-C(1)	-86.7(7)
N(1)-Cu-N(2)-C(6)	0.7(5)	C(12)-Cu-N(2)-C(6)	164.8(5)
C(11)-Cu-N(2)-C(6)	140.6(10)	O(3)-Cu-N(2)-C(6)	-83.1(5)
N(1)-Cu-N(2)-C(10)	-176.2(8)	C(12)-Cu-N(2)-C(10)	-12.1(9)
C(11)-Cu-N(2)-C(10)	-36.3(14)	O(3)-Cu-N(2)-C(10)	100.0(8)
C(5)-N(1)-C(1)-C(2)	-4.1(13)	Cu-N(1)-C(1)-C(2)	171.1(7)
N(1)-C(1)-C(2)-C(3)	4(2)	C(1)-C(2)-C(3)-C(4)	0(2)
C(2)-C(3)-C(4)-C(5)	-4(2)	C(1)-N(1)-C(5)-C(4)	0.5(11)
Cu-N(1)-C(5)-C(4)	-175.4(6)	C(1)-N(1)-C(5)-C(6)	-178.8(7)
Cu-N(1)-C(5)-C(6)	5.3(8)	C(3)-C(4)-C(5)-N(1)	3.7(14)
C(3)-C(4)-C(5)-C(6)	-177.1(9)	C(10)-N(2)-C(6)-C(7)	-2.3(13)
Cu-N(2)-C(6)-C(7)	-179.4(7)	C(10)-N(2)-C(6)-C(5)	179.0(8)
Cu-N(2)-C(6)-C(5)	2.0(8)	N(1)-C(5)-C(6)-N(2)	-4.9(9)
C(4)-C(5)-C(6)-N(2)	175.9(8)	N(1)-C(5)-C(6)-C(7)	176.4(7)
C(4)-C(5)-C(6)-C(7)	-2.8(12)	N(2)-C(6)-C(7)-C(8)	1.8(14)
C(5)-C(6)-C(7)-C(8)	-179.6(8)	C(6)-C(7)-C(8)-C(9)	-2(2)
C(7)-C(8)-C(9)-C(10)	2(2)	C(6)-N(2)-C(10)-C(9)	2.5(14)
Cu-N(2)-C(10)-C(9)	179.2(7)	C(8)-C(9)-C(10)-N(2)	-2(2)
N(1)-Cu-C(11)-C(12)	169.5(5)	N(2)-Cu-C(11)-C(12)	34.4(13)
O(3)-Cu-C(11)-C(12)	-99.9(5)	Cu-C(11)-C(12)-C(13)	-99.0(8)
N(1)-Cu-C(12)-C(11)	-21.1(9)	N(2)-Cu-C(12)-C(11)	-164.9(6)
O(3)-Cu-C(12)-C(11)	92.2(6)	N(1)-Cu-C(12)-C(13)	100.9(8)
N(2)-Cu-C(12)-C(13)	-42.9(8)	C(11)-Cu-C(12)-C(13)	122.0(9)
O(3)-Cu-C(12)-C(13)	-145.8(6)	C(11)-C(12)-C(13)-C(18)	-172.4(11)
Cu-C(12)-C(13)-C(18)	108.8(11)	C(11)-C(12)-C(13)-C(14)	8(2)
Cu-C(12)-C(13)-C(14)	-71.1(12)	C(18)-C(13)-C(14)-C(15)	-2(2)
C(12)-C(13)-C(14)-C(15)	178.2(13)	C(13)-C(14)-C(15)-C(16)	8(3)
C(14)-C(15)-C(16)-C(17)	-11(4)	C(15)-C(16)-C(17)-C(18)	7(5)
C(14)-C(13)-C(18)-C(17)	-2(2)	C(12)-C(13)-C(18)-C(17)	178(2)
C(16)-C(17)-C(18)-C(13)	-1(4)	O(2)-B-O(1)-C(19)	-45.2(8)
O(4)-B-O(1)-C(19)	72.3(6)	O(3)-B-O(1)-C(19)	-168.0(5)
O(1)-B-O(2)-C(29)	-41.1(8)	O(4)-B-O(2)-C(29)	-165.4(5)
O(3)-B-O(2)-C(29)	75.1(7)	O(1)-B-O(3)-C(39)	-161.9(5)
O(2)-B-O(3)-C(39)	74.4(7)	O(4)-B-O(3)-C(39)	-39.8(7)
O(1)-B-O(3)-Cu	12.1(5)	O(2)-B-O(3)-Cu	-111.7(5)
O(4)-B-O(3)-Cu	134.1(4)	N(1)-Cu-O(3)-C(39)	13.9(5)
N(2)-Cu-O(3)-C(39)	95.8(5)	C(12)-Cu-O(3)-C(39)	-141.0(5)
C(11)-Cu-O(3)-C(39)	-100.7(6)	N(1)-Cu-O(3)-B	-159.6(4)
N(2)-Cu-O(3)-B	-77.7(4)	C(12)-Cu-O(3)-B	45.5(5)
C(11)-Cu-O(3)-B	85.8(5)	O(1)-B-O(4)-C(49)	68.9(7)
O(2)-B-O(4)-C(49)	-166.5(5)	O(3)-B-O(4)-C(49)	-45.5(7)
B-O(1)-C(19)-C(20)	70.0(8)	B-O(1)-C(19)-C(28)	-115.5(7)
O(1)-C(19)-C(20)-C(21)	-176.3(5)	C(28)-C(19)-C(20)-C(21)	9.3(10)
O(1)-C(19)-C(20)-C(30)	-1.6(9)	C(28)-C(19)-C(20)-C(30)	-176.0(6)
C(19)-C(20)-C(21)-C(22)	170.0(6)	C(30)-C(20)-C(21)-C(22)	-4.6(10)
C(19)-C(20)-C(21)-C(26)	-10.2(9)	C(30)-C(20)-C(21)-C(26)	175.2(6)
C(20)-C(21)-C(22)-C(23)	-178.7(7)	C(26)-C(21)-C(22)-C(23)	1.5(11)
C(21)-C(22)-C(23)-C(24)	-0.6(14)	C(22)-C(23)-C(24)-C(25)	-1(2)
C(23)-C(24)-C(25)-C(26)	2(2)	C(24)-C(25)-C(26)-C(27)	174.2(11)
C(24)-C(25)-C(26)-C(21)	-2(2)	C(22)-C(21)-C(26)-C(27)	-176.3(8)
C(20)-C(21)-C(26)-C(27)	3.9(12)	C(22)-C(21)-C(26)-C(25)	-0.4(12)
C(20)-C(21)-C(26)-C(25)	179.8(8)	C(25)-C(26)-C(27)-C(28)	-171.9(10)
C(21)-C(26)-C(27)-C(28)	4(2)	C(26)-C(27)-C(28)-C(19)	-5(2)

O(1)-C(19)-C(28)-C(27)	-176.1(8)	C(20)-C(19)-C(28)-C(27)	-1.7(12)
B-O(2)-C(29)-C(38)	-113.9(7)	B-O(2)-C(29)-C(30)	68.8(8)
O(2)-C(29)-C(30)-C(31)	-175.1(5)	C(38)-C(29)-C(30)-C(31)	7.7(9)
O(2)-C(29)-C(30)-C(20)	-2.3(9)	C(38)-C(29)-C(30)-C(20)	-179.5(6)
C(19)-C(20)-C(30)-C(29)	-45.9(8)	C(21)-C(20)-C(30)-C(29)	128.6(7)
C(19)-C(20)-C(30)-C(31)	126.4(7)	C(21)-C(20)-C(30)-C(31)	-59.1(8)
C(29)-C(30)-C(31)-C(32)	172.6(6)	C(20)-C(30)-C(31)-C(32)	0.0(9)
C(29)-C(30)-C(31)-C(36)	-4.9(9)	C(20)-C(30)-C(31)-C(36)	-177.5(6)
C(36)-C(31)-C(32)-C(33)	0.5(11)	C(30)-C(31)-C(32)-C(33)	-177.1(8)
C(31)-C(32)-C(33)-C(34)	-3(2)	C(32)-C(33)-C(34)-C(35)	4(2)
C(33)-C(34)-C(35)-C(36)	-3(2)	C(32)-C(31)-C(36)-C(37)	-177.0(7)
C(30)-C(31)-C(36)-C(37)	0.5(10)	C(32)-C(31)-C(36)-C(35)	0.5(10)
C(30)-C(31)-C(36)-C(35)	178.0(7)	C(34)-C(35)-C(36)-C(31)	0.8(13)
C(34)-C(35)-C(36)-C(37)	178.3(9)	C(31)-C(36)-C(37)-C(38)	1.2(11)
C(35)-C(36)-C(37)-C(38)	-176.2(8)	C(36)-C(37)-C(38)-C(29)	1.6(12)
O(2)-C(29)-C(38)-C(37)	176.4(7)	C(30)-C(29)-C(38)-C(37)	-6.4(11)
B-O(3)-C(39)-C(40)	65.1(8)	Cu-O(3)-C(39)-C(40)	-108.2(6)
B-O(3)-C(39)-C(48)	-116.9(6)	Cu-O(3)-C(39)-C(48)	69.8(7)
O(3)-C(39)-C(40)-C(41)	-175.3(6)	C(48)-C(39)-C(40)-C(41)	6.8(10)
O(3)-C(39)-C(40)-C(50)	2.3(9)	C(48)-C(39)-C(40)-C(50)	-175.5(6)
C(39)-C(40)-C(41)-C(42)	170.8(6)	C(50)-C(40)-C(41)-C(42)	-6.8(10)
C(39)-C(40)-C(41)-C(46)	-8.3(9)	C(50)-C(40)-C(41)-C(46)	174.1(6)
C(46)-C(41)-C(42)-C(43)	-2.4(12)	C(40)-C(41)-C(42)-C(43)	178.5(8)
C(41)-C(42)-C(43)-C(44)	-6(2)	C(42)-C(43)-C(44)-C(45)	13(2)
C(43)-C(44)-C(45)-C(46)	-12(2)	C(44)-C(45)-C(46)-C(47)	-176.9(11)
C(44)-C(45)-C(46)-C(41)	4(2)	C(42)-C(41)-C(46)-C(47)	-175.6(8)
C(40)-C(41)-C(46)-C(47)	3.6(11)	C(42)-C(41)-C(46)-C(45)	3.2(11)
C(40)-C(41)-C(46)-C(45)	-177.7(7)	C(45)-C(46)-C(47)-C(48)	-175.6(9)
C(41)-C(46)-C(47)-C(48)	3.1(14)	C(46)-C(47)-C(48)-C(39)	-4.7(13)
O(3)-C(39)-C(48)-C(47)	-178.4(7)	C(40)-C(39)-C(48)-C(47)	-0.4(11)
B-O(4)-C(49)-C(50)	71.9(7)	B-O(4)-C(49)-C(58)	-112.5(6)
O(4)-C(49)-C(50)-C(51)	-176.8(5)	C(58)-C(49)-C(50)-C(51)	7.8(9)
O(4)-C(49)-C(50)-C(40)	-2.1(9)	C(58)-C(49)-C(50)-C(40)	-177.6(6)
C(39)-C(40)-C(50)-C(49)	-47.6(8)	C(41)-C(40)-C(50)-C(49)	129.9(6)
C(39)-C(40)-C(50)-C(51)	126.8(6)	C(41)-C(40)-C(50)-C(51)	-55.6(9)
C(49)-C(50)-C(51)-C(52)	173.3(6)	C(40)-C(50)-C(51)-C(52)	-1.1(10)
C(49)-C(50)-C(51)-C(56)	-8.0(9)	C(40)-C(50)-C(51)-C(56)	177.5(6)
C(56)-C(51)-C(52)-C(53)	0.6(10)	C(50)-C(51)-C(52)-C(53)	179.3(7)
C(51)-C(52)-C(53)-C(54)	0.4(12)	C(52)-C(53)-C(54)-C(55)	-1.1(14)
C(53)-C(54)-C(55)-C(56)	1.0(14)	C(52)-C(51)-C(56)-C(57)	-176.0(6)
C(50)-C(51)-C(56)-C(57)	5.3(10)	C(52)-C(51)-C(56)-C(55)	-0.7(10)
C(50)-C(51)-C(56)-C(55)	-179.5(6)	C(54)-C(55)-C(56)-C(57)	175.2(8)
C(54)-C(55)-C(56)-C(51)	-0.1(12)	C(51)-C(56)-C(57)-C(58)	-2.1(11)
C(55)-C(56)-C(57)-C(58)	-177.2(7)	C(56)-C(57)-C(58)-C(49)	1.6(11)
O(4)-C(49)-C(58)-C(57)	179.8(6)	C(50)-C(49)-C(58)-C(57)	-4.6(10)