SUPPORTING INFORMATION ACCOMPANYING:

A Bis-Acetonitrile Two-Coordinate Copper(I) Complex: Synthesis and Characterization of Highly Soluble $B(C_6F_5)_4^-$ Salts of $[Cu(MeCN)_2]^+$ and $[Cu(MeCN)_4]^+$

Hong-Chang Liang,[a] Eunsuk Kim,[a] Chris D. Incarvito,[b] Arnold L. Rheingold,[b] and Kenneth D. Karlin,*[a]

Diagram of $[Cu^I(MeCN)_2]B(C_6F_5)_4$ (**2**), with full atom labelling.

Table 1S. Crystal data and structure refinement.

Table 2S. Atomic Coordinates.

Table 3S. Bond lengths and bond angles.

Table 4S. Anisotropic displacement coefficients.

Table 5S. H-atom coordinates.

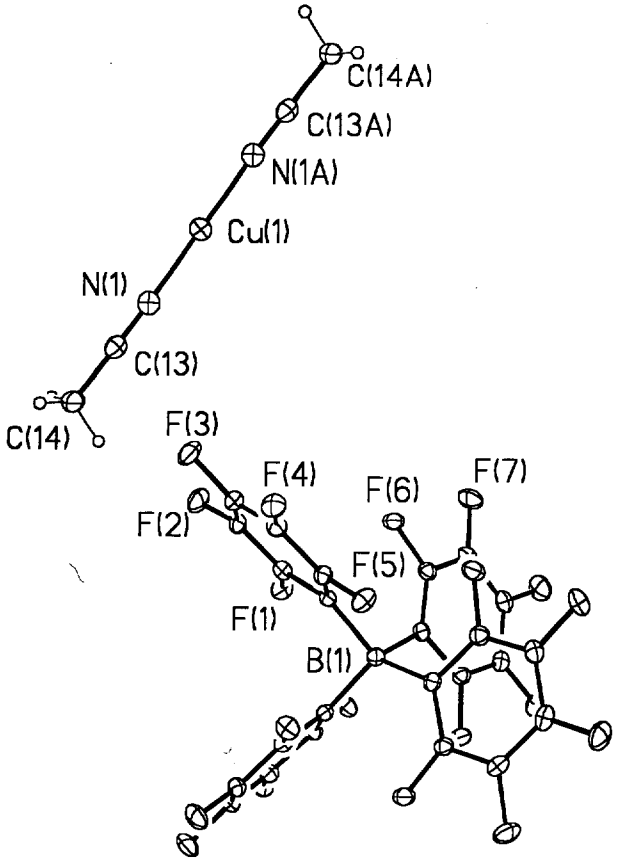
C(14A)
C(13A)
N(1A)
Cu(1)
N(1)
C(13)
C(14)
F(3)
F(4)
F(6)
F(7)
F(2)
F(5)
F(1)
B(1)

Table 1S. Crystal data and structure refinement.

Identification code	kdk43	
Empirical formula	C_{28} H_6 B Cu F_{20} N_2	
Formula weight	824.70	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.7183(16) Å	α= 90°.
	b = 8.2444(7) Å	β= 118.2620(10)°.
	c = 19.8057(16) Å	γ = 90°.
Volume	2835.9(4) $Å^3$	
Z	4	
Density (calculated)	1.932 g/cm^3	
Absorption coefficient	0.928 mm^{-1}	
F(000)	1608	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.33 to 28.32°.	
Index ranges	-26<=h<=25, -10<=k<=10, -25<=l<=22	
Reflections collected	6814	
Independent reflections	3156 [R(int) = 0.0285]	
Completeness to theta = 28.32°	89.4 %	
Absorption correction	Empirical from SADABS	
Max. and min. transmission	0.8733 and 0.8361	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3156 / 0 / 238	
Goodness-of-fit on F^2	1.178	
Final R indices [I>2sigma(I)] [a]	R1 = 0.0343, wR2 = 0.0903	
R indices (all data)	R1 = 0.0465, wR2 = 0.0972	
Largest diff. peak and hole	0.301 and -0.411 $e.Å^{-3}$	

[a]Quantity minimized = $R(wF^2) = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[(wF_o^2)^2]^{1/2}$; $R = \Sigma\Delta/\Sigma(F_o)$, $\Delta = |(F_o-F_c)|$

$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = [2F_c^2 + \mathrm{Max}(F_o, 0)]/3$

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

	x	y	z	U(eq)
Cu(1)	5000	5000	0	33(1)
B(1)	10000	531(4)	2500	22(1)
N(1)	5854(1)	6287(2)	543(1)	34(1)
F(1)	9267(1)	2831(2)	3047(1)	32(1)
F(2)	8193(1)	5022(2)	2243(1)	39(1)
F(3)	7624(1)	5245(2)	691(1)	43(1)
F(4)	8183(1)	3254(2)	-19(1)	35(1)
F(5)	9234(1)	1076(2)	748(1)	34(1)
F(6)	8443(1)	-39(1)	2506(1)	32(1)
F(7)	8190(1)	-2283(2)	3309(1)	41(1)
F(8)	9335(1)	-4304(2)	4260(1)	44(1)
F(9)	10760(1)	-4012(2)	4379(1)	38(1)
F(10)	11044(1)	-1759(2)	3586(1)	34(1)
C(1)	9297(1)	1779(2)	1947(1)	22(1)
C(2)	9005(1)	2870(2)	2277(1)	25(1)
C(3)	8451(1)	4019(2)	1877(1)	28(1)
C(4)	8162(1)	4141(3)	1097(1)	29(1)
C(5)	8440(1)	3126(3)	739(1)	26(1)
C(6)	8993(1)	1983(2)	1165(1)	24(1)
C(7)	9767(1)	-748(2)	3006(1)	23(1)
C(8)	9054(1)	-970(2)	2967(1)	25(1)
C(9)	8899(1)	-2145(3)	3377(1)	29(1)
C(10)	9470(1)	-3180(3)	3853(1)	30(1)
C(11)	10189(1)	-3021(3)	3906(1)	28(1)
C(12)	10318(1)	-1846(3)	3490(1)	26(1)
C(13)	6364(1)	7119(3)	857(1)	33(1)
C(14)	7022(1)	8188(3)	1263(2)	44(1)

Table 3S. Bond lengths [Å] and angles [°].

Cu(1)-N(1)#1	1.8443(19)
Cu(1)-N(1)	1.8443(19)
B(1)-C(1)#2	1.656(3)
B(1)-C(1)	1.656(3)
B(1)-C(7)#2	1.662(3)
B(1)-C(7)	1.662(3)
N(1)-C(13)	1.131(3)
F(1)-C(2)	1.358(2)
F(2)-C(3)	1.348(2)
F(3)-C(4)	1.339(2)
F(4)-C(5)	1.341(2)
F(5)-C(6)	1.357(2)
F(6)-C(8)	1.355(2)
F(7)-C(9)	1.345(2)
F(8)-C(10)	1.335(2)
F(9)-C(11)	1.346(2)
F(10)-C(12)	1.354(2)
C(1)-C(6)	1.382(3)
C(1)-C(2)	1.387(3)
C(2)-C(3)	1.379(3)
C(3)-C(4)	1.373(3)
C(4)-C(5)	1.370(3)
C(5)-C(6)	1.384(3)
C(7)-C(8)	1.382(3)
C(7)-C(12)	1.391(3)
C(8)-C(9)	1.388(3)
C(9)-C(10)	1.370(3)
C(10)-C(11)	1.379(3)
C(11)-C(12)	1.371(3)
C(13)-C(14)	1.455(3)
N(1)#1-Cu(1)-N(1)	180.00(19)
C(1)#2-B(1)-C(1)	103.2(2)
C(1)#2-B(1)-C(7)#2	114.11(9)

C(1)-B(1)-C(7)#2	112.33(9)
C(1)#2-B(1)-C(7)	112.33(9)
C(1)-B(1)-C(7)	114.11(9)
C(7)#2-B(1)-C(7)	101.2(2)
C(13)-N(1)-Cu(1)	177.5(2)
C(6)-C(1)-C(2)	113.12(17)
C(6)-C(1)-B(1)	126.89(15)
C(2)-C(1)-B(1)	119.72(15)
F(1)-C(2)-C(3)	115.97(17)
F(1)-C(2)-C(1)	119.41(17)
C(3)-C(2)-C(1)	124.61(18)
F(2)-C(3)-C(4)	119.90(18)
F(2)-C(3)-C(2)	120.71(18)
C(4)-C(3)-C(2)	119.39(18)
F(3)-C(4)-C(5)	120.09(18)
F(3)-C(4)-C(3)	120.98(18)
C(5)-C(4)-C(3)	118.93(18)
F(4)-C(5)-C(4)	119.99(17)
F(4)-C(5)-C(6)	120.48(18)
C(4)-C(5)-C(6)	119.52(18)
F(5)-C(6)-C(1)	121.61(17)
F(5)-C(6)-C(5)	113.98(16)
C(1)-C(6)-C(5)	124.40(18)
C(8)-C(7)-C(12)	113.20(18)
C(8)-C(7)-B(1)	127.95(16)
C(12)-C(7)-B(1)	118.64(15)
F(6)-C(8)-C(7)	121.24(17)
F(6)-C(8)-C(9)	114.72(17)
C(7)-C(8)-C(9)	124.03(18)
F(7)-C(9)-C(10)	119.49(19)
F(7)-C(9)-C(8)	120.43(19)
C(10)-C(9)-C(8)	120.08(19)
F(8)-C(10)-C(9)	120.96(19)
F(8)-C(10)-C(11)	120.82(19)
C(9)-C(10)-C(11)	118.21(19)
F(9)-C(11)-C(12)	121.01(18)

F(9)-C(11)-C(10)	119.06(19)
C(12)-C(11)-C(10)	119.92(19)
F(10)-C(12)-C(11)	115.99(17)
F(10)-C(12)-C(7)	119.43(17)
C(11)-C(12)-C(7)	124.55(18)
N(1)-C(13)-C(14)	179.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+2,y,-z+1/2

Table 4S. Anisotropic displacement parameters ($Å^2 x\ 10^3$). 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)	36(1)	35(1)	31(1)	-2(1)	18(1)	-3(1)
B(1)	22(1)	24(2)	22(1)	0	12(1)	0
N(1)	38(1)	35(1)	30(1)	0(1)	18(1)	0(1)
F(1)	35(1)	37(1)	24(1)	-3(1)	15(1)	4(1)
F(2)	43(1)	35(1)	44(1)	-7(1)	23(1)	11(1)
F(3)	39(1)	36(1)	43(1)	7(1)	12(1)	17(1)
F(4)	35(1)	39(1)	23(1)	5(1)	8(1)	4(1)
F(5)	39(1)	39(1)	26(1)	1(1)	18(1)	12(1)
F(6)	21(1)	36(1)	37(1)	7(1)	11(1)	0(1)
F(7)	30(1)	50(1)	48(1)	5(1)	22(1)	-10(1)
F(8)	54(1)	36(1)	47(1)	12(1)	29(1)	-8(1)
F(9)	47(1)	30(1)	38(1)	11(1)	20(1)	13(1)
F(10)	25(1)	39(1)	38(1)	9(1)	16(1)	7(1)
C(1)	20(1)	21(1)	26(1)	-2(1)	12(1)	-3(1)
C(2)	25(1)	26(1)	23(1)	-2(1)	12(1)	-4(1)
C(3)	28(1)	22(1)	36(1)	-5(1)	17(1)	0(1)
C(4)	24(1)	24(1)	36(1)	2(1)	11(1)	3(1)
C(5)	26(1)	28(1)	22(1)	2(1)	9(1)	-1(1)
C(6)	24(1)	24(1)	26(1)	-3(1)	13(1)	-1(1)
C(7)	26(1)	21(1)	22(1)	-2(1)	11(1)	-2(1)
C(8)	23(1)	25(1)	24(1)	-2(1)	10(1)	-1(1)
C(9)	28(1)	30(1)	30(1)	-5(1)	16(1)	-9(1)
C(10)	41(1)	23(1)	29(1)	-1(1)	19(1)	-7(1)
C(11)	34(1)	23(1)	25(1)	0(1)	13(1)	3(1)
C(12)	25(1)	27(1)	28(1)	-2(1)	14(1)	0(1)
C(13)	36(1)	34(1)	29(1)	0(1)	15(1)	7(1)
C(14)	33(1)	39(1)	49(1)	-9(1)	11(1)	1(1)

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

	x	y	z	U(eq)
H(14A)	6972	8754	1672	66
H(14B)	7040	8984	904	66
H(14C)	7497	7546	1486	66