Electronic and Structural Variation Among Copper(II) Complexes with Substituted Phenanthrolines

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Supplementary Material

Table S1. Experimental Details of the X-ray Diffraction Studies of [Cu(5-NO_2-phen)$_2$(CH_3CN)](BF_4)$_2$, (**1**), [Cu(5-Cl-phen)$_2$(CH_3CN)](BF_4)$_2$, (**2**), [Cu(o-phen)$_2$(CH_3CN)](BF_4)$_2$, (**3**), [Cu(5-Me-phen)$_2$(CH_3CN)](BF_4)$_2$, (**4**) and [Cu(5,6-Me_2-phen)$_2$(CH_3CN)](BF_4)$_2$, (**5**)

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Figure S1. ORTEP diagram of $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$, **1**, showing 50% probability ellipsoids. The hydrogen atoms and counterions are omitted for clarity.

Figure S2. ORTEP diagram of $[Cu(5\text{-}Cl\text{-}phen)_2(CH_3CN)]^+$, **4**, showing 50% probability ellipsoids. The hydrogen atoms and counterions are omitted for clarity.

Table S1. Experimental Details of the X-ray Diffraction Studies of $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**1**), $[Cu(5\text{-}Cl\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**2**), $[Cu(o\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**3**), $[Cu(5\text{-}Me\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**4**) and $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**5**)

compound	**1**	**2**	**3**	**4**	**5**
formula	$C_{26}H_{17}B_2CuF_8N_7O_4$	$C_{26}H_{17}B_2Cl_2CuF_8N_5$	$C_{26}H_{19}N_5B_2CuF_8$	$C_{28}H_{23}B_2CuF_8N_5$	$C_{30}H_{27}B_2CuF_8N_5O_{0.5}$
formula weight, g mol^{-1}	728.625	707.514	638.624	666.677	703.739
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	C2/c (15)	C2/c (15)	C2/c (15)	C2/c (15)	$P2_1/c$ (14)
a, Å	23.225(7)	24.10(1)	19.433(8)	23.94(1)	11.482(2)
b, Å	9.307(3)	8.861(4)	8.784(4)	8.904(5)	15.756(3)
c, Å	26.984(5)	16.977(8)	14.874(6)	16.850(9)	17.410(3)
b, deg	130.309(4)	131.108(7)	97.426(7)	130.380(7)	109.14(1)
V, $Å^3$	2800(10)	2732(2)	2518(2)	2736(2)	2975.5(9)
Z	4	4	4	4	4
T, deg C	23	23	23	23	-75
ρ_{calcd}, g cm^{-1}	1.729	1.720	1.685	1.618	1.569
crystal dimensions, mm^3	0.2 x 0.2 x 0.3	0.5 x 0.3 x 0.2	0.2 x 0.2 x 0.6	0.4 x 0.3 x 0.2	0.16 x 0.21 x 0.24

Table S1. con't Experimental Details of the X-ray Diffraction Studies of $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**1**), $[Cu(5\text{-}Cl\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**2**), $[Cu(o\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**3**), $[Cu(5\text{-}Me\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**4**) and $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$, (**5**)

compound	**1**	**2**	**3**	**4**	**5**
trans. factor range	0.7010 - 1.000	0.3683 - 1.000	0.6092 - 1.000	0.7627 - 1.00	0.905 - 1.000
linear abs. coeff., cm^{-1}	8.830	10.787	9.555	8.829	8.175
data collected	-27 h 27 -11 k 6 -20 l 20	-24 h 24 -10 k 10 -10 l 20	-22 h 20 -8 k 10 -17 l 17	-28 h 28 -10 k 10 -19 l 17	3° 2θ 48; +h, +k, ±l
reflections collected	7064	5900	6685	4804	5397
R_{avg}	0.050	0.085	0.030	0.044	0.038
no. of independent data	2469	2514	2384	2147	4866
no. of unique data with $I > 3\sigma(I)$	1404 with $Fo>4\sigma(Fo)$	841	1737	996	2276
no. of variables	219	141	192	166	323
F(0,0,0)	1460	1412	1284	1348	1432
R^a	0.084	0.080	0.032	0.054	0.078
$R_w{}^b$	0.134[c]	0.092	0.044	0.062	0.084

Table S1. con't

$^{a}R = \Sigma \, | \, |F_o| - |F_c| \, | / \Sigma |F_o|$. $^{b}R_w = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w |F_o|^2]^{1/2}$, where $w = 4F^2/\sigma^2(F^2)$ and $\sigma^2(F^2) = [S^2(C+4B) + (pI)^2]/(Lp)^2$ with S = scan rate, C = peak counts, B = sum of left and right background counts, I = reflection intensity, Lp = Lorentz-polarization factor and p is a constant employed to avoid overweighting of intense reflections. $^{c}wR^2 = [\ (wFo^2 - Fc^2)^2 / (wFo^4)]^{1/2}$ and $w = 1/\sigma^2 (F_o^2) + (0.0482*P)^2 + 0 * P$, where $P = (\max (F_o^2, 0) + 2 *F_c^2)/3$

Table S2. Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**1**)[a]

atom	atom	distance	atom	atom	distance
Cu(1)	N(3)	1.984(10)	C(6)	N(4)	1.469(11)
Cu(1)	N(2)	2.001(7)	N(4)	O(2)	1.140(11)
Cu(1)	N(2a)	2.001(7)	N(4)	O(1)	1.235(12)
Cu(1)	N(1)	2.098(7)	C(7)	C(8)	1.379(14)
Cu(1)	N(1a)	2.098(7)	C(7)	C(6a)	1.418(12)
N(1)	C(12)	1.309(10)	C(7)	C(11)	1.430(11)
N(1)	C(1)	1.348(10)	C(8)	C(9)	1.352(15)
N(2)	C(10)	1.322(12)	C(9)	C(10)	1.507(14)
N(2)	C(11)	1.397(11)	C(11)	C(12a)	1.387(12)
C(1)	C(2)	1.417(13)	C(12)	C(11a)	1.387(12)
C(2)	C(3)	1.304(13)	N(3)	C(13)	1.127(14)
C(3)	C(4)	1.377(12)	C(13)	C(14)	1.443(17)
C(4)	C(5)	1.359(12)	B(1)	F(1)	1.296(13)
C(4)	C(12)	1.482(12)	B(1)	F(3)	1.321(12)
C(5)	C(6)	1.352(12)	B(1)	F(4)	1.359(12)
C(6)	C(7a)	1.418(12)	B(1)	F(2)	1.372(12)

[a]Numbers in parentheses are errors in the last significant digit

Table S3. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**1**)[a]

atom	atom	atom	angle	atom	atom	atom	angle
N(3)	Cu(1)	N(2)	93.77(19)	C(7a)	C(6)	N(4)	125.0(9)
N(3)	Cu(1)	N(2a)	93.77(19)	O(2)	N(4)	O(1)	119.9(11)
N(2)	Cu(1)	N(2a)	172.5(4)	O(2)	N(4)	C(6)	123.8(11)
N(3)	Cu(1)	N(1)	129.25(17)	O(1)	N(4)	C(6)	116.3(10)
N(2)	Cu(1)	N(1)	95.1(3)	C(8)	C(7)	C(6a)	131.1(9)
N(2a)	Cu(1)	N(1)	80.1(3)	C(8)	C(7)	C(11)	113.0(10)
N(3)	Cu(1)	N(1a)	129.25(17)	C(6a)	C(7)	C(11)	115.8(8)
N(2)	Cu(1)	N(1a)	80.1(3)	C(9)	C(8)	C(7)	129.1(10)
N(2a)	Cu(1)	N(1a)	95.1(3)	C(8)	C(9)	C(10)	115.3(9)
N(1)	Cu(1)	N(1a)	101.5(3)	N(2)	C(10)	C(9)	117.3(11)
C(12)	N(1)	C(1)	119.4(8)	C(12a)	C(11)	N(2)	117.8(7)
C(12)	N(1)	Cu(1)	112.4(6)	C(12a)	C(11)	C(7)	121.1(9)
C(1)	N(1)	Cu(1)	127.9(6)	N(2)	C(11)	C(7)	121.2(9)
C(10)	N(2)	C(11)	124.1(9)	N(1)	C(12)	C(11a)	117.3(8)
C(10)	N(2)	Cu(1)	123.8(8)	N(1)	C(12)	C(4)	122.4(8)
C(11)	N(2)	Cu(1)	112.0(5)	C(11a)	C(12)	C(4)	120.3(8)
N(1)	C(1)	C(2)	122.0(9)	C(13)	N(3)	Cu(1)	180.000(4)
C(3)	C(2)	C(1)	117.0(9)	N(3)	C(13)	C(14)	180.000(6)
C(2)	C(3)	C(4)	126.3(10)	F(1)	B(1)	F(3)	108.6(10)
C(5)	C(4)	C(3)	130.9(10)	F(1)	B(1)	F(4)	115.6(10)
C(5)	C(4)	C(12)	116.2(9)	F(3)	B(1)	F(4)	108.4(9)
C(3)	C(4)	C(12)	112.9(8)	F(1)	B(1)	F(2)	108.1(10)
C(6)	C(5)	C(4)	123.3(10)	F(3)	B(1)	F(2)	108.8(9)
C(5)	C(6)	C(7a)	123.1(8)	F(4)	B(1)	F(2)	107.2(9)
C(5)	C(6)	N(4)	111.9(9)				

[a]Numbers in parentheses are errors in the last significant digit. Symmetry transformations used to generate equivalent atoms: -x, y, -z+1/2

Table S4. Atomic Positional parameters (x 10^4) and Equivalent Isotropic Thermal Parameters (Å^2 x 10^3) for the Nonhydrogen Atoms of [Cu(5-NO_2-phen)$_2$(CH_3CN)](BF_4)$_2$ (**1**).[a]

atom	x	y	z	U(eq)
Cu(1)	0	5473(1)	2500	50(1)
N(1)	-582(4)	4047(7)	2724(5)	61(2)
N(2)	-738(4)	5332(7)	959(5)	65(2)
C(1)	-1260(5)	3427(9)	1999(8)	74(2)
C(2)	-1569(5)	2409(10)	2256(8)	93(3)
C(3)	-1161(5)	2073(10)	3230(7)	77(2)
C(4)	-457(5)	2606(9)	4033(7)	72(2)
C(5)	25(6)	2281(10)	5056(7)	84(3)
C(6)	702(5)	2928(8)	5753(6)	57(2)
N(4)	1101(6)	2387(11)	6804(8)	109(3)
O(1)	1493(8)	3266(12)	7511(7)	187(6)
O(2)	1056(5)	1235(11)	6986(7)	126(3)
C(7)	-977(5)	4012(10)	-484(6)	73(3)
C(8)	-1648(6)	4762(11)	-1077(8)	87(3)
C(9)	-1899(6)	5758(11)	-781(8)	92(3)
C(10)	-1379(6)	6057(12)	362(8)	93(3)
C(11)	-512(5)	4329(9)	593(6)	69(3)
C(12)	-184(5)	3671(8)	3692(7)	63(2)
N(3)	0	7605(10)	2500	67(3)
C(13)	0	8816(14)	2500	69(3)
C(14)	0	10367(12)	2500	87(4)
B(1)	1732(6)	10349(13)	5324(8)	71(3)
F(1)	2161(6)	9654(11)	5217(8)	198(4)
F(2)	1572(5)	11664(8)	4859(6)	141(3)
F(3)	1096(4)	9627(9)	4849(5)	152(3)
F(4)	2032(4)	10592(9)	6314(5)	140(3)

[a] Numbers in parentheses are errors in the last significant digit. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S5. Anisotropic Thermal Parameters for $[Cu(5\text{-}NO_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**1**).[a]

atom	U11	U22	U33	U23	U13	U12
Cu(1)	54(1)	42(1)	42(1)	0	26(1)	0
N(1)	70(4)	43(3)	74(4)	13(3)	49(4)	15(3)
N(2)	58(4)	60(4)	56(4)	12(3)	27(3)	-8(3)
C(1)	61(5)	57(5)	99(7)	-4(5)	50(5)	-10(4)
C(2)	67(6)	73(6)	100(8)	3(6)	36(6)	-15(5)
C(3)	64(5)	84(6)	71(6)	-7(5)	39(5)	1(5)
C(4)	84(6)	57(5)	82(6)	11(4)	56(6)	27(5)
C(5)	90(7)	79(6)	81(7)	-3(5)	55(6)	13(5)
C(6)	75(5)	53(4)	52(4)	15(4)	46(4)	24(4)
N(4)	142(9)	78(6)	105(7)	31(6)	79(7)	52(6)
O(1)	238(13)	139(9)	73(5)	-1(6)	51(7)	20(8)
O(2)	138(7)	133(7)	133(7)	64(6)	99(6)	42(6)
C(7)	69(6)	70(5)	62(5)	11(4)	34(5)	-20(4)
C(8)	72(6)	86(7)	81(6)	16(6)	39(6)	-19(5)
C(9)	70(6)	86(8)	102(8)	41(6)	47(6)	13(5)
C(10)	67(6)	97(7)	72(6)	18(5)	26(5)	-10(5)
C(11)	96(7)	69(6)	54(4)	-24(4)	54(5)	-46(5)
C(12)	71(6)	49(5)	74(5)	6(4)	49(5)	14(4)
N(3)	91(7)	49(6)	56(5)	0	45(5)	0
C(13)	77(8)	60(8)	61(7)	0	41(7)	0
C(14)	126(12)	48(7)	78(9)	0	62(9)	0
B(1)	64(6)	80(8)	70(6)	-4(6)	44(5)	-5(6)
F(1)	177(9)	241(12)	209(11)	-31(8)	140(9)	48(8)
F(2)	210(8)	95(5)	120(5)	4(4)	109(6)	-13(5)
F(3)	127(6)	196(9)	94(5)	-3(5)	54(5)	-76(6)
F(4)	118(5)	202(8)	70(4)	1(4)	47(4)	-26(5)

[a]Numbers in parentheses are errors in the last significant digit. The anisotropic thermal parameters are of the form $\exp[-2\pi^2(U_{11}h^2a^{*2} \ldots + 2U_{12}hka^*b^* + \ldots)]$

Table S6. Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for $[Cu(5\text{-Cl-phen})_2(CH_3CN)](BF_4)_2$ (**2**)[a]

atom	atom	distance	atom	atom	distance
Cu1	N1	2.05(1)	C6	C7	1.40(2)
Cu1	N2	1.988(8)	C7	C8	1.41(1)
Cu1	N3	1.99(2)	C7	C11	1.43(2)
Cl1	C6	1.74(1)	C8	C9	1.30(2)
N1	C1	1.32(1)	C9	C10	1.41(2)
N1	C12	1.40(1)	C11	C12	1.43(1)
N2	C10	1.34(1)	C13	C14	1.34(3)
N2	C11	1.35(2)	B1	F1	1.21(2)
N3	C13	1.07(3)	B1	F2	1.39(2)
C1	C2	1.34(2)	B1	F3	1.33(3)
C2	C3	1.39(2)	B1	F4	1.55(3)
C3	C4	1.36(1)	B1	F5	1.30(2)
C4	C5	1.45(2)	B1	F6	1.38(3)
C4	C12	1.37(2)	B1	F7	1.32(2)
C5	C6	1.37(2)	B1	F8	1.44(4)

[a]Numbers in parentheses are errors in the last significant digit

Table S7. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for $[Cu(5\text{-Cl-phen})_2(CH_3CN)](BF_4)_2$ (**2**)[a]

atom	atom	atom	angle	atom	atom	atom	angle
N1	Cu1	N1′	108.1(5)	C6	C7	C11	118.5(9)
N1	Cu1	N2	81.6(4)	C8	C7	C11	114(1)
N1	Cu1	N2′	96.0(4)	C7	C8	C9	122(1)
N1	Cu1	N3	126.0(3)	C8	C9	C10	122(1)
N2	Cu1	N2′	175.9(5)	N2	C10	C9	119(2)
N2	Cu1	N3	92.0(3)	N2	C11	C7	123.6(9)
Cu1	N1	C1	133.4(9)	N2	C11	C12	119(1)
Cu1	N1	C12	112.6(6)	C7	C11	C12	118(1)
C1	N1	C12	114(1)	N1	C12	C4	124.0(8)
Cu1	N2	C10	127(1)	N1	C12	C11	113(1)
Cu1	N2	C11	113.5(6)	C4	C12	C11	123(1)
C10	N2	C11	119(1)	N3	C13	C14	180.00
Cu1	N3	C13	180.00	F1	B1	F2	117(2)
N1	C1	C2	125(1)	F1	B1	F3	122(3)
C1	C2	C3	120.1(9)	F1	B1	F4	106(2)
C2	C3	C4	118(1)	F2	B1	F3	109(2)
C3	C4	C5	124(1)	F2	B1	F4	98(2)
C3	C4	C12	118(1)	F3	B1	F4	100(2)
C5	C4	C12	118.4(9)	F5	B1	F6	112(2)
C4	C5	C6	119(1)	F5	B1	F7	116(1)
Cl1	C6	C5	118(1)	F5	B1	F8	108(2)
Cl1	C6	C7	118.2(7)	F6	B1	F7	110(2)
C5	C6	C7	123(1)	F6	B1	F8	104(2)
C6	C7	C8	128(1)	F7	B1	F8	107(2)

[a]Numbers in parentheses are errors in the last significant digit

Table S9. Anisotropic Thermal Parameters for $[Cu(5\text{-}Cl\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**2**).[a]

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.040(1)	0.046(1)	0.0302(9)	0.0000	0.0083(8)	0.0000
Cl(1)	0.077(3)	0.143(4)	0.045(2)	0.021(2)	0.027(2)	0.013(2)
N(1)	0.030(5)	0.033(6)	0.049(5)	-0.002(4)	0.018(4)	-0.008(4)
N(2)	0.038(5)	0.051(7)	0.056(6)	-0.016(5)	0.026(5)	-0.013(6)
N(3)	0.08(1)	0.04(1)	0.044(8)	0.0000	0.030(7)	0.0000
C(4)	0.033(6)	0.043(8)	0.043(7)	-0.006(5)	0.018(6)	0.001(6)
C(5)	0.054(7)	0.071(9)	0.044(7)	-0.009(6)	0.028(6)	0.002(7)
C(6)	0.058(8)	0.068(9)	0.040(6)	0.019(6)	0.033(6)	0.008(7)
C(7)	0.034(6)	0.050(8)	0.048(7)	0.001(5)	0.021(6)	-0.004(6)
C(11)	0.038(7)	0.042(8)	0.053(7)	0.014(5)	0.024(6)	-0.004(6)
C(12)	0.033(6)	0.028(7)	0.034(6)	0.004(5)	0.011(5)	-0.009(5)
C(13)	0.06(1)	0.03(1)	0.05(1)	0.0000	0.037(9)	0.0000
C(14)	0.13(2)	0.14(2)	0.033(9)	0.0000	0.04(1)	0.0000

[a]Numbers in parentheses are errors in the last significant digit. The anisotropic temperature factors are of the form $\exp[-2\pi^2(U_{11}h^2a^{*2} \ldots + 2U_{12}hka^*b^* + \ldots)]$

Table S8. Atomic Positional parameters and Equivalent Isotropic Thermal Parameters for the Nonhydrogen Atoms of $[Cu(5\text{-Cl-phen})_2(CH_3CN)](BF_4)_2$ (**2**). [a]

atom	x	y	z	B(eq)[b]
Cu(1)	0.5000	0.4770(2)	0.7500	3.97(5)
Cl(1)	0.3743(2)	0.7546(4)	0.2820(2)	7.7(1)
F(1)	0.332(1)	0.853(2)	0.514(1)	8.7(3)
F(2)	0.3801(7)	1.069(2)	0.514(1)	8.7(5)
F(3)	0.2666(9)	1.064(2)	0.457(2)	8.7(3)
F(4)	0.290(1)	0.956(2)	0.364(1)	9(1)
F(5)	0.2715(9)	1.034(2)	0.382(1)	9.4(3)
F(6)	0.3909(7)	1.003(2)	0.517(2)	9.4(2)
F(7)	0.310(1)	0.835(1)	0.486(2)	9.4(3)
F(8)	0.315(1)	1.063(2)	0.545(2)	9.4(3)
N(1)	0.5589(4)	0.6127(8)	0.7303(6)	3.5(2)
N(2)	0.4284(4)	0.485(1)	0.5947(6)	4.1(2)
N(3)	0.5000	0.252(2)	0.7500	4.9(4)
C(1)	0.6251(6)	0.673(1)	0.7957(8)	4.0(2)
C(2)	0.6533(5)	0.769(1)	0.7695(8)	3.9(2)
C(3)	0.6127(6)	0.810(1)	0.6655(9)	4.7(2)
C(4)	0.5443(5)	0.750(1)	0.5924(8)	3.5(3)
C(5)	0.4976(6)	0.780(1)	0.4816(8)	4.7(3)
C(6)	0.4302(6)	0.713(1)	0.4142(8)	4.3(3)
C(7)	0.4040(5)	0.610(1)	0.4458(8)	3.8(3)
C(8)	0.3367(5)	0.531(1)	0.3825(8)	4.4(2)
C(9)	0.3178(6)	0.439(1)	0.4210(9)	5.1(3)
C(10)	0.3637(7)	0.413(1)	0.529(1)	6.1(3)
C(11)	0.4486(5)	0.580(1)	0.5553(9)	3.8(3)
C(12)	0.5193(5)	0.651(1)	0.6256(7)	3.2(3)
C(13)	0.5000	0.132(2)	0.7500	3.8(4)
C(14)	0.5000	-0.020(3)	0.7500	9.0(6)
B(1)	0.3196(8)	0.978(2)	0.476(1)	6.4(4)

[a] Numbers in parentheses are errors in the last significant digit. [b] $B_{eq} = 4/3[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + 2ab\cos(\gamma)\beta_{12} + 2ac\cos(\beta)\beta_{13} + 2bc\cos(\alpha)\beta_{23}]$.

Table S10. Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for [Cu(o-phen)$_2$(CH$_3$CN)](BF$_4$)$_2$ (**3**)[a]

atom	atom	distance	atom	atom	distance
Cu(1)	N(1)	2.094(2)	C(2)	C(3)	1.369(4)
Cu(1)	N(2)	1.986(2)	C(3)	C(4)	1.408(4)
Cu(1)	N(3)	2.048(4)	C(4)	C(5)	1.432(4)
F(1)	B(1)	1.371(4)	C(4)	C(12)	1.398(4)
F(2)	B(1)	1.349(4)	C(5)	C(6)	1.349(4)
F(3)	B(1)	1.374(4)	C(6)	C(7)	1.434(4)
F(4)	B(1)	1.373(4)	C(7)	C(8)	1.411(4)
N(1)	C(1)	1.326(3)	C(7)	C(11)	1.395(3)
N(1)	C(12)	1.368(3)	C(8)	C(9)	1.357(4)
N(2)	C(10)	1.324(4)	C(9)	C(10)	1.395(4)
N(2)	C(11)	1.366(3)	C(11)	C(12)	1.435(4)
N(3)	C(13)	1.109(5)	C(13)	C(14)	1.464(6)
C(1)	C(2)	1.394(4)			

[a]Numbers in parentheses are errors in the last significant digit

Table S11. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for $[Cu\text{-}o\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**3**)[a]

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(1a)	113.4(1)	C(5)	C(6)	C(7)	121.1(3)
N(1)	Cu(1)	N(2)	81.63(9)	C(6)	C(7)	C(8)	124.5(3)
N(1)	Cu(1)	N(2a)	96.25(9)	C(6)	C(7)	C(11)	118.7(3)
N(1)	Cu(1)	N(3)	123.29(6)	C(8)	C(7)	C(11)	116.8(3)
N(2)	Cu(1)	N(2a)	176.2(1)	C(7)	C(8)	C(9)	119.7(2)
N(2)	Cu(1)	N(3)	91.92(6)	C(8)	C(9)	C(10)	120.1(3)
Cu(1)	N(1)	C(1)	131.6(2)	N(2)	C(10)	C(9)	122.0(3)
Cu(1)	N(1)	C(12)	110.3(2)	N(2)	C(11)	C(7)	123.0(2)
C(1)	N(1)	C(12)	117.9(2)	N(2)	C(11)	C(12)	116.7(2)
Cu(1)	N(2)	C(10)	127.5(2)	C(7)	C(11)	C(12)	120.3(3)
Cu(1)	N(2)	C(11)	114.1(2)	N(1)	C(12)	C(4)	123.4(2)
C(10)	N(2)	C(11)	118.4(2)	N(1)	C(12)	C(11)	116.9(2)
Cu(1)	N(3)	C(13)	180.00	C(4)	C(12)	C(11)	119.7(2)
N(1)	C(1)	C(2)	122.3(3)	N(3)	C(13)	C(14)	180.00
C(1)	C(2)	C(3)	120.0(3)	F(1)	B(1)	F(2)	109.8(3)
C(2)	C(3)	C(4)	119.5(3)	F(1)	B(1)	F(3)	109.0(3)
C(3)	C(4)	C(5)	124.3(3)	F(1)	B(1)	F(4)	110.0(3)
C(3)	C(4)	C(12)	116.7(2)	F(2)	B(1)	F(3)	108.8(3)
C(5)	C(4)	C(12)	119.0(3)	F(2)	B(1)	F(4)	109.4(3)
C(4)	C(5)	C(6)	121.1(3)	F(3)	B(1)	F(4)	109.9(3)

[a]Numbers in parentheses are errors in the last significant digit

Table S12. Atomic Positional parameters and Equivalent Isotropic Thermal Parameters for the Nonhydrogen Atoms of $[Cu(o\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**3**).[a]

atom	x	y	z	B(eq)[b]
Cu(1)	1.0000	0.47333(4)	0.7500	2.841(9)
F(1)	1.14447(8)	1.0315(2)	0.8802(1)	7.81(5)
F(2)	1.1863(1)	0.8389(2)	0.8066(1)	8.83(6)
F(3)	1.24936(8)	1.0475(2)	0.8345(1)	7.33(5)
F(4)	1.15387(8)	1.0510(2)	0.7316(1)	6.24(4)
N(1)	0.97069(8)	0.6042(2)	0.8565(1)	2.55(4)
N(2)	1.09128(8)	0.4809(2)	0.8272(1)	2.77(4)
N(3)	1.0000	0.2402(3)	0.7500	3.24(6)
C(1)	0.9101(1)	0.6633(3)	0.8700(2)	3.27(5)
C(2)	0.9031(1)	0.7601(3)	0.9425(2)	3.95(6)
C(3)	0.9599(1)	0.7972(3)	1.0028(2)	3.79(6)
C(4)	1.0251(1)	0.7353(2)	0.9916(1)	2.92(5)
C(5)	1.0876(1)	0.7635(3)	1.0515(1)	3.48(6)
C(6)	1.1478(1)	0.6949(3)	1.0390(1)	3.47(5)
C(7)	1.1518(1)	0.5952(2)	0.9635(1)	2.87(5)
C(8)	1.2125(1)	0.5184(3)	0.9462(2)	3.62(5)
C(9)	1.2108(1)	0.4277(3)	0.8721(2)	4.01(6)
C(10)	1.1493(1)	0.4109(3)	0.8132(2)	3.66(6)
C(11)	1.0921(1)	0.5703(2)	0.9024(1)	2.47(5)
C(12)	1.0275(1)	0.6387(2)	0.9173(1)	2.39(4)
C(13)	1.0000	0.1139(4)	0.7500	3.15(8)
C(14)	1.0000	-0.0527(4)	0.7500	5.0(1)
B(1)	1.1832(1)	0.9918(3)	0.8131(2)	4.02(7)

[a] Numbers in parentheses are errors in the last significant digit. [b] $Beq = 4/3[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + 2ab\cos(\gamma)\beta_{12} + 2ac\cos(\beta)\beta_{13} + 2bc\cos(\alpha)\beta_{23}]$.

Table S13. Anisotropic Thermal Parameters for $[Cu(o\text{-}phen)_2(CH_3CN)](BF_4)_2$ (3)[a]

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.0328(2)	0.0379(2)	0.0352(2)	0.0000	-0.0031(2)	0.0000
F(1)	0.079(1)	0.160(2)	0.062(1)	0.027(1)	0.0256(9)	-0.011(1)
F(2)	0.159(2)	0.061(1)	0.114(2)	0.010(1)	0.015(1)	0.009(1)
F(3)	0.056(1)	0.139(2)	0.081(1)	-0.012(1)	-0.0027(9)	0.010(1)
F(4)	0.068(1)	0.110(1)	0.057(1)	0.0209(9)	-0.0008(8)	0.026(1)
N(1)	0.0295(9)	0.034(1)	0.033(1)	0.0001(8)	0.0010(8)	0.0029(8)
N(2)	0.0314(9)	0.038(1)	0.035(1)	0.0040(8)	0.0003(7)	-0.0001(8)
N(3)	0.043(2)	0.034(2)	0.045(2)	0.0000	0.004(1)	0.0000
C(1)	0.034(1)	0.046(1)	0.043(1)	0.001(1)	0.003(1)	0.003(1)
C(2)	0.040(1)	0.062(2)	0.049(2)	0.014(1)	0.010(1)	0.000(1)
C(3)	0.059(2)	0.050(1)	0.037(1)	0.008(1)	0.012(1)	-0.004(1)
C(4)	0.045(1)	0.036(1)	0.030(1)	-0.001(1)	0.006(1)	0.002(1)
C(5)	0.053(2)	0.048(1)	0.030(1)	-0.006(1)	0.001(1)	-0.004(1)
C(6)	0.045(1)	0.051(1)	0.032(1)	-0.013(1)	-0.007(1)	0.002(1)
C(7)	0.032(1)	0.043(1)	0.033(1)	-0.005(1)	-0.001(1)	0.009(1)
C(8)	0.033(1)	0.061(2)	0.041(1)	-0.003(1)	-0.006(1)	0.007(1)
C(9)	0.031(1)	0.071(2)	0.050(2)	0.013(1)	0.004(1)	0.005(1)
C(10)	0.040(1)	0.056(2)	0.043(1)	0.011(1)	0.003(1)	-0.005(1)
C(11)	0.031(1)	0.031(1)	0.031(1)	-0.0021(9)	0.0009(9)	0.0045(9)
C(12)	0.032(1)	0.029(1)	0.029(1)	-0.0023(9)	0.0022(9)	0.0065(9)
C(13)	0.038(2)	0.045(2)	0.038(2)	0.0000	0.008(1)	0.0000
C(14)	0.064(3)	0.042(2)	0.087(3)	0.0000	0.011(2)	0.0000
B(1)	0.045(2)	0.061(2)	0.046(2)	0.012(1)	0.005(1)	0.007(1)

[a]Numbers in parentheses are errors in the last significant digit. The anisotropic temperature factors are of the form $\exp[-2\pi^2(U_{11}h^2a^{*2} \ldots + 2U_{12}hka^*b^* + \ldots)]$

Table S14. Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for $[Cu(5\text{-Me-phen})_2(CH_3CN)](BF_4)_2$ (**4**).[a]

atom	atom	distance	atom	atom	distance
Cu(1)	N(1)	2.066(7)	C(1)	C(2)	1.38(1)
Cu(1)	N(1)′	2.066(7)	C(2)	C(3)	1.33(1)
Cu(1)	N(2)	1.971(7)	C(3)	C(4)	1.39(1)
Cu(1)	N(2)′	1.971(7)	C(4)	C(5)	1.40(1)
Cu(1)	N(3)	2.03(1)	C(4)	C(12)	1.41(1)
F(1)	B(1)	1.31(1)	C(5)	C(6)	1.35(1)
F(2)	B(1)	1.25(2)	C(6)	C(7)	1.42(1)
F(3)	B(1)	1.31(1)	C(6)	C(13)	1.50(1)
F(4)	B(1)	1.33(2)	C(7)	C(8)	1.42(1)
N(1)	C(1)	1.33(1)	C(7)	C(11)	1.42(1)
N(1)	C(12)	1.35(1)	C(8)	C(9)	1.32(1)
N(2)	C(10)	1.34(1)	C(9)	C(10)	1.40(1)
N(2)	C(11)	1.34(1)	C(11)	C(12)	1.43(1)
N(3)	C(14)	1.07(1)	C(14)	C(15)	1.40(2)

[a]Numbers in parentheses are errors in the last significant digit

Table S15. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for $[Cu(5\text{-Me-phen})_2(CH_3CN)](BF_4)_2$ (**4**).[a]

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(1)	109.1(4)	C(4)	C(5)	C(6)	123(1)
N(1)	Cu(1)	N(2)	81.3(3)	C(5)	C(6)	C(7)	119.9(9)
N(1)	Cu(1)	N(2)	95.8(3)	C(5)	C(6)	C(13)	121(1)
N(1)	Cu(1)	N(3)	125.4(2)	C(7)	C(6)	C(13)	119(1)
N(1)	Cu(1)	N(2)	95.8(3)	C(6)	C(7)	C(8)	127.3(9)
N(1)	Cu(1)	N(2)	81.3(3)	C(6)	C(7)	C(11)	119.1(8)
N(1)	Cu(1)	N(3)	125.4(2)	C(8)	C(7)	C(11)	113.6(9)
N(2)	Cu(1)	N(2)	175.2(4)	C(7)	C(8)	C(9)	122.9(9)
N(2)	Cu(1)	N(3)	92.4(2)	C(8)	C(9)	C(10)	120.0(9)
N(2)	Cu(1)	N(3)	92.4(2)	N(2)	C(10)	C(9)	120.3(9)
Cu(1)	N(1)	C(1)	132.2(7)	N(2)	C(11)	C(7)	123.4(8)
Cu(1)	N(1)	C(12)	110.9(5)	N(2)	C(11)	C(12)	117.0(9)
C(1)	N(1)	C(12)	116.6(8)	C(7)	C(11)	C(12)	119.6(9)
Cu(1)	N(2)	C(10)	126.1(7)	N(1)	C(12)	C(4)	124.4(8)
Cu(1)	N(2)	C(11)	114.0(6)	N(1)	C(12)	C(11)	116.2(8)
C(10)	N(2)	C(11)	119.7(8)	C(4)	C(12)	C(11)	119.3(9)
Cu(1)	N(3)	C(14)	180.0000(2)	N(3)	C(14)	C(15)	180.0000(2)
N(1)	C(1)	C(2)	122.0(9)	F(1)	B(1)	F(2)	108(1)
C(1)	C(2)	C(3)	121.4(9)	F(1)	B(1)	F(3)	117(1)
C(2)	C(3)	C(4)	120(1)	F(1)	B(1)	F(4)	109(1)
C(3)	C(4)	C(5)	126(1)	F(2)	B(1)	F(3)	107(1)
C(3)	C(4)	C(12)	115.3(9)	F(2)	B(1)	F(4)	111(1)
C(5)	C(4)	C(12)	119.0(9)	F(3)	B(1)	F(4)	105(1)

[a]Numbers in parentheses are errors in the last significant digit

Table S16. Atomic Positional parameters and Equivalent Isotropic Thermal Parameters for the Nonhydrogen Atoms of $[Cu(5\text{-Me-phen})_2(CH_3CN)](BF_4)_2$ (**4**).[a]

atom	x	y	z	B(eq)
Cu(1)	0.5000	0.0289(1)	0.7500	3.53(3)
F(1)	0.8178(4)	0.1549(6)	0.4988(5)	11.2(2)
F(2)	0.7933(7)	-0.0652(9)	0.506(1)	23.0(6)
F(3)	0.8846(3)	-0.0395(7)	0.5183(4)	10.7(2)
F(4)	0.7814(4)	0.004(1)	0.3742(5)	17.4(3)
N(1)	0.5582(3)	-0.1057(5)	0.7261(5)	3.2(1)
N(2)	0.4278(3)	0.0195(6)	0.5967(4)	3.5(1)
N(3)	0.5000	0.2573(9)	0.7500	4.4(2)
C(1)	0.6243(4)	-0.1688(8)	0.7916(6)	3.9(2)
C(2)	0.6497(4)	-0.2667(8)	0.7581(6)	4.7(2)
C(3)	0.6088(4)	-0.3047(8)	0.6586(6)	4.7(2)
C(4)	0.5392(4)	-0.2431(8)	0.5849(6)	3.5(2)
C(5)	0.4906(4)	-0.2754(8)	0.4782(7)	4.3(2)
C(6)	0.4236(4)	-0.2122(9)	0.4105(6)	3.9(2)
C(7)	0.4000(4)	-0.1068(8)	0.4465(6)	3.6(2)
C(8)	0.3324(4)	-0.0280(8)	0.3862(6)	4.3(1)
C(9)	0.3146(4)	0.0656(8)	0.4273(6)	4.6(2)
C(10)	0.3627(4)	0.0887(8)	0.5351(6)	4.7(2)
C(11)	0.4465(4)	-0.0741(7)	0.5548(6)	2.8(2)
C(12)	0.5167(4)	-0.1438(7)	0.6247(6)	3.2(2)
C(13)	0.3717(5)	-0.256(1)	0.2975(7)	6.3(3)
C(14)	0.5000	0.378(1)	0.7500	3.8(3)
C(15)	0.5000	0.535(2)	0.7500	6.4(3)
B(1)	0.8199(6)	0.015(1)	0.476(1)	5.9(2)

[a] Numbers in parentheses are errors in the last significant digit. [b] $Beq = 4/3[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + 2ab\cos(\gamma)\beta_{12} + 2ac\cos(\beta)\beta_{13} + 2bc\cos(\alpha)\beta_{23}]$.

Table S17. Anisotropic Thermal Parameters for $[Cu(5\text{-Me-phen})_2(CH_3CN)](BF_4)_2$ (**4**).[a]

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.0412(7)	0.0328(7)	0.0385(9)	0.0000	0.0161(6)	0.0000
F(1)	0.194(7)	0.077(4)	0.146(6)	0.012(4)	0.107(5)	-0.021(4)
F(2)	0.41(2)	0.127(7)	0.63(2)	0.021(8)	0.47(2)	0.062(9)
F(3)	0.076(3)	0.202(6)	0.094(4)	0.048(4)	0.039(3)	-0.014(4)
F(4)	0.133(5)	0.28(1)	0.101(6)	0.083(7)	0.008(4)	-0.069(6)
N(1)	0.038(3)	0.032(3)	0.036(4)	-0.001(3)	0.016(3)	0.004(3)
N(2)	0.038(3)	0.038(3)	0.039(4)	0.004(3)	0.017(3)	0.003(3)
N(3)	0.054(6)	0.030(5)	0.062(6)	0.0000	0.028(5)	0.0000
C(4)	0.042(4)	0.044(5)	0.043(6)	-0.005(4)	0.027(4)	-0.003(4)
C(5)	0.052(5)	0.052(5)	0.057(7)	-0.006(4)	0.034(5)	-0.003(4)
C(6)	0.063(5)	0.052(5)	0.044(6)	-0.023(4)	0.040(5)	-0.009(4)
C(7)	0.045(5)	0.039(4)	0.050(6)	-0.010(4)	0.030(5)	0.004(4)
C(11)	0.042(4)	0.027(4)	0.035(6)	-0.009(3)	0.024(4)	0.002(3)
C(12)	0.043(4)	0.034(4)	0.040(6)	-0.003(4)	0.026(4)	0.008(4)
C(13)	0.086(6)	0.097(7)	0.060(7)	-0.017(6)	0.049(6)	-0.007(5)
C(14)	0.054(7)	0.019(6)	0.063(8)	0.0000	0.034(6)	0.0000
C(15)	0.065(8)	0.073(8)	0.081(9)	0.0000	0.037(7)	0.0000

[a]Numbers in parentheses are errors in the last significant digit. The anisotropic temperature factors are of the form $\exp[-2\pi^2(U_{11}h^2a^{*2} \ldots + 2U_{12}hka^*b^* + \ldots)]$

Table S18. Intramolecular Distances (Å) Involving the Nonhydrogen Atoms for $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$. (**5**)[a]

atom	atom	distance	atom	atom	distance
Cu(1)	N(1)	2.050(6)	C(15)	C(16)	1.42(1)
Cu(1)	N(2)	1.993(7)	C(16)	C(17)	1.35(1)
Cu(1)	N(3)	1.986(8)	C(17)	C(18)	1.41(1)
Cu(1)	N(4)	2.015(6)	C(18)	C(19)	1.45(1)
Cu(1)	N(5)	2.201(7)	C(18)	C(26)	1.40(1)
N(1)	C(1)	1.31(1)	C(19)	C(20)	1.34(1)
N(1)	C(12)	1.38(1)	C(19)	C(27)	1.51(2)
N(2)	C(10)	1.30(1)	C(20)	C(21)	1.46(1)
N(2)	C(11)	1.37(1)	C(20)	C(28)	1.53(1)
N(3)	C(15)	1.32(1)	C(21)	C(22)	1.38(1)
N(3)	C(26)	1.35(1)	C(21)	C(25)	1.40(1)
N(4)	C(24)	1.31(1)	C(22)	C(23)	1.37(2)
N(4)	C(25)	1.36(1)	C(23)	C(24)	1.40(1)
N(5)	C(29)	1.08(1)	C(25)	C(26)	1.42(1)
C(1)	C(2)	1.41(1)	C(29)	C(30)	1.51(2)
C(2)	C(3)	1.34(1)	F(1)	B(1)	1.42(2)
C(3)	C(4)	1.39(1)	F(2)	B(1)	1.32(2)
C(4)	C(5)	1.46(1)	F(3)	B(1)	1.43(2)
C(4)	C(12)	1.41(1)	F(4)	B(1)	1.29(2)
C(5)	C(6)	1.36(1)	B(2)	F(5)	1.36(1)
C(5)	C(13)	1.50(1)	B(2)	F(6)	1.36(1)
C(6)	C(7)	1.45(1)	B(2)	F(7)	1.36(1)
C(6)	C(14)	1.51(1)	B(2)	F(8)	1.36(1)
C(7)	C(8)	1.40(1)	B(3)	F(11)	1.36(3)
C(7)	C(11)	1.42(1)	B(3)	F(12)	1.36(2)
C(8)	C(9)	1.35(1)	B(3)	F(9)	1.36(2)
C(9)	C(10)	1.40(2)	B(3)	F(10)	1.36(2)
C(11)	C(12)	1.40(1)			

[a]Numbers in parentheses are errors in the last significant digit

Table S19. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**5**).[a]

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(2)	82.0(3)	C(3)	C(4)	C(5)	125.5(7)
N(1)	Cu(1)	N(3)	98.3(3)	C(3)	C(4)	C(12)	116.0(8)
N(1)	Cu(1)	N(4)	136.3(2)	C(5)	C(4)	C(12)	118.5(8)
N(1)	Cu(1)	N(5)	107.2(3)	C(4)	C(5)	C(6)	121.1(7)
N(2)	Cu(1)	N(3)	176.9(2)	C(4)	C(5)	C(13)	117.0(8)
N(2)	Cu(1)	N(4)	100.7(3)	C(6)	C(5)	C(13)	121.9(9)
N(2)	Cu(1)	N(5)	86.6(3)	C(5)	C(6)	C(7)	120.0(8)
N(3)	Cu(1)	N(4)	81.3(3)	C(5)	C(6)	C(14)	123.6(8)
N(3)	Cu(1)	N(5)	90.4(3)	C(7)	C(6)	C(14)	116.5(8)
N(4)	Cu(1)	N(5)	116.5(3)	C(6)	C(7)	C(8)	124.0(8)
Cu(1)	N(1)	C(1)	130.7(6)	C(6)	C(7)	C(11)	119.5(8)
Cu(1)	N(1)	C(12)	111.3(5)	C(8)	C(7)	C(11)	116.5(7)
C(1)	N(1)	C(12)	118.0(7)	C(7)	C(8)	C(9)	120.1(9)
Cu(1)	N(2)	C(10)	128.9(6)	C(8)	C(9)	C(10)	119.6(9)
Cu(1)	N(2)	C(11)	112.7(6)	N(2)	C(10)	C(9)	122.9(8)
C(10)	N(2)	C(11)	118.2(8)	N(2)	C(11)	C(7)	122.6(8)
Cu(1)	N(3)	C(15)	126.2(6)	N(2)	C(11)	C(12)	117.6(8)
Cu(1)	N(3)	C(26)	113.6(5)	C(7)	C(11)	C(12)	119.8(7)
C(15)	N(3)	C(26)	120.2(8)	N(1)	C(12)	C(4)	122.6(8)
Cu(1)	N(4)	C(24)	130.2(6)	N(1)	C(12)	C(11)	116.4(7)
Cu(1)	N(4)	C(25)	112.6(5)	C(4)	C(12)	C(11)	121.0(8)
C(24)	N(4)	C(25)	116.7(7)	N(3)	C(15)	C(16)	120.6(8)
Cu(1)	N(5)	C(29)	157.1(9)	C(15)	C(16)	C(17)	119.2(8)
N(1)	C(1)	C(2)	122.9(9)	C(16)	C(17)	C(18)	121.1(9)
C(1)	C(2)	C(3)	118.2(9)	C(17)	C(18)	C(19)	125.2(9)
C(2)	C(3)	C(4)	122.4(8)	C(17)	C(18)	C(26)	115.8(7)

Table S19, continued. Intramolecular Bond Angles (deg) Involving the Nonhydrogen Atoms for [Cu(5,6-Me_2-phen)$_2$(CH_3CN)](BF_4)$_2$ (**5**).[a]

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(18)	C(26)	119.0(8)	N(5)	C(29)	C(30)	173(1)
C(18)	C(19)	C(20)	120.4(9)	F(1)	B(1)	F(2)	106(1)
C(18)	C(19)	C(27)	118.8(8)	F(1)	B(1)	F(3)	106(1)
C(20)	C(19)	C(27)	120.8(8)	F(1)	B(1)	F(4)	109(2)
C(19)	C(20)	C(21)	121.3(8)	F(2)	B(1)	F(3)	108(2)
C(19)	C(20)	C(28)	121.2(9)	F(2)	B(1)	F(4)	118(1)
C(21)	C(20)	C(28)	117.5(8)	F(3)	B(1)	F(4)	109(1)
C(20)	C(21)	C(22)	125.1(8)	F(5)	B(2)	F(6)	109.5(8)
C(20)	C(21)	C(25)	118.5(8)	F(5)	B(2)	F(7)	109.5(7)
C(22)	C(21)	C(25)	116.4(9)	F(5)	B(2)	F(8)	109.5(7)
C(21)	C(22)	C(23)	121.0(9)	F(6)	B(2)	F(7)	109.4(7)
C(22)	C(23)	C(24)	117.6(9)	F(6)	B(2)	F(8)	109.4(7)
N(4)	C(24)	C(23)	124.1(9)	F(7)	B(2)	F(8)	109.4(9)
N(4)	C(25)	C(21)	124.2(7)	F(11)	B(3)	F(9)	110(2)
N(4)	C(25)	C(26)	115.7(7)	F(11)	B(3)	F(12)	110(2)
C(21)	C(25)	C(26)	120.2(8)	F(11)	B(3)	F(10)	110(2)
N(3)	C(26)	C(18)	123.0(7)	F(9)	B(3)	F(12)	109(2)
N(3)	C(26)	C(25)	116.3(8)	F(9)	B(3)	F(10)	109(2)
C(18)	C(26)	C(25)	120.6(7)	F(12)	B(3)	F(10)	109(2)

[a]Numbers in parentheses are errors in the least significant digit

Table S20. Atomic Positional parameters and Equivalent Isotropic Thermal Parameters for the Nonhydrogen Atoms of $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (**5**).[a]

atom	x	y	z	B(eq)
Cu(1)	0.65974(9)	0.24244(6)	0.38851(6)	2.39(2)
N(1)	0.7222(6)	0.3622(4)	0.4265(4)	2.4(2)
N(2)	0.5768(5)	0.2569(4)	0.4719(3)	2.2(1)
N(3)	0.7340(6)	0.2302(4)	0.3009(4)	2.4(2)
N(4)	0.7250(6)	0.1233(3)	0.4131(4)	1.9(1)
N(5)	0.4755(7)	0.2559(5)	0.2971(4)	3.8(2)
C(1)	0.7976(7)	0.4118(5)	0.4049(5)	2.4(2)
C(2)	0.8307(8)	0.4936(5)	0.4380(5)	3.3(2)
C(3)	0.7856(8)	0.5201(5)	0.4956(5)	2.9(2)
C(4)	0.7083(7)	0.4704(5)	0.5234(5)	2.6(2)
C(5)	0.6560(8)	0.4947(5)	0.5859(5)	2.8(2)
C(6)	0.5787(7)	0.4421(5)	0.6077(5)	2.4(2)
C(7)	0.5463(7)	0.3604(5)	0.5683(4)	2.5(2)
C(8)	0.4645(8)	0.3029(5)	0.5852(5)	3.2(2)
C(9)	0.4407(8)	0.2272(6)	0.5462(5)	3.5(2)
C(10)	0.4996(8)	0.2063(5)	0.4897(5)	3.2(2)
C(11)	0.5996(7)	0.3348(5)	0.5092(5)	2.3(2)
C(12)	0.6773(7)	0.3906(5)	0.4860(4)	2.1(2)
C(13)	0.6914(8)	0.5803(6)	0.6245(5)	3.5(2)
C(14)	0.5228(9)	0.4634(6)	0.6725(5)	4.6(3)
C(15)	0.7250(8)	0.2851(5)	0.2418(5)	3.0(2)
C(16)	0.7852(7)	0.2697(5)	0.1839(5)	3.0(2)
C(17)	0.8541(8)	0.1985(5)	0.1907(6)	3.2(2)
C(18)	0.8605(7)	0.1373(5)	0.2511(5)	2.5(2)
C(19)	0.9268(7)	0.0575(5)	0.2609(5)	2.9(2)
C(20)	0.9269(7)	0.0037(5)	0.3207(5)	2.9(2)
C(21)	0.8583(7)	0.0226(5)	0.3761(5)	2.8(2)
C(22)	0.8508(8)	-0.0302(6)	0.4379(6)	4.0(2)
C(23)	0.7842(9)	-0.0072(6)	0.4868(6)	4.0(2)
C(24)	0.7231(7)	0.0713(5)	0.4716(5)	2.8(2)

Table S20, continued. Atomic Positional parameters and Equivalent Isotropic Thermal Parameters for the Nonhydrogen Atoms of $[Cu(5,6\text{-}Me_2\text{-}phen)_2(CH_3CN)](BF_4)_2$ (5)[a]

atom	x	y	z	B(eq)
C(25)	0.7934(7)	0.0990(5)	0.3664(5)	2.1(2)
C(26)	0.7972(7)	0.1574(5)	0.3051(5)	2.2(2)
C(27)	0.9996(9)	0.0379(7)	0.2049(6)	4.5(3)
C(28)	0.9972(9)	-0.0802(6)	0.3325(7)	5.4(3)
C(29)	0.379(1)	0.2426(7)	0.2673(6)	4.9(3)
C(30)	0.245(1)	0.216(1)	0.234(1)	12.9(6)
F(1)	0.0184(7)	0.1658(4)	0.0510(4)	8.6(2)
F(2)	0.1596(6)	0.2524(6)	0.0375(5)	10.8(3)
F(3)	0.0296(7)	0.1940(5)	-0.0745(5)	9.3(3)
F(4)	-0.0394(7)	0.2900(4)	-0.0068(5)	10.6(3)
B(1)	0.043(2)	0.231(1)	0.003(1)	6.7(3)
F(5)	0.3100(9)	0.0024(7)	0.2548(4)	7.7(3)
F(6)	0.4762(6)	0.0489(7)	0.3523(6)	7.7(7)
F(7)	0.367(1)	-0.0574(5)	0.3771(6)	7.7(6)
F(8)	0.2899(8)	0.0733(6)	0.3600(6)	7.7(7)
F(9)	0.291(1)	-0.035(1)	0.328(1)	5(1)
F(10)	0.460(2)	-0.012(2)	0.4338(9)	4.7(9)
F(11)	0.476(2)	-0.062(1)	0.318(1)	4.7(4)
F(12)	0.417(2)	0.072(1)	0.326(1)	4.7(6)
B(2)	0.3607(6)	0.0168(4)	0.3360(4)	7.7(4)
B(3)	0.411(1)	-0.0094(9)	0.3514(9)	4.7(6)
O(1)	0.146(3)	0.267(2)	-0.156(2)	19.0(9)

[a] Numbers in parentheses are errors in the last significant digit. [b]$Beq = 4/3[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + 2ab\cos(\gamma)\beta_{12} + 2ac\cos(\beta)\beta_{13} + 2bc\cos(\alpha)\beta_{23}]$.

Table S21. Anisotropic Thermal Parameters for [Cu(5,6-Me_2-phen)$_2$(CH_3CN)](BF_4)$_2$ (**5**).[a]

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.0440(6)	0.0242(5)	0.0286(5)	0.0009(6)	0.0196(4)	-0.0010(5)
N(1)	0.038(4)	0.029(4)	0.027(4)	0.001(3)	0.016(4)	-0.001(3)
N(2)	0.025(4)	0.029(4)	0.029(4)	-0.004(3)	0.008(3)	-0.000(3)
N(3)	0.041(4)	0.024(4)	0.029(4)	-0.008(3)	0.016(3)	-0.004(3)
N(4)	0.029(4)	0.019(3)	0.024(4)	0.002(3)	0.007(3)	-0.002(3)
N(5)	0.052(5)	0.060(5)	0.025(4)	-0.002(5)	0.003(4)	-0.017(4)
C(4)	0.038(5)	0.033(5)	0.024(5)	0.009(4)	0.004(4)	-0.007(4)
C(5)	0.040(6)	0.034(5)	0.032(5)	0.014(4)	0.010(4)	0.005(4)
C(6)	0.023(5)	0.049(5)	0.017(4)	0.013(4)	0.003(4)	-0.004(4)
C(7)	0.030(5)	0.041(5)	0.019(4)	0.015(4)	0.004(4)	0.012(4)
C(11)	0.037(5)	0.036(5)	0.018(4)	0.007(4)	0.011(4)	0.007(4)
C(12)	0.028(5)	0.038(5)	0.018(4)	0.014(4)	0.010(4)	0.003(4)
C(13)	0.060(7)	0.044(5)	0.032(5)	0.023(5)	0.016(5)	-0.000(4)
C(14)	0.083(8)	0.064(7)	0.027(5)	0.021(6)	0.019(6)	-0.001(5)
C(18)	0.021(5)	0.042(5)	0.029(5)	-0.016(4)	0.006(4)	-0.014(4)
C(19)	0.027(5)	0.045(6)	0.034(5)	-0.011(4)	0.004(4)	-0.023(5)
C(20)	0.033(5)	0.026(5)	0.044(6)	-0.002(4)	0.005(5)	-0.014(4)
C(21)	0.037(6)	0.036(5)	0.028(5)	-0.001(4)	0.005(4)	0.002(4)
C(25)	0.019(5)	0.031(4)	0.026(5)	-0.005(4)	0.002(4)	-0.002(4)
C(26)	0.024(5)	0.028(4)	0.026(5)	-0.002(4)	0.001(4)	-0.014(4)
C(27)	0.045(6)	0.071(7)	0.060(7)	-0.005(6)	0.024(6)	-0.012(6)
C(28)	0.066(8)	0.045(6)	0.095(9)	0.021(5)	0.026(7)	-0.016(6)
C(29)	0.070(8)	0.063(7)	0.041(6)	-0.012(7)	0.003(6)	-0.031(6)
C(30)	0.11(1)	0.13(2)	0.19(2)	-0.01(1)	-0.03(1)	-0.05(1)
F(1)	0.151(7)	0.085(5)	0.090(6)	0.001(5)	0.037(5)	-0.004(4)
F(2)	0.067(5)	0.144(7)	0.178(8)	-0.016(6)	0.007(5)	0.009(7)
F(3)	0.136(7)	0.096(6)	0.121(7)	-0.035(5)	0.042(6)	-0.002(5)
F(4)	0.109(6)	0.070(5)	0.173(9)	0.049(5)	-0.021(5)	0.009(5)

[a]Numbers in parentheses are errors in the last significant digit. The anisotropic temperature factors are of the form $\exp[-2\pi^2(U_{11}h^2a^{*2} \ldots + 2U_{12}hka^*b^* + \ldots)]$

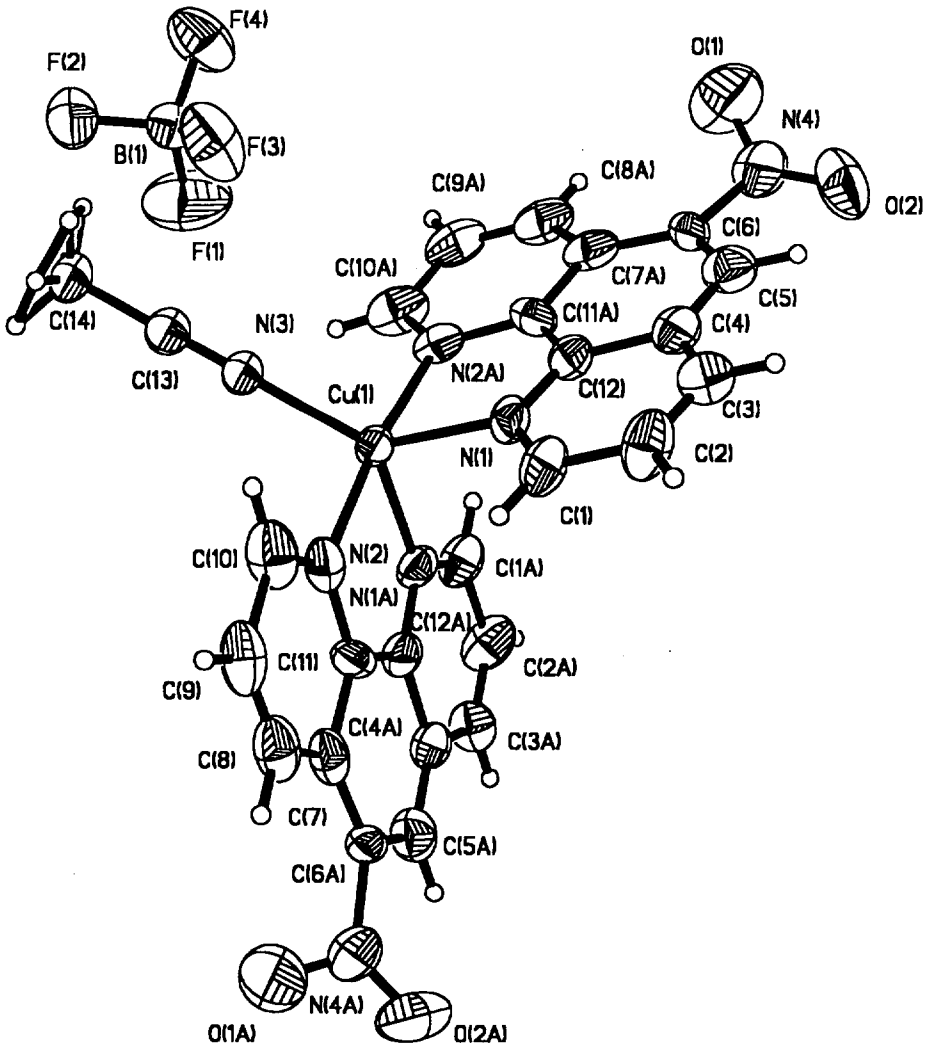

Figure S1. Bush, Whitehead, Pink *et al.*

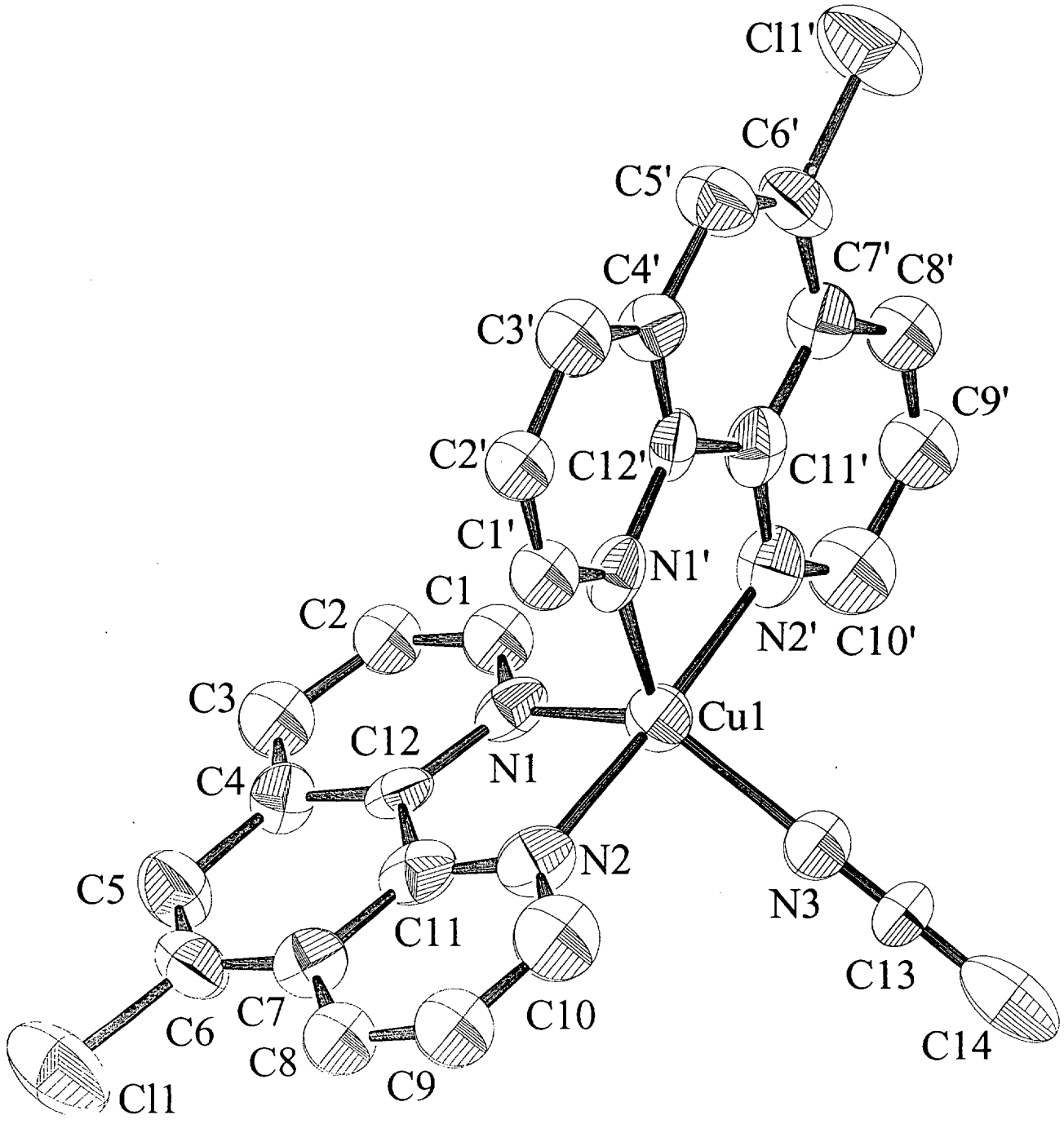

Figure S2. Bush, Whitehead, Pink *et al.*