Supplementary Information

Trinuclear copper(I) complexes with triscarbene ligands: catalysis of C-N and C-C coupling reactions

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Full listing of atomic coordinates, bond distances and angles for the reported structure of complex $[Cu_3\{HB(MeIm)_3\}_2](PF_6)$ **1-PF$_6$**.

Table 1. Crystal data and structure refinement for [Cu$_3${HB(MeIm)$_3$}$_2$](PF$_6$).

Empirical formula	C$_{24}$H$_{32}$B$_2$Cu$_3$F$_6$N$_{12}$P
	[C$_{24}$H$_{32}$B$_2$Cu$_3$N$_{12}$, F$_6$P]
Formula weight	845.83
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P$\bar{1}$
Unit cell dimensions	a = 14.1659(6) Å α= 86.9100(10)°.
	b = 15.2179(8) Å β= 76.3670(10)°.
	c = 16.9149(9) Å γ = 73.9790(10)°.
Volume	3405.8(3) Å^3
Z	4
Density (calculated)	1.650 Mg/m^3
Absorption coefficient	1.973 mm^{-1}
F(000)	1704
Crystal size	0.25 x 0.13 x 0.13 mm^3
Theta range for data collection	1.77 to 30.42°.
Index ranges	-20<=h<=14, -21<=k<=21, -24<=l<=24
Reflections collected	55191
Independent reflections	20099 [R(int) = 0.0306]
Completeness to theta = 30.42°	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7735 and 0.7382
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	20099 / 0 / 865
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1281
R indices (all data)	R1 = 0.0623, wR2 = 0.1459
Largest diff. peak and hole	1.447 and -0.956 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ea03305b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	6627(1)	8053(1)	4842(1)	31(1)
Cu(2)	7929(1)	6459(1)	4207(1)	32(1)
Cu(3)	5938(1)	6853(1)	4265(1)	27(1)
N(1)	5689(4)	7080(4)	6248(3)	38(1)
N(2)	4726(4)	8409(4)	6055(3)	39(1)
N(3)	7597(4)	6362(4)	5997(3)	42(1)
N(4)	9029(4)	6594(4)	5427(4)	47(1)
N(5)	6483(4)	5525(3)	5545(3)	38(1)
N(6)	6338(4)	4881(3)	4477(3)	40(1)
N(7)	7754(4)	8402(3)	3178(3)	33(1)
N(8)	8293(4)	8825(3)	4152(3)	34(1)
N(9)	7664(4)	6959(3)	2528(3)	32(1)
N(10)	8333(4)	5523(4)	2677(3)	41(1)
N(11)	6056(4)	8277(3)	3002(3)	30(1)
N(12)	4544(4)	8413(3)	3720(3)	34(1)
B(1)	6534(5)	6184(6)	6185(4)	43(2)
B(2)	7206(5)	8008(5)	2651(4)	33(1)
C(1)	5651(4)	7824(4)	5767(3)	33(1)
C(2)	4790(5)	7208(6)	6842(4)	51(2)
C(3)	4196(5)	8035(5)	6711(4)	48(2)
C(4)	4353(6)	9320(5)	5766(5)	49(2)
C(5)	8190(4)	6445(4)	5260(4)	37(1)
C(6)	8055(6)	6476(6)	6606(4)	58(2)
C(7)	8954(6)	6609(7)	6250(5)	61(2)
C(8)	9920(5)	6643(6)	4807(5)	59(2)
C(9)	6234(4)	5713(4)	4809(3)	31(1)
C(10)	6741(5)	4570(5)	5632(6)	59(2)
C(11)	6656(5)	4190(4)	4987(6)	55(2)
C(12)	6113(6)	4764(5)	3694(5)	53(2)
C(13)	7580(4)	8452(4)	4005(3)	29(1)
C(14)	8568(5)	8744(5)	2829(4)	45(2)
C(15)	8903(5)	9011(5)	3429(4)	47(2)
C(16)	8377(6)	9033(5)	4961(4)	49(2)

C(17)	7959(4)	6338(4)	3085(3)	32(1)
C(18)	7880(5)	6526(5)	1783(3)	40(1)
C(19)	8295(5)	5637(6)	1870(4)	51(2)
C(20)	8768(6)	4654(5)	3027(5)	58(2)
C(21)	5516(4)	7897(3)	3627(3)	26(1)
C(22)	5405(5)	9023(4)	2716(4)	40(1)
C(23)	4469(6)	9100(4)	3161(4)	46(2)
C(24)	3688(4)	8233(5)	4318(4)	41(1)
Cu(4)	1549(1)	8357(1)	937(1)	28(1)
Cu(5)	3212(1)	8896(1)	1043(1)	27(1)
Cu(6)	3331(1)	7223(1)	441(1)	33(1)
N(13)	1823(3)	7003(3)	2259(3)	31(1)
N(14)	852(4)	6769(4)	1525(3)	40(1)
N(15)	2227(3)	8414(3)	2703(3)	28(1)
N(16)	1943(3)	9867(3)	2522(3)	29(1)
N(17)	3655(3)	7006(3)	2130(3)	30(1)
N(18)	5038(4)	6650(3)	1193(3)	37(1)
N(19)	2063(3)	9638(3)	-395(2)	26(1)
N(20)	862(3)	10267(3)	618(3)	30(1)
N(21)	3949(3)	8829(3)	-761(3)	32(1)
N(22)	5133(3)	8711(4)	-126(3)	35(1)
N(23)	2677(3)	8046(3)	-1035(3)	28(1)
N(24)	2385(4)	6722(3)	-770(3)	41(1)
B(3)	2551(5)	7357(4)	2627(4)	31(1)
B(4)	2925(4)	8962(4)	-999(3)	29(1)
C(25)	1404(4)	7341(4)	1627(3)	31(1)
C(26)	1523(5)	6228(5)	2546(4)	47(2)
C(27)	899(6)	6093(5)	2105(5)	52(2)
C(28)	202(6)	6916(6)	950(5)	53(2)
C(29)	2442(4)	9050(3)	2142(3)	26(1)
C(30)	1612(4)	8843(4)	3415(3)	34(1)
C(31)	1437(4)	9759(4)	3300(3)	36(1)
C(32)	1989(5)	10752(4)	2168(4)	40(1)
C(33)	4017(4)	6950(4)	1311(3)	31(1)
C(34)	4463(4)	6726(4)	2504(4)	38(1)
C(35)	5312(5)	6506(5)	1929(4)	44(1)
C(36)	5737(5)	6443(6)	398(5)	57(2)
C(37)	1494(4)	9446(3)	324(3)	26(1)

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C(38)	1804(5)	10566(4)	-535(4)	37(1)
C(39)	1047(5)	10970(4)	90(4)	39(1)
C(40)	75(5)	10397(5)	1360(4)	43(1)
C(41)	4116(4)	8855(4)	-2(3)	29(1)
C(42)	4851(4)	8667(5)	-1329(4)	43(1)
C(43)	5596(5)	8591(5)	-939(4)	45(2)
C(44)	5654(5)	8749(5)	521(4)	48(2)
C(45)	2789(4)	7340(4)	-508(3)	34(1)
C(46)	2186(4)	7864(4)	-1604(3)	35(1)
C(47)	2009(5)	7043(5)	-1443(4)	45(1)
C(48)	2386(8)	5833(5)	-405(5)	61(2)
P(1)	8762(1)	1752(1)	3901(1)	39(1)
F(1)	8347(4)	2291(3)	4745(3)	68(1)
F(2)	9188(4)	1164(4)	3083(3)	70(1)
F(3)	9814(5)	1942(6)	3801(4)	112(3)
F(4)	7757(5)	1471(7)	4024(4)	133(3)
F(5)	9199(5)	870(4)	4385(3)	89(2)
F(6)	8323(9)	2592(5)	3434(4)	163(5)
P(2)	1301(1)	3458(1)	921(1)	37(1)
F(7)	2275(7)	3693(9)	1053(7)	178(5)
F(8)	384(6)	3224(9)	810(8)	193(6)
F(9)	1872(11)	2790(8)	207(7)	224(8)
F(10)	723(8)	4135(8)	1568(9)	239(8)
F(11)	1513(19)	2704(10)	1426(11)	319(12)
F(12)	1457(13)	4153(9)	266(8)	228(7)

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Table 3.   Bond lengths [Å] and angles [°] for ea03305b.

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Cu(1)-C(13)	1.912(5)	N(10)-C(17)	1.361(7)
Cu(1)-C(1)	1.915(5)	N(10)-C(19)	1.379(9)
Cu(1)-Cu(3)	2.6199(9)	N(10)-C(20)	1.455(10)
Cu(1)-Cu(2)	2.7049(10)	N(11)-C(21)	1.354(6)
Cu(2)-C(5)	1.901(6)	N(11)-C(22)	1.394(7)
Cu(2)-C(17)	1.905(5)	N(11)-B(2)	1.542(8)
Cu(2)-Cu(3)	2.6965(9)	N(12)-C(21)	1.361(7)
Cu(3)-C(9)	1.908(5)	N(12)-C(23)	1.370(8)
Cu(3)-C(21)	1.908(5)	N(12)-C(24)	1.465(8)
N(1)-C(1)	1.355(7)	B(1)-H(1)	1.0000
N(1)-C(2)	1.397(8)	B(2)-H(2)	1.0000
N(1)-B(1)	1.535(10)	C(2)-C(3)	1.348(11)
N(2)-C(1)	1.360(8)	C(2)-H(2A)	0.9500
N(2)-C(3)	1.376(8)	C(3)-H(3)	0.9500
N(2)-C(4)	1.443(9)	C(4)-H(4A)	0.9800
N(3)-C(5)	1.350(8)	C(4)-H(4B)	0.9800
N(3)-C(6)	1.382(8)	C(4)-H(4C)	0.9800
N(3)-B(1)	1.558(9)	C(6)-C(7)	1.339(11)
N(4)-C(5)	1.362(7)	C(6)-H(6)	0.9500
N(4)-C(7)	1.372(9)	C(7)-H(7)	0.9500
N(4)-C(8)	1.456(9)	C(8)-H(8A)	0.9800
N(5)-C(9)	1.366(7)	C(8)-H(8B)	0.9800
N(5)-C(10)	1.406(8)	C(8)-H(8C)	0.9800
N(5)-B(1)	1.543(10)	C(10)-C(11)	1.308(13)
N(6)-C(11)	1.369(9)	C(10)-H(10)	0.9500
N(6)-C(9)	1.370(7)	C(11)-H(11)	0.9500
N(6)-C(12)	1.463(9)	C(12)-H(12A)	0.9800
N(7)-C(13)	1.364(7)	C(12)-H(12B)	0.9800
N(7)-C(14)	1.388(7)	C(12)-H(12C)	0.9800
N(7)-B(2)	1.548(7)	C(14)-C(15)	1.341(9)
N(8)-C(13)	1.363(6)	C(14)-H(14)	0.9500
N(8)-C(15)	1.386(8)	C(15)-H(15)	0.9500
N(8)-C(16)	1.459(7)	C(16)-H(16A)	0.9800
N(9)-C(17)	1.352(8)	C(16)-H(16B)	0.9800
N(9)-C(18)	1.382(7)	C(16)-H(16C)	0.9800
N(9)-B(2)	1.553(8)	C(18)-C(19)	1.333(11)

C(18)-H(18)	0.9500	N(19)-C(37)	1.359(6)
C(19)-H(19)	0.9500	N(19)-C(38)	1.381(7)
C(20)-H(20A)	0.9800	N(19)-B(4)	1.558(7)
C(20)-H(20B)	0.9800	N(20)-C(37)	1.360(7)
C(20)-H(20C)	0.9800	N(20)-C(39)	1.396(7)
C(22)-C(23)	1.339(10)	N(20)-C(40)	1.451(7)
C(22)-H(22)	0.9500	N(21)-C(41)	1.364(6)
C(23)-H(23)	0.9500	N(21)-C(42)	1.374(7)
C(24)-H(24A)	0.9800	N(21)-B(4)	1.553(7)
C(24)-H(24B)	0.9800	N(22)-C(41)	1.362(7)
C(24)-H(24C)	0.9800	N(22)-C(43)	1.375(7)
Cu(4)-C(37)	1.900(5)	N(22)-C(44)	1.468(7)
Cu(4)-C(25)	1.914(5)	N(23)-C(45)	1.357(7)
Cu(4)-Cu(6)	2.6088(9)	N(23)-C(46)	1.392(6)
Cu(4)-Cu(5)	2.7455(9)	N(23)-B(4)	1.536(7)
Cu(5)-C(29)	1.911(5)	N(24)-C(45)	1.368(8)
Cu(5)-C(41)	1.915(5)	N(24)-C(47)	1.378(8)
Cu(5)-Cu(6)	2.7404(9)	N(24)-C(48)	1.456(8)
Cu(6)-C(45)	1.916(5)	B(3)-H(3A)	1.0000
Cu(6)-C(33)	1.916(5)	B(4)-H(4)	1.0000
N(13)-C(25)	1.353(7)	C(26)-C(27)	1.345(9)
N(13)-C(26)	1.387(7)	C(26)-H(26)	0.9500
N(13)-B(3)	1.546(7)	C(27)-H(27)	0.9500
N(14)-C(25)	1.362(7)	C(28)-H(28A)	0.9800
N(14)-C(27)	1.381(8)	C(28)-H(28B)	0.9800
N(14)-C(28)	1.460(8)	C(28)-H(28C)	0.9800
N(15)-C(29)	1.363(6)	C(30)-C(31)	1.359(8)
N(15)-C(30)	1.383(7)	C(30)-H(30)	0.9500
N(15)-B(3)	1.549(8)	C(31)-H(31)	0.9500
N(16)-C(29)	1.359(6)	C(32)-H(32A)	0.9800
N(16)-C(31)	1.366(7)	C(32)-H(32B)	0.9800
N(16)-C(32)	1.455(7)	C(32)-H(32C)	0.9800
N(17)-C(33)	1.358(7)	C(34)-C(35)	1.329(9)
N(17)-C(34)	1.391(6)	C(34)-H(34)	0.9500
N(17)-B(3)	1.551(8)	C(35)-H(35)	0.9500
N(18)-C(33)	1.359(7)	C(36)-H(36A)	0.9800
N(18)-C(35)	1.378(8)	C(36)-H(36B)	0.9800
N(18)-C(36)	1.461(8)	C(36)-H(36C)	0.9800

C(38)-C(39)	1.349(9)	C(5)-Cu(2)-Cu(3)	112.05(18)
C(38)-H(38)	0.9500	C(17)-Cu(2)-Cu(3)	79.52(16)
C(39)-H(39)	0.9500	C(5)-Cu(2)-Cu(1)	78.92(19)
C(40)-H(40A)	0.9800	C(17)-Cu(2)-Cu(1)	111.16(18)
C(40)-H(40B)	0.9800	Cu(3)-Cu(2)-Cu(1)	58.03(2)
C(40)-H(40C)	0.9800	C(9)-Cu(3)-C(21)	170.2(2)
C(42)-C(43)	1.348(9)	C(9)-Cu(3)-Cu(1)	111.16(17)
C(42)-H(42)	0.9500	C(21)-Cu(3)-Cu(1)	78.61(14)
C(43)-H(43)	0.9500	C(9)-Cu(3)-Cu(2)	75.37(15)
C(44)-H(44A)	0.9800	C(21)-Cu(3)-Cu(2)	111.35(15)
C(44)-H(44B)	0.9800	Cu(1)-Cu(3)-Cu(2)	61.15(3)
C(44)-H(44C)	0.9800	C(1)-N(1)-C(2)	109.9(6)
C(46)-C(47)	1.343(9)	C(1)-N(1)-B(1)	128.8(5)
C(46)-H(46)	0.9500	C(2)-N(1)-B(1)	121.3(5)
C(47)-H(47)	0.9500	C(1)-N(2)-C(3)	110.3(6)
C(48)-H(48A)	0.9800	C(1)-N(2)-C(4)	126.2(5)
C(48)-H(48B)	0.9800	C(3)-N(2)-C(4)	123.4(6)
C(48)-H(48C)	0.9800	C(5)-N(3)-C(6)	110.1(5)
P(1)-F(6)	1.525(6)	C(5)-N(3)-B(1)	127.7(5)
P(1)-F(4)	1.563(6)	C(6)-N(3)-B(1)	122.2(6)
P(1)-F(3)	1.565(6)	C(5)-N(4)-C(7)	111.2(6)
P(1)-F(5)	1.587(5)	C(5)-N(4)-C(8)	123.7(6)
P(1)-F(1)	1.588(5)	C(7)-N(4)-C(8)	124.9(6)
P(1)-F(2)	1.588(4)	C(9)-N(5)-C(10)	107.5(6)
P(2)-F(11)	1.401(9)	C(9)-N(5)-B(1)	129.4(5)
P(2)-F(10)	1.470(7)	C(10)-N(5)-B(1)	123.0(6)
P(2)-F(8)	1.493(7)	C(11)-N(6)-C(9)	110.5(6)
P(2)-F(12)	1.511(9)	C(11)-N(6)-C(12)	125.6(6)
P(2)-F(9)	1.539(8)	C(9)-N(6)-C(12)	123.9(5)
P(2)-F(7)	1.583(8)	C(13)-N(7)-C(14)	109.4(5)
		C(13)-N(7)-B(2)	128.9(4)
C(13)-Cu(1)-C(1)	171.1(2)	C(14)-N(7)-B(2)	121.6(5)
C(13)-Cu(1)-Cu(3)	110.66(15)	C(13)-N(8)-C(15)	110.8(5)
C(1)-Cu(1)-Cu(3)	77.68(16)	C(13)-N(8)-C(16)	124.5(5)
C(13)-Cu(1)-Cu(2)	77.32(16)	C(15)-N(8)-C(16)	124.7(5)
C(1)-Cu(1)-Cu(2)	110.25(18)	C(17)-N(9)-C(18)	109.4(5)
Cu(3)-Cu(1)-Cu(2)	60.82(2)	C(17)-N(9)-B(2)	127.6(4)
C(5)-Cu(2)-C(17)	168.0(3)	C(18)-N(9)-B(2)	123.0(5)

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C(17)-N(10)-C(19)	110.8(6)	N(4)-C(5)-Cu(2)	125.4(5)
C(17)-N(10)-C(20)	125.1(6)	C(7)-C(6)-N(3)	107.8(6)
C(19)-N(10)-C(20)	124.1(6)	C(7)-C(6)-H(6)	126.1
C(21)-N(11)-C(22)	109.1(5)	N(3)-C(6)-H(6)	126.1
C(21)-N(11)-B(2)	128.6(4)	C(6)-C(7)-N(4)	106.3(6)
C(22)-N(11)-B(2)	122.3(5)	C(6)-C(7)-H(7)	126.8
C(21)-N(12)-C(23)	111.1(5)	N(4)-C(7)-H(7)	126.9
C(21)-N(12)-C(24)	124.2(5)	N(4)-C(8)-H(8A)	109.4
C(23)-N(12)-C(24)	124.7(5)	N(4)-C(8)-H(8B)	109.5
N(1)-B(1)-N(5)	111.6(5)	H(8A)-C(8)-H(8B)	109.5
N(1)-B(1)-N(3)	111.7(6)	N(4)-C(8)-H(8C)	109.4
N(5)-B(1)-N(3)	110.3(6)	H(8A)-C(8)-H(8C)	109.5
N(1)-B(1)-H(1)	107.6	H(8B)-C(8)-H(8C)	109.5
N(5)-B(1)-H(1)	107.6	N(5)-C(9)-N(6)	105.4(5)
N(3)-B(1)-H(1)	107.7	N(5)-C(9)-Cu(3)	129.5(4)
N(11)-B(2)-N(7)	111.3(5)	N(6)-C(9)-Cu(3)	124.8(4)
N(11)-B(2)-N(9)	112.8(4)	C(11)-C(10)-N(5)	109.3(6)
N(7)-B(2)-N(9)	111.0(5)	C(11)-C(10)-H(10)	125.3
N(11)-B(2)-H(2)	107.2	N(5)-C(10)-H(10)	125.4
N(7)-B(2)-H(2)	107.1	C(10)-C(11)-N(6)	107.2(6)
N(9)-B(2)-H(2)	107.1	C(10)-C(11)-H(11)	126.4
N(1)-C(1)-N(2)	105.6(5)	N(6)-C(11)-H(11)	126.4
N(1)-C(1)-Cu(1)	129.8(4)	N(6)-C(12)-H(12A)	109.4
N(2)-C(1)-Cu(1)	124.5(4)	N(6)-C(12)-H(12B)	109.4
C(3)-C(2)-N(1)	106.7(6)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-H(2A)	126.7	N(6)-C(12)-H(12C)	109.5
N(1)-C(2)-H(2A)	126.6	H(12A)-C(12)-H(12C)	109.5
C(2)-C(3)-N(2)	107.5(6)	H(12B)-C(12)-H(12C)	109.5
C(2)-C(3)-H(3)	126.3	N(8)-C(13)-N(7)	105.2(4)
N(2)-C(3)-H(3)	126.2	N(8)-C(13)-Cu(1)	123.7(4)
N(2)-C(4)-H(4A)	109.5	N(7)-C(13)-Cu(1)	131.1(4)
N(2)-C(4)-H(4B)	109.5	C(15)-C(14)-N(7)	108.3(5)
H(4A)-C(4)-H(4B)	109.5	C(15)-C(14)-H(14)	125.9
N(2)-C(4)-H(4C)	109.5	N(7)-C(14)-H(14)	125.9
H(4A)-C(4)-H(4C)	109.5	C(14)-C(15)-N(8)	106.4(5)
H(4B)-C(4)-H(4C)	109.5	C(14)-C(15)-H(15)	126.8
N(3)-C(5)-N(4)	104.6(5)	N(8)-C(15)-H(15)	126.8
N(3)-C(5)-Cu(2)	129.8(4)	N(8)-C(16)-H(16A)	109.5

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N(8)-C(16)-H(16B)	109.5	C(37)-Cu(4)-Cu(5)	73.95(14)
H(16A)-C(16)-H(16B)	109.5	C(25)-Cu(4)-Cu(5)	111.44(16)
N(8)-C(16)-H(16C)	109.5	Cu(6)-Cu(4)-Cu(5)	61.51(2)
H(16A)-C(16)-H(16C)	109.5	C(29)-Cu(5)-C(41)	170.4(2)
H(16B)-C(16)-H(16C)	109.5	C(29)-Cu(5)-Cu(6)	110.42(15)
N(9)-C(17)-N(10)	105.2(5)	C(41)-Cu(5)-Cu(6)	77.46(16)
N(9)-C(17)-Cu(2)	131.9(4)	C(29)-Cu(5)-Cu(4)	78.21(14)
N(10)-C(17)-Cu(2)	122.9(5)	C(41)-Cu(5)-Cu(4)	111.13(15)
C(19)-C(18)-N(9)	108.6(6)	Cu(6)-Cu(5)-Cu(4)	56.79(2)
C(19)-C(18)-H(18)	125.7	C(45)-Cu(6)-C(33)	171.5(2)
N(9)-C(18)-H(18)	125.7	C(45)-Cu(6)-Cu(4)	77.67(17)
C(18)-C(19)-N(10)	106.0(5)	C(33)-Cu(6)-Cu(4)	110.49(16)
C(18)-C(19)-H(19)	127.0	C(45)-Cu(6)-Cu(5)	111.57(17)
N(10)-C(19)-H(19)	127.0	C(33)-Cu(6)-Cu(5)	75.29(16)
N(10)-C(20)-H(20A)	109.5	Cu(4)-Cu(6)-Cu(5)	61.70(2)
N(10)-C(20)-H(20B)	109.4	C(25)-N(13)-C(26)	109.3(5)
H(20A)-C(20)-H(20B)	109.5	C(25)-N(13)-B(3)	128.6(4)
N(10)-C(20)-H(20C)	109.5	C(26)-N(13)-B(3)	122.1(5)
H(20A)-C(20)-H(20C)	109.5	C(25)-N(14)-C(27)	110.5(5)
H(20B)-C(20)-H(20C)	109.5	C(25)-N(14)-C(28)	124.5(5)
N(11)-C(21)-N(12)	105.3(4)	C(27)-N(14)-C(28)	124.6(5)
N(11)-C(21)-Cu(3)	130.3(4)	C(29)-N(15)-C(30)	109.9(4)
N(12)-C(21)-Cu(3)	124.3(4)	C(29)-N(15)-B(3)	129.5(4)
C(23)-C(22)-N(11)	108.0(5)	C(30)-N(15)-B(3)	120.5(4)
C(23)-C(22)-H(22)	126.0	C(29)-N(16)-C(31)	111.7(4)
N(11)-C(22)-H(22)	126.0	C(29)-N(16)-C(32)	124.5(5)
C(22)-C(23)-N(12)	106.5(5)	C(31)-N(16)-C(32)	123.7(5)
C(22)-C(23)-H(23)	126.8	C(33)-N(17)-C(34)	108.8(5)
N(12)-C(23)-H(23)	126.8	C(33)-N(17)-B(3)	129.3(4)
N(12)-C(24)-H(24A)	109.5	C(34)-N(17)-B(3)	121.9(5)
N(12)-C(24)-H(24B)	109.5	C(33)-N(18)-C(35)	110.5(5)
H(24A)-C(24)-H(24B)	109.5	C(33)-N(18)-C(36)	124.4(5)
N(12)-C(24)-H(24C)	109.5	C(35)-N(18)-C(36)	124.9(5)
H(24A)-C(24)-H(24C)	109.5	C(37)-N(19)-C(38)	110.4(5)
H(24B)-C(24)-H(24C)	109.5	C(37)-N(19)-B(4)	128.1(4)
C(37)-Cu(4)-C(25)	171.7(2)	C(38)-N(19)-B(4)	121.5(4)
C(37)-Cu(4)-Cu(6)	108.52(15)	C(37)-N(20)-C(39)	110.7(5)
C(25)-Cu(4)-Cu(6)	79.77(17)	C(37)-N(20)-C(40)	125.0(5)

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C(39)-N(20)-C(40)	124.3(5)	H(28A)-C(28)-H(28C)	109.5
C(41)-N(21)-C(42)	109.6(5)	H(28B)-C(28)-H(28C)	109.5
C(41)-N(21)-B(4)	128.0(4)	N(16)-C(29)-N(15)	104.7(4)
C(42)-N(21)-B(4)	122.3(5)	N(16)-C(29)-Cu(5)	125.2(4)
C(41)-N(22)-C(43)	111.3(5)	N(15)-C(29)-Cu(5)	130.1(4)
C(41)-N(22)-C(44)	124.1(5)	C(31)-C(30)-N(15)	107.5(5)
C(43)-N(22)-C(44)	124.5(5)	C(31)-C(30)-H(30)	126.3
C(45)-N(23)-C(46)	109.0(5)	N(15)-C(30)-H(30)	126.2
C(45)-N(23)-B(4)	128.2(4)	C(30)-C(31)-N(16)	106.2(5)
C(46)-N(23)-B(4)	122.5(4)	C(30)-C(31)-H(31)	126.9
C(45)-N(24)-C(47)	110.7(5)	N(16)-C(31)-H(31)	126.9
C(45)-N(24)-C(48)	124.5(5)	N(16)-C(32)-H(32A)	109.5
C(47)-N(24)-C(48)	124.8(6)	N(16)-C(32)-H(32B)	109.4
N(13)-B(3)-N(15)	111.6(4)	H(32A)-C(32)-H(32B)	109.5
N(13)-B(3)-N(17)	111.1(5)	N(16)-C(32)-H(32C)	109.5
N(15)-B(3)-N(17)	111.0(4)	H(32A)-C(32)-H(32C)	109.5
N(13)-B(3)-H(3A)	107.6	H(32B)-C(32)-H(32C)	109.5
N(15)-B(3)-H(3A)	107.6	N(17)-C(33)-N(18)	105.6(4)
N(17)-B(3)-H(3A)	107.6	N(17)-C(33)-Cu(6)	130.8(4)
N(23)-B(4)-N(21)	111.6(4)	N(18)-C(33)-Cu(6)	123.6(4)
N(23)-B(4)-N(19)	110.6(4)	C(35)-C(34)-N(17)	108.4(5)
N(21)-B(4)-N(19)	110.4(4)	C(35)-C(34)-H(34)	125.8
N(23)-B(4)-H(4)	108.0	N(17)-C(34)-H(34)	125.8
N(21)-B(4)-H(4)	108.1	C(34)-C(35)-N(18)	106.7(5)
N(19)-B(4)-H(4)	108.0	C(34)-C(35)-H(35)	126.7
N(13)-C(25)-N(14)	105.7(4)	N(18)-C(35)-H(35)	126.7
N(13)-C(25)-Cu(4)	130.6(4)	N(18)-C(36)-H(36A)	109.5
N(14)-C(25)-Cu(4)	123.6(4)	N(18)-C(36)-H(36B)	109.5
C(27)-C(26)-N(13)	108.2(5)	H(36A)-C(36)-H(36B)	109.5
C(27)-C(26)-H(26)	125.9	N(18)-C(36)-H(36C)	109.5
N(13)-C(26)-H(26)	125.9	H(36A)-C(36)-H(36C)	109.5
C(26)-C(27)-N(14)	106.2(5)	H(36B)-C(36)-H(36C)	109.5
C(26)-C(27)-H(27)	126.9	N(19)-C(37)-N(20)	105.0(4)
N(14)-C(27)-H(27)	126.9	N(19)-C(37)-Cu(4)	132.5(4)
N(14)-C(28)-H(28A)	109.5	N(20)-C(37)-Cu(4)	122.1(4)
N(14)-C(28)-H(28B)	109.5	C(39)-C(38)-N(19)	107.8(5)
H(28A)-C(28)-H(28B)	109.5	C(39)-C(38)-H(38)	126.1
N(14)-C(28)-H(28C)	109.4	N(19)-C(38)-H(38)	126.1

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C(38)-C(39)-N(20)	106.0(5)	H(48A)-C(48)-H(48B)	109.5
C(38)-C(39)-H(39)	127.0	N(24)-C(48)-H(48C)	109.5
N(20)-C(39)-H(39)	127.0	H(48A)-C(48)-H(48C)	109.5
N(20)-C(40)-H(40A)	109.5	H(48B)-C(48)-H(48C)	109.5
N(20)-C(40)-H(40B)	109.5	F(6)-P(1)-F(4)	89.7(6)
H(40A)-C(40)-H(40B)	109.5	F(6)-P(1)-F(3)	95.4(6)
N(20)-C(40)-H(40C)	109.5	F(4)-P(1)-F(3)	174.7(5)
H(40A)-C(40)-H(40C)	109.5	F(6)-P(1)-F(5)	178.8(6)
H(40B)-C(40)-H(40C)	109.5	F(4)-P(1)-F(5)	89.0(5)
N(22)-C(41)-N(21)	104.8(4)	F(3)-P(1)-F(5)	85.8(4)
N(22)-C(41)-Cu(5)	124.7(4)	F(6)-P(1)-F(1)	92.3(3)
N(21)-C(41)-Cu(5)	129.9(4)	F(4)-P(1)-F(1)	90.0(4)
C(43)-C(42)-N(21)	108.5(5)	F(3)-P(1)-F(1)	91.1(3)
C(43)-C(42)-H(42)	125.7	F(5)-P(1)-F(1)	88.0(3)
N(21)-C(42)-H(42)	125.8	F(6)-P(1)-F(2)	90.7(4)
C(42)-C(43)-N(22)	105.8(5)	F(4)-P(1)-F(2)	89.3(4)
C(42)-C(43)-H(43)	127.1	F(3)-P(1)-F(2)	89.3(3)
N(22)-C(43)-H(43)	127.1	F(5)-P(1)-F(2)	89.1(3)
N(22)-C(44)-H(44A)	109.4	F(1)-P(1)-F(2)	177.0(3)
N(22)-C(44)-H(44B)	109.5	F(11)-P(2)-F(10)	97.2(11)
H(44A)-C(44)-H(44B)	109.5	F(11)-P(2)-F(8)	91.1(10)
N(22)-C(44)-H(44C)	109.5	F(10)-P(2)-F(8)	93.4(6)
H(44A)-C(44)-H(44C)	109.5	F(11)-P(2)-F(12)	160.3(13)
H(44B)-C(44)-H(44C)	109.5	F(10)-P(2)-F(12)	95.4(9)
N(23)-C(45)-N(24)	105.5(5)	F(8)-P(2)-F(12)	103.2(9)
N(23)-C(45)-Cu(6)	128.8(4)	F(11)-P(2)-F(9)	86.2(10)
N(24)-C(45)-Cu(6)	125.6(4)	F(10)-P(2)-F(9)	176.4(10)
C(47)-C(46)-N(23)	108.5(5)	F(8)-P(2)-F(9)	85.2(7)
C(47)-C(46)-H(46)	125.8	F(12)-P(2)-F(9)	81.7(8)
N(23)-C(46)-H(46)	125.7	F(11)-P(2)-F(7)	87.8(10)
C(46)-C(47)-N(24)	106.3(5)	F(10)-P(2)-F(7)	86.6(6)
C(46)-C(47)-H(47)	126.8	F(8)-P(2)-F(7)	178.9(8)
N(24)-C(47)-H(47)	126.9	F(12)-P(2)-F(7)	77.9(8)
N(24)-C(48)-H(48A)	109.5	F(9)-P(2)-F(7)	95.0(7)
N(24)-C(48)-H(48B)	109.4		

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Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for ea03305b. 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)	35(1)	33(1)	26(1)	1(1)	-5(1)	-15(1)
Cu(2)	30(1)	37(1)	31(1)	3(1)	-8(1)	-9(1)
Cu(3)	29(1)	25(1)	30(1)	7(1)	-11(1)	-11(1)
N(1)	38(2)	54(3)	25(2)	7(2)	-5(2)	-20(2)
N(2)	37(2)	44(3)	37(2)	-11(2)	-5(2)	-14(2)
N(3)	40(3)	59(3)	37(2)	19(2)	-23(2)	-19(2)
N(4)	35(3)	62(4)	50(3)	12(3)	-19(2)	-16(2)
N(5)	30(2)	38(3)	49(3)	22(2)	-14(2)	-13(2)
N(6)	33(2)	28(2)	56(3)	-2(2)	-7(2)	-9(2)
N(7)	41(2)	36(2)	29(2)	5(2)	-6(2)	-24(2)
N(8)	38(2)	36(2)	36(2)	-2(2)	-11(2)	-21(2)
N(9)	34(2)	41(2)	26(2)	-4(2)	-2(2)	-21(2)
N(10)	34(2)	42(3)	45(3)	-14(2)	4(2)	-16(2)
N(11)	39(2)	31(2)	28(2)	9(2)	-17(2)	-16(2)
N(12)	33(2)	31(2)	41(2)	1(2)	-18(2)	-7(2)
B(1)	41(3)	61(4)	32(3)	22(3)	-15(3)	-20(3)
B(2)	43(3)	41(3)	24(2)	8(2)	-12(2)	-25(3)
C(1)	34(3)	44(3)	27(2)	0(2)	-9(2)	-17(2)
C(2)	48(4)	81(5)	27(3)	0(3)	1(2)	-33(4)
C(3)	38(3)	70(5)	36(3)	-10(3)	4(2)	-24(3)
C(4)	54(4)	42(3)	55(4)	-17(3)	-14(3)	-12(3)
C(5)	35(3)	44(3)	39(3)	12(2)	-18(2)	-14(2)
C(6)	57(4)	88(6)	40(3)	21(4)	-28(3)	-29(4)
C(7)	59(4)	93(6)	54(4)	24(4)	-39(4)	-39(4)
C(8)	37(3)	79(5)	65(5)	5(4)	-12(3)	-24(3)
C(9)	27(2)	27(2)	40(3)	11(2)	-9(2)	-10(2)
C(10)	46(4)	42(4)	90(6)	42(4)	-26(4)	-12(3)
C(11)	41(3)	24(3)	97(6)	10(3)	-12(4)	-8(2)
C(12)	47(4)	46(4)	67(5)	-15(3)	-5(3)	-20(3)
C(13)	31(2)	30(2)	31(2)	-1(2)	-9(2)	-14(2)
C(14)	51(4)	57(4)	36(3)	4(3)	-3(2)	-38(3)
C(15)	48(3)	61(4)	42(3)	3(3)	-7(3)	-36(3)
C(16)	64(4)	56(4)	42(3)	-1(3)	-23(3)	-32(3)

C(17)	29(2)	37(3)	31(2)	-6(2)	1(2)	-16(2)
C(18)	40(3)	61(4)	26(2)	-13(2)	0(2)	-28(3)
C(19)	40(3)	72(5)	46(3)	-28(3)	3(3)	-29(3)
C(20)	45(4)	38(3)	78(5)	-9(3)	5(3)	-5(3)
C(21)	29(2)	27(2)	27(2)	4(2)	-13(2)	-11(2)
C(22)	59(4)	33(3)	40(3)	16(2)	-31(3)	-19(3)
C(23)	56(4)	31(3)	56(4)	5(3)	-34(3)	-5(3)
C(24)	29(3)	46(3)	45(3)	-4(3)	-10(2)	-6(2)
Cu(4)	26(1)	29(1)	30(1)	9(1)	-9(1)	-9(1)
Cu(5)	29(1)	30(1)	23(1)	1(1)	-6(1)	-11(1)
Cu(6)	38(1)	29(1)	31(1)	-2(1)	-15(1)	0(1)
N(13)	34(2)	32(2)	33(2)	11(2)	-13(2)	-16(2)
N(14)	44(3)	42(3)	47(3)	14(2)	-20(2)	-28(2)
N(15)	29(2)	31(2)	25(2)	3(2)	-8(2)	-10(2)
N(16)	30(2)	27(2)	31(2)	-2(2)	-12(2)	-5(2)
N(17)	33(2)	26(2)	33(2)	4(2)	-18(2)	-7(2)
N(18)	31(2)	37(3)	39(2)	1(2)	-8(2)	-2(2)
N(19)	29(2)	25(2)	25(2)	4(2)	-10(2)	-7(2)
N(20)	28(2)	29(2)	31(2)	-2(2)	-10(2)	1(2)
N(21)	25(2)	43(3)	26(2)	-3(2)	-3(2)	-11(2)
N(22)	27(2)	46(3)	34(2)	-1(2)	-7(2)	-12(2)
N(23)	25(2)	33(2)	26(2)	-5(2)	-7(2)	-5(2)
N(24)	57(3)	30(2)	41(3)	-3(2)	-21(2)	-8(2)
B(3)	34(3)	31(3)	34(3)	9(2)	-15(2)	-12(2)
B(4)	31(3)	34(3)	22(2)	1(2)	-7(2)	-9(2)
C(25)	32(2)	35(3)	31(2)	9(2)	-10(2)	-16(2)
C(26)	57(4)	45(3)	53(4)	27(3)	-26(3)	-29(3)
C(27)	61(4)	48(4)	63(4)	28(3)	-26(3)	-38(3)
C(28)	50(4)	68(5)	59(4)	17(3)	-28(3)	-34(4)
C(29)	25(2)	26(2)	28(2)	2(2)	-9(2)	-7(2)
C(30)	33(3)	40(3)	25(2)	0(2)	-7(2)	-7(2)
C(31)	32(3)	40(3)	33(3)	-5(2)	-9(2)	-5(2)
C(32)	47(3)	26(3)	48(3)	1(2)	-13(3)	-8(2)
C(33)	30(2)	28(2)	34(2)	2(2)	-12(2)	-5(2)
C(34)	37(3)	41(3)	41(3)	3(2)	-25(2)	-4(2)
C(35)	37(3)	47(3)	54(4)	8(3)	-28(3)	-8(3)
C(36)	38(3)	65(5)	49(4)	1(3)	0(3)	9(3)
C(37)	22(2)	30(2)	29(2)	1(2)	-10(2)	-8(2)

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C(38)	45(3)	27(3)	41(3)	14(2)	-16(2)	-12(2)
C(39)	48(3)	23(2)	49(3)	3(2)	-22(3)	-5(2)
C(40)	33(3)	52(4)	36(3)	-7(3)	-5(2)	0(2)
C(41)	28(2)	36(3)	25(2)	1(2)	-9(2)	-11(2)
C(42)	32(3)	65(4)	28(3)	-5(3)	1(2)	-16(3)
C(43)	30(3)	74(5)	32(3)	-5(3)	-3(2)	-17(3)
C(44)	42(3)	66(4)	45(3)	3(3)	-21(3)	-23(3)
C(45)	38(3)	29(2)	31(2)	-5(2)	-10(2)	-2(2)
C(46)	34(3)	42(3)	29(2)	-4(2)	-12(2)	-8(2)
C(47)	54(4)	41(3)	47(3)	-9(3)	-22(3)	-13(3)
C(48)	100(7)	31(3)	63(5)	3(3)	-36(5)	-21(4)
P(1)	37(1)	45(1)	32(1)	-4(1)	-7(1)	-7(1)
F(1)	78(3)	62(3)	47(2)	-15(2)	-7(2)	5(2)
F(2)	82(3)	84(3)	40(2)	-21(2)	-8(2)	-16(3)
F(3)	85(4)	156(7)	105(5)	-47(5)	20(4)	-78(5)
F(4)	61(4)	252(11)	101(5)	-50(6)	-5(3)	-72(5)
F(5)	125(5)	68(3)	54(3)	5(2)	-19(3)	6(3)
F(6)	275(12)	70(4)	77(4)	16(3)	-39(6)	58(6)
P(2)	39(1)	38(1)	31(1)	-2(1)	-6(1)	-8(1)
F(7)	102(7)	274(14)	183(10)	-76(10)	-11(6)	-95(8)
F(8)	79(5)	276(13)	254(12)	-119(11)	-19(6)	-89(7)
F(9)	284(15)	156(9)	191(11)	-122(8)	132(10)	-126(10)
F(10)	164(9)	220(11)	297(14)	-212(11)	144(9)	-119(8)
F(11)	580(40)	165(12)	310(20)	159(13)	-300(20)	-119(17)
F(12)	335(19)	165(10)	197(12)	107(10)	-39(12)	-126(12)

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

for ea03305b.

	x	y	z	U(eq)
H(1)	6437	5879	6725	52
H(2)	7328	8291	2103	39
H(2A)	4629	6792	7257	61
H(3)	3532	8311	7016	57
H(4A)	4604	9749	6015	74
H(4B)	3613	9499	5912	74
H(4C)	4588	9329	5173	74
H(6)	7782	6461	7174	69
H(7)	9443	6699	6516	73
H(8A)	10387	6030	4704	88
H(8B)	10254	7049	4995	88
H(8C)	9720	6881	4304	88
H(10)	6945	4251	6088	71
H(11)	6790	3554	4889	66
H(12A)	6226	5274	3339	79
H(12B)	5408	4754	3781	79
H(12C)	6556	4188	3438	79
H(14)	8841	8782	2263	53
H(15)	9451	9274	3371	56
H(16A)	8063	9685	5084	73
H(16B)	9091	8883	4977	73
H(16C)	8033	8669	5365	73
H(18)	7755	6815	1292	48
H(19)	8518	5176	1458	61
H(20A)	8608	4715	3621	87
H(20B)	9502	4477	2819	87
H(20C)	8486	4184	2876	87
H(22)	5594	9409	2283	48
H(23)	3870	9543	3099	55
H(24A)	3934	7856	4755	61
H(24B)	3336	7908	4053	61
H(24C)	3223	8813	4547	61

H(3A)	2522	7106	3189	38
H(4)	2980	9235	-1553	35
H(26)	1725	5857	2979	57
H(27)	557	5628	2179	62
H(28A)	-462	7319	1199	80
H(28B)	125	6329	806	80
H(28C)	506	7201	458	80
H(30)	1358	8550	3897	40
H(31)	1043	10229	3682	43
H(32A)	2510	10953	2342	61
H(32B)	1334	11199	2351	61
H(32C)	2155	10699	1574	61
H(34)	4415	6697	3074	46
H(35)	5979	6291	2010	53
H(36A)	5772	5831	219	86
H(36B)	6409	6465	439	86
H(36C)	5499	6894	3	86
H(38)	2106	10868	-991	44
H(39)	708	11603	158	47
H(40A)	-503	10217	1265	64
H(40B)	-140	11042	1527	64
H(40C)	335	10020	1791	64
H(42)	4934	8619	-1900	51
H(43)	6298	8476	-1177	55
H(44A)	5766	9356	532	72
H(44B)	6306	8284	416	72
H(44C)	5240	8635	1047	72
H(46)	2007	8254	-2034	42
H(47)	1687	6743	-1734	54
H(48A)	2858	5350	-775	92
H(48B)	1706	5752	-305	92
H(48C)	2594	5800	112	92

Table 6. Torsion angles [°] for ea03305b.

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C(13)-Cu(1)-Cu(2)-C(5)	112.4(2)
C(1)-Cu(1)-Cu(2)-C(5)	-62.8(2)
Cu(3)-Cu(1)-Cu(2)-C(5)	-124.98(18)
C(13)-Cu(1)-Cu(2)-C(17)	-60.8(2)
C(1)-Cu(1)-Cu(2)-C(17)	124.1(2)
Cu(3)-Cu(1)-Cu(2)-C(17)	61.86(16)
C(13)-Cu(1)-Cu(2)-Cu(3)	-122.67(16)
C(1)-Cu(1)-Cu(2)-Cu(3)	62.20(17)
C(13)-Cu(1)-Cu(3)-C(9)	119.9(2)
C(1)-Cu(1)-Cu(3)-C(9)	-63.3(3)
Cu(2)-Cu(1)-Cu(3)-C(9)	58.50(18)
C(13)-Cu(1)-Cu(3)-C(21)	-61.0(2)
C(1)-Cu(1)-Cu(3)-C(21)	115.8(2)
Cu(2)-Cu(1)-Cu(3)-C(21)	-122.34(16)
C(13)-Cu(1)-Cu(3)-Cu(2)	61.37(17)
C(1)-Cu(1)-Cu(3)-Cu(2)	-121.84(18)
C(5)-Cu(2)-Cu(3)-C(9)	-64.6(3)
C(17)-Cu(2)-Cu(3)-C(9)	112.0(3)
Cu(1)-Cu(2)-Cu(3)-C(9)	-124.74(19)
C(5)-Cu(2)-Cu(3)-C(21)	123.0(3)
C(17)-Cu(2)-Cu(3)-C(21)	-60.5(2)
Cu(1)-Cu(2)-Cu(3)-C(21)	62.78(16)
C(5)-Cu(2)-Cu(3)-Cu(1)	60.2(2)
C(17)-Cu(2)-Cu(3)-Cu(1)	-123.25(17)
C(1)-N(1)-B(1)-N(5)	-81.3(7)
C(2)-N(1)-B(1)-N(5)	96.3(6)
C(1)-N(1)-B(1)-N(3)	42.8(8)
C(2)-N(1)-B(1)-N(3)	-139.7(6)
C(9)-N(5)-B(1)-N(1)	37.4(8)
C(10)-N(5)-B(1)-N(1)	-145.1(6)
C(9)-N(5)-B(1)-N(3)	-87.5(7)
C(10)-N(5)-B(1)-N(3)	90.0(7)
C(5)-N(3)-B(1)-N(1)	-87.8(8)
C(6)-N(3)-B(1)-N(1)	90.8(7)
C(5)-N(3)-B(1)-N(5)	37.0(9)
C(6)-N(3)-B(1)-N(5)	-144.4(7)

C(21)-N(11)-B(2)-N(7)	-80.0(7)
C(22)-N(11)-B(2)-N(7)	96.7(6)
C(21)-N(11)-B(2)-N(9)	45.5(7)
C(22)-N(11)-B(2)-N(9)	-137.8(5)
C(13)-N(7)-B(2)-N(11)	41.4(8)
C(14)-N(7)-B(2)-N(11)	-141.1(6)
C(13)-N(7)-B(2)-N(9)	-85.1(7)
C(14)-N(7)-B(2)-N(9)	92.4(6)
C(17)-N(9)-B(2)-N(11)	-84.6(6)
C(18)-N(9)-B(2)-N(11)	99.0(6)
C(17)-N(9)-B(2)-N(7)	41.1(7)
C(18)-N(9)-B(2)-N(7)	-135.3(5)
C(2)-N(1)-C(1)-N(2)	-0.6(6)
B(1)-N(1)-C(1)-N(2)	177.1(6)
C(2)-N(1)-C(1)-Cu(1)	-178.6(4)
B(1)-N(1)-C(1)-Cu(1)	-0.8(9)
C(3)-N(2)-C(1)-N(1)	0.2(6)
C(4)-N(2)-C(1)-N(1)	176.5(5)
C(3)-N(2)-C(1)-Cu(1)	178.3(4)
C(4)-N(2)-C(1)-Cu(1)	-5.4(8)
Cu(3)-Cu(1)-C(1)-N(1)	72.7(5)
Cu(2)-Cu(1)-C(1)-N(1)	20.5(5)
Cu(3)-Cu(1)-C(1)-N(2)	-104.9(5)
Cu(2)-Cu(1)-C(1)-N(2)	-157.2(4)
C(1)-N(1)-C(2)-C(3)	0.8(7)
B(1)-N(1)-C(2)-C(3)	-177.2(6)
N(1)-C(2)-C(3)-N(2)	-0.6(7)
C(1)-N(2)-C(3)-C(2)	0.2(7)
C(4)-N(2)-C(3)-C(2)	-176.1(6)
C(6)-N(3)-C(5)-N(4)	1.2(8)
B(1)-N(3)-C(5)-N(4)	179.9(6)
C(6)-N(3)-C(5)-Cu(2)	-174.2(6)
B(1)-N(3)-C(5)-Cu(2)	4.5(10)
C(7)-N(4)-C(5)-N(3)	-0.4(8)
C(8)-N(4)-C(5)-N(3)	174.2(7)
C(7)-N(4)-C(5)-Cu(2)	175.2(6)
C(8)-N(4)-C(5)-Cu(2)	-10.2(10)
C(17)-Cu(2)-C(5)-N(3)	-144.3(10)

Cu(3)-Cu(2)-C(5)-N(3)	19.4(7)
Cu(1)-Cu(2)-C(5)-N(3)	68.0(6)
C(17)-Cu(2)-C(5)-N(4)	41.2(15)
Cu(3)-Cu(2)-C(5)-N(4)	-155.2(5)
Cu(1)-Cu(2)-C(5)-N(4)	-106.6(6)
C(5)-N(3)-C(6)-C(7)	-1.5(10)
B(1)-N(3)-C(6)-C(7)	179.6(7)
N(3)-C(6)-C(7)-N(4)	1.2(10)
C(5)-N(4)-C(7)-C(6)	-0.5(10)
C(8)-N(4)-C(7)-C(6)	-175.0(8)
C(10)-N(5)-C(9)-N(6)	0.5(6)
B(1)-N(5)-C(9)-N(6)	178.3(5)
C(10)-N(5)-C(9)-Cu(3)	-173.5(5)
B(1)-N(5)-C(9)-Cu(3)	4.3(9)
C(11)-N(6)-C(9)-N(5)	-0.8(6)
C(12)-N(6)-C(9)-N(5)	177.9(5)
C(11)-N(6)-C(9)-Cu(3)	173.5(4)
C(12)-N(6)-C(9)-Cu(3)	-7.8(8)
Cu(1)-Cu(3)-C(9)-N(5)	19.2(5)
Cu(2)-Cu(3)-C(9)-N(5)	69.8(5)
Cu(1)-Cu(3)-C(9)-N(6)	-153.6(4)
Cu(2)-Cu(3)-C(9)-N(6)	-103.1(5)
C(9)-N(5)-C(10)-C(11)	0.0(8)
B(1)-N(5)-C(10)-C(11)	-177.9(6)
N(5)-C(10)-C(11)-N(6)	-0.5(8)
C(9)-N(6)-C(11)-C(10)	0.8(8)
C(12)-N(6)-C(11)-C(10)	-177.9(6)
C(15)-N(8)-C(13)-N(7)	0.2(7)
C(16)-N(8)-C(13)-N(7)	178.1(6)
C(15)-N(8)-C(13)-Cu(1)	177.3(5)
C(16)-N(8)-C(13)-Cu(1)	-4.8(8)
C(14)-N(7)-C(13)-N(8)	0.0(7)
B(2)-N(7)-C(13)-N(8)	177.8(6)
C(14)-N(7)-C(13)-Cu(1)	-176.8(5)
B(2)-N(7)-C(13)-Cu(1)	0.9(9)
Cu(3)-Cu(1)-C(13)-N(8)	-157.9(4)
Cu(2)-Cu(1)-C(13)-N(8)	-106.1(5)
Cu(3)-Cu(1)-C(13)-N(7)	18.4(6)

Cu(2)-Cu(1)-C(13)-N(7)	70.2(5)
C(13)-N(7)-C(14)-C(15)	-0.3(8)
B(2)-N(7)-C(14)-C(15)	-178.2(6)
N(7)-C(14)-C(15)-N(8)	0.4(8)
C(13)-N(8)-C(15)-C(14)	-0.4(8)
C(16)-N(8)-C(15)-C(14)	-178.3(7)
C(18)-N(9)-C(17)-N(10)	-1.5(6)
B(2)-N(9)-C(17)-N(10)	-178.2(5)
C(18)-N(9)-C(17)-Cu(2)	177.9(4)
B(2)-N(9)-C(17)-Cu(2)	1.1(8)
C(19)-N(10)-C(17)-N(9)	1.5(6)
C(20)-N(10)-C(17)-N(9)	178.3(6)
C(19)-N(10)-C(17)-Cu(2)	-177.9(4)
C(20)-N(10)-C(17)-Cu(2)	-1.2(8)
C(5)-Cu(2)-C(17)-N(9)	-127.4(11)
Cu(3)-Cu(2)-C(17)-N(9)	68.0(5)
Cu(1)-Cu(2)-C(17)-N(9)	18.5(5)
C(5)-Cu(2)-C(17)-N(10)	51.9(14)
Cu(3)-Cu(2)-C(17)-N(10)	-112.7(4)
Cu(1)-Cu(2)-C(17)-N(10)	-162.2(4)
C(17)-N(9)-C(18)-C(19)	1.0(6)
B(2)-N(9)-C(18)-C(19)	177.9(5)
N(9)-C(18)-C(19)-N(10)	0.0(7)
C(17)-N(10)-C(19)-C(18)	-1.0(7)
C(20)-N(10)-C(19)-C(18)	-177.7(6)
C(22)-N(11)-C(21)-N(12)	-0.2(6)
B(2)-N(11)-C(21)-N(12)	176.9(5)
C(22)-N(11)-C(21)-Cu(3)	178.4(4)
B(2)-N(11)-C(21)-Cu(3)	-4.5(8)
C(23)-N(12)-C(21)-N(11)	0.5(6)
C(24)-N(12)-C(21)-N(11)	178.3(5)
C(23)-N(12)-C(21)-Cu(3)	-178.2(4)
C(24)-N(12)-C(21)-Cu(3)	-0.4(7)
Cu(1)-Cu(3)-C(21)-N(11)	74.3(5)
Cu(2)-Cu(3)-C(21)-N(11)	21.7(5)
Cu(1)-Cu(3)-C(21)-N(12)	-107.3(4)
Cu(2)-Cu(3)-C(21)-N(12)	-159.9(4)
C(21)-N(11)-C(22)-C(23)	-0.2(7)

B(2)-N(11)-C(22)-C(23)	-177.5(5)
N(11)-C(22)-C(23)-N(12)	0.6(7)
C(21)-N(12)-C(23)-C(22)	-0.7(7)
C(24)-N(12)-C(23)-C(22)	-178.4(5)
C(37)-Cu(4)-Cu(5)-C(29)	113.6(2)
C(25)-Cu(4)-Cu(5)-C(29)	-59.7(2)
Cu(6)-Cu(4)-Cu(5)-C(29)	-124.23(15)
C(37)-Cu(4)-Cu(5)-C(41)	-64.2(2)
C(25)-Cu(4)-Cu(5)-C(41)	122.4(3)
Cu(6)-Cu(4)-Cu(5)-C(41)	57.92(18)
C(37)-Cu(4)-Cu(5)-Cu(6)	-122.16(16)
C(25)-Cu(4)-Cu(5)-Cu(6)	64.52(19)
C(37)-Cu(4)-Cu(6)-C(45)	-63.9(2)
C(25)-Cu(4)-Cu(6)-C(45)	115.6(2)
Cu(5)-Cu(4)-Cu(6)-C(45)	-123.03(18)
C(37)-Cu(4)-Cu(6)-C(33)	118.5(2)
C(25)-Cu(4)-Cu(6)-C(33)	-62.0(2)
Cu(5)-Cu(4)-Cu(6)-C(33)	59.40(17)
C(37)-Cu(4)-Cu(6)-Cu(5)	59.10(15)
C(25)-Cu(4)-Cu(6)-Cu(5)	-121.37(16)
C(29)-Cu(5)-Cu(6)-C(45)	121.5(2)
C(41)-Cu(5)-Cu(6)-C(45)	-64.2(2)
Cu(4)-Cu(5)-Cu(6)-C(45)	61.73(19)
C(29)-Cu(5)-Cu(6)-C(33)	-63.8(2)
C(41)-Cu(5)-Cu(6)-C(33)	110.5(2)
Cu(4)-Cu(5)-Cu(6)-C(33)	-123.53(17)
C(29)-Cu(5)-Cu(6)-Cu(4)	59.72(15)
C(41)-Cu(5)-Cu(6)-Cu(4)	-125.94(16)
C(25)-N(13)-B(3)-N(15)	42.3(8)
C(26)-N(13)-B(3)-N(15)	-139.5(6)
C(25)-N(13)-B(3)-N(17)	-82.2(7)
C(26)-N(13)-B(3)-N(17)	96.0(7)
C(29)-N(15)-B(3)-N(13)	-85.8(6)
C(30)-N(15)-B(3)-N(13)	92.8(6)
C(29)-N(15)-B(3)-N(17)	38.8(7)
C(30)-N(15)-B(3)-N(17)	-142.6(5)
C(33)-N(17)-B(3)-N(13)	42.8(7)
C(34)-N(17)-B(3)-N(13)	-140.3(5)

C(33)-N(17)-B(3)-N(15)	-82.1(6)
C(34)-N(17)-B(3)-N(15)	94.8(6)
C(45)-N(23)-B(4)-N(21)	42.6(7)
C(46)-N(23)-B(4)-N(21)	-144.3(5)
C(45)-N(23)-B(4)-N(19)	-80.8(6)
C(46)-N(23)-B(4)-N(19)	92.4(5)
C(41)-N(21)-B(4)-N(23)	-91.6(6)
C(42)-N(21)-B(4)-N(23)	88.8(6)
C(41)-N(21)-B(4)-N(19)	31.8(7)
C(42)-N(21)-B(4)-N(19)	-147.7(5)
C(37)-N(19)-B(4)-N(23)	37.1(7)
C(38)-N(19)-B(4)-N(23)	-145.4(5)
C(37)-N(19)-B(4)-N(21)	-86.9(6)
C(38)-N(19)-B(4)-N(21)	90.6(6)
C(26)-N(13)-C(25)-N(14)	-0.4(7)
B(3)-N(13)-C(25)-N(14)	178.0(5)
C(26)-N(13)-C(25)-Cu(4)	-177.3(5)
B(3)-N(13)-C(25)-Cu(4)	1.1(9)
C(27)-N(14)-C(25)-N(13)	1.9(7)
C(28)-N(14)-C(25)-N(13)	174.8(6)
C(27)-N(14)-C(25)-Cu(4)	179.1(5)
C(28)-N(14)-C(25)-Cu(4)	-8.0(9)
Cu(6)-Cu(4)-C(25)-N(13)	70.4(5)
Cu(5)-Cu(4)-C(25)-N(13)	16.7(6)
Cu(6)-Cu(4)-C(25)-N(14)	-106.0(5)
Cu(5)-Cu(4)-C(25)-N(14)	-159.7(5)
C(25)-N(13)-C(26)-C(27)	-1.3(8)
B(3)-N(13)-C(26)-C(27)	-179.8(6)
N(13)-C(26)-C(27)-N(14)	2.3(9)
C(25)-N(14)-C(27)-C(26)	-2.7(9)
C(28)-N(14)-C(27)-C(26)	-175.6(7)
C(31)-N(16)-C(29)-N(15)	0.6(6)
C(32)-N(16)-C(29)-N(15)	177.0(5)
C(31)-N(16)-C(29)-Cu(5)	178.4(4)
C(32)-N(16)-C(29)-Cu(5)	-5.2(7)
C(30)-N(15)-C(29)-N(16)	-0.4(5)
B(3)-N(15)-C(29)-N(16)	178.3(5)
C(30)-N(15)-C(29)-Cu(5)	-178.0(4)

B(3)-N(15)-C(29)-Cu(5)	0.7(8)
Cu(6)-Cu(5)-C(29)-N(16)	-155.7(4)
Cu(4)-Cu(5)-C(29)-N(16)	-108.1(4)
Cu(6)-Cu(5)-C(29)-N(15)	21.5(5)
Cu(4)-Cu(5)-C(29)-N(15)	69.1(4)
C(29)-N(15)-C(30)-C(31)	0.1(6)
B(3)-N(15)-C(30)-C(31)	-178.7(5)
N(15)-C(30)-C(31)-N(16)	0.3(6)
C(29)-N(16)-C(31)-C(30)	-0.6(6)
C(32)-N(16)-C(31)-C(30)	-177.0(5)
C(34)-N(17)-C(33)-N(18)	-0.9(6)
B(3)-N(17)-C(33)-N(18)	176.3(5)
C(34)-N(17)-C(33)-Cu(6)	179.8(4)
B(3)-N(17)-C(33)-Cu(6)	-3.0(8)
C(35)-N(18)-C(33)-N(17)	1.0(6)
C(36)-N(18)-C(33)-N(17)	176.5(6)
C(35)-N(18)-C(33)-Cu(6)	-179.6(4)
C(36)-N(18)-C(33)-Cu(6)	-4.1(9)
Cu(4)-Cu(6)-C(33)-N(17)	22.4(6)
Cu(5)-Cu(6)-C(33)-N(17)	74.0(5)
Cu(4)-Cu(6)-C(33)-N(18)	-156.8(4)
Cu(5)-Cu(6)-C(33)-N(18)	-105.2(5)
C(33)-N(17)-C(34)-C(35)	0.5(7)
B(3)-N(17)-C(34)-C(35)	-177.0(5)
N(17)-C(34)-C(35)-N(18)	0.2(7)
C(33)-N(18)-C(35)-C(34)	-0.7(7)
C(36)-N(18)-C(35)-C(34)	-176.2(7)
C(38)-N(19)-C(37)-N(20)	1.5(5)
B(4)-N(19)-C(37)-N(20)	179.2(4)
C(38)-N(19)-C(37)-Cu(4)	-172.0(4)
B(4)-N(19)-C(37)-Cu(4)	5.7(8)
C(39)-N(20)-C(37)-N(19)	-1.0(6)
C(40)-N(20)-C(37)-N(19)	176.8(5)
C(39)-N(20)-C(37)-Cu(4)	173.4(4)
C(40)-N(20)-C(37)-Cu(4)	-8.8(7)
Cu(6)-Cu(4)-C(37)-N(19)	18.3(5)
Cu(5)-Cu(4)-C(37)-N(19)	70.0(4)
Cu(6)-Cu(4)-C(37)-N(20)	-154.3(4)

Cu(5)-Cu(4)-C(37)-N(20)	-102.6(4)
C(37)-N(19)-C(38)-C(39)	-1.5(6)
B(4)-N(19)-C(38)-C(39)	-179.4(5)
N(19)-C(38)-C(39)-N(20)	0.8(6)
C(37)-N(20)-C(39)-C(38)	0.1(6)
C(40)-N(20)-C(39)-C(38)	-177.7(5)
C(43)-N(22)-C(41)-N(21)	-0.5(7)
C(44)-N(22)-C(41)-N(21)	175.3(6)
C(43)-N(22)-C(41)-Cu(5)	171.5(5)
C(44)-N(22)-C(41)-Cu(5)	-12.7(8)
C(42)-N(21)-C(41)-N(22)	0.4(6)
B(4)-N(21)-C(41)-N(22)	-179.2(5)
C(42)-N(21)-C(41)-Cu(5)	-171.1(5)
B(4)-N(21)-C(41)-Cu(5)	9.3(9)
Cu(6)-Cu(5)-C(41)-N(22)	-105.2(5)
Cu(4)-Cu(5)-C(41)-N(22)	-151.8(4)
Cu(6)-Cu(5)-C(41)-N(21)	64.7(5)
Cu(4)-Cu(5)-C(41)-N(21)	18.1(6)
C(41)-N(21)-C(42)-C(43)	-0.1(8)
B(4)-N(21)-C(42)-C(43)	179.5(6)
N(21)-C(42)-C(43)-N(22)	-0.2(8)
C(41)-N(22)-C(43)-C(42)	0.5(8)
C(44)-N(22)-C(43)-C(42)	-175.3(6)
C(46)-N(23)-C(45)-N(24)	1.3(6)
B(4)-N(23)-C(45)-N(24)	175.2(5)
C(46)-N(23)-C(45)-Cu(6)	-175.9(4)
B(4)-N(23)-C(45)-Cu(6)	-2.0(8)
C(47)-N(24)-C(45)-N(23)	-1.0(7)
C(48)-N(24)-C(45)-N(23)	176.9(7)
C(47)-N(24)-C(45)-Cu(6)	176.2(5)
C(48)-N(24)-C(45)-Cu(6)	-5.8(10)
Cu(4)-Cu(6)-C(45)-N(23)	75.5(5)
Cu(5)-Cu(6)-C(45)-N(23)	23.0(6)
Cu(4)-Cu(6)-C(45)-N(24)	-101.1(5)
Cu(5)-Cu(6)-C(45)-N(24)	-153.7(5)
C(45)-N(23)-C(46)-C(47)	-1.0(7)
B(4)-N(23)-C(46)-C(47)	-175.4(5)
N(23)-C(46)-C(47)-N(24)	0.4(7)

C(45)-N(24)-C(47)-C(46)	0.4(8)
C(48)-N(24)-C(47)-C(46)	-177.5(7)

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Symmetry transformations used to generate equivalent atoms: