

**Multifrequency EPR Studies of $[\text{Cu}^{1.5}\text{Cu}^{1.5}]^{1+}$
for $\text{Cu}_2(\mu\text{-NR}_2)_2$ and $\text{Cu}_2(\mu\text{-PR}_2)_2$ Diamond
Cores**

SUPPORTING INFORMATION

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Supplementary Figures

Figure S1. Second derivative of S-band spectrum for $[\text{Cu}_2\text{PPP}_2]^{+1}$ and simulations. EPR parameters for Simulation1: g_{iso} , 2.01; $A^{\text{Cu}}_{\text{iso}} \sim A^{\text{P-bridging}} = 45$ G; $A^{\text{P-non-bridging}} = 12.5$ G; line width 5 G; microwave frequency, 3.358 GHz. Simulation2: $A^{\text{Cu}} = 45$ G, $A^{\text{P-bridging}} = 25$ G, and $A^{\text{P-non-bridging}} = 12.5$ G. Simulation3: $A^{\text{Cu}} = 25$ G, $A^{\text{P-bridging}} = 25$ G, and $A^{\text{P-non-bridging}} = 12.5$ G. The simulations establish that the hyperfine coupling constants for both Cu and P are about 45 G because the lines are too close together if either the coupling constant for Cu or P are decreased. Also, the wings of the spectra are not simulated if the coupling constants for Cu and/or P are less than 45 G.

Figure S2. Q-band spectrum for $[\text{Cu}_2\text{PNP}_2]^{+1}$ and simulation. EPR parameters for simulation: g_{max} , g_{mid} , g_{min} , 2.085, 2.060, 2.000; $A^{\text{Cu}}_{\text{max}}$, $A^{\text{Cu}}_{\text{mid}}$, $A^{\text{Cu}}_{\text{min}}$, 40, 27, 15 G; $A^{\text{N}}_{\text{max}}$, $A^{\text{N}}_{\text{mid}}$, $A^{\text{N}}_{\text{min}}$, 12, 24, 15 G; line width 20, 25, 10 G; microwave frequency, 35.028 GHz.

Figure S3. Second derivative of S-band spectrum for $[\text{Cu}_2\text{PNP}_2]^{+1}$ and simulations. EPR parameters for simulations: g_{max} , g_{mid} , g_{min} , 2.085, 2.057, 2.000; $A^{\text{Cu}}_{\text{max}}$, $A^{\text{Cu}}_{\text{mid}}$, $A^{\text{Cu}}_{\text{min}}$, 40, 27, 15 G; $A^{\text{N}}_{\text{max}}$, $A^{\text{N}}_{\text{mid}}$, $A^{\text{N}}_{\text{min}}$, 12, 24, 15 G; line width 15, 11, 10 G (top simulation) 5, 5, 5 G (bottom simulation); microwave frequency, 3.364 GHz.

Figure S4. Second derivative of S-band spectrum for $[\text{Cu}_2\text{SNS}_2]^{+1}$ and simulation. EPR parameters for simulations: g_{max} , g_{mid} , g_{min} , 2.069, 2.066, 2.00; $A^{\text{Cu}}_{\text{max}}$, $A^{\text{Cu}}_{\text{mid}}$, $A^{\text{Cu}}_{\text{min}}$, 44, 17, 5 G; $A^{\text{N}}_{\text{max}}$, $A^{\text{N}}_{\text{mid}}$, $A^{\text{N}}_{\text{min}}$, 12, 17, 5 G; line width 7, 7, 4 G; microwave frequency, 3.366 GHz.

Figure S1

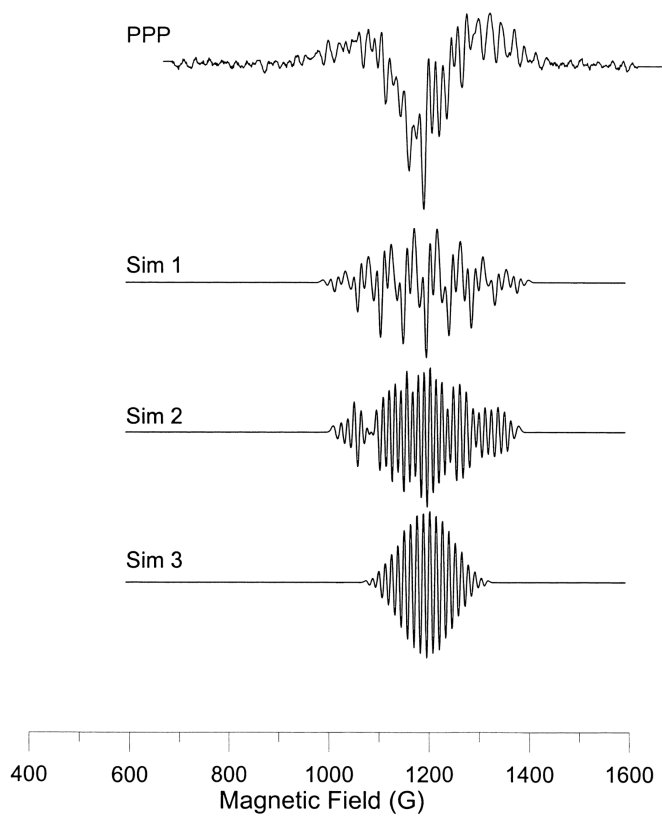


Figure S2

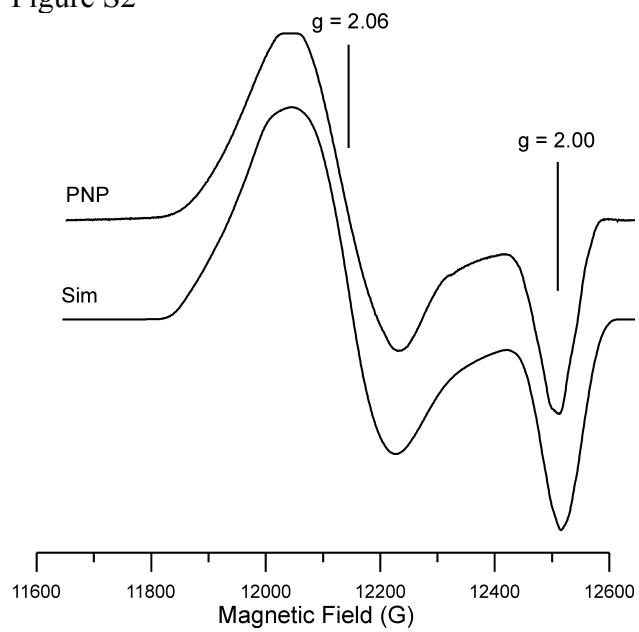


Figure S3

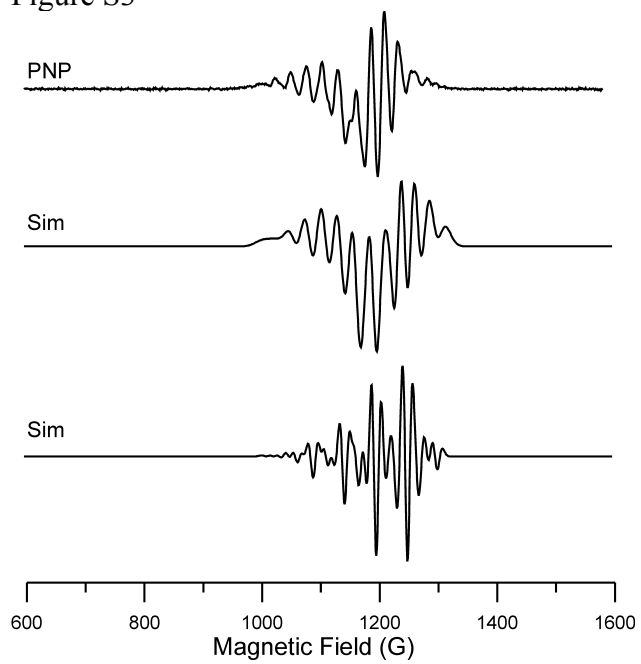


Figure S4

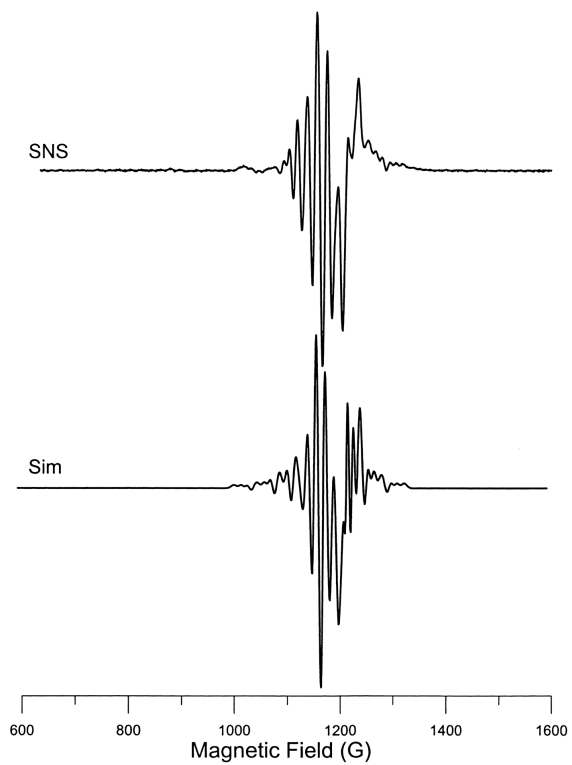


Table 1. Crystal data and structure refinement for [(PNP)Cu]₂[B(3,5-(CF₃)₂-C₆H₃)₄].

Identification code	sbh50	
Empirical formula	C ₈₈ H ₁₀₀ B Cu ₂ F ₂₄ N ₂ P ₄	
Formula weight	1903.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 21.1306(12) Å	α = 90°.
	b = 16.4994(9) Å	β = 91.9760(10)°.
	c = 25.8125(15) Å	γ = 90°.
Volume	8994.0(9) Å ³	
Z	4	
Density (calculated)	1.406 Mg/m ³	
Absorption coefficient	0.638 mm ⁻¹	
F(000)	3924	
Crystal size	0.37 x 0.35 x 0.33 mm ³	
Theta range for data collection	1.47 to 32.97°.	
Index ranges	-32 ≤ h ≤ 32, -24 ≤ k ≤ 24, -36 ≤ l ≤ 36	
Reflections collected	149170	
Independent reflections	30305 [R(int) = 0.0731]	
Completeness to theta = 32.97°	89.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	30305 / 0 / 1183	
Goodness-of-fit on F ²	1.033	
Final R indices [I > 2σ(I)]	R1 = 0.0709, wR2 = 0.1866	
R indices (all data)	R1 = 0.1335, wR2 = 0.2279	
Largest diff. peak and hole	3.424 and -1.467 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(\text{PNP})\text{Cu}]_2[\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Cu(1)	1941(1)	2217(1)	629(1)	21(1)
Cu(2)	3044(1)	2678(1)	399(1)	31(1)
N(1)	2488(1)	2835(2)	1170(1)	25(1)
N(2)	2404(1)	1969(2)	-43(1)	17(1)
P(1)	1913(1)	1183(1)	1195(1)	20(1)
P(2)	3047(1)	4025(1)	385(1)	21(1)
P(3)	3717(1)	1618(1)	415(1)	24(1)
P(4)	1188(1)	2860(1)	137(1)	18(1)
B	2356(2)	7283(2)	3126(1)	20(1)
C(1)	2673(2)	2380(2)	1616(1)	25(1)
C(2)	2477(1)	1575(2)	1680(1)	21(1)
C(3)	2702(2)	1136(2)	2112(1)	30(1)
C(4)	3102(2)	1469(2)	2479(1)	33(1)
C(5)	3296(2)	2263(3)	2420(2)	38(1)
C(6)	3078(2)	2717(2)	2000(2)	38(1)
C(7)	2359(2)	3669(2)	1267(1)	24(1)
C(8)	2551(1)	4281(2)	927(1)	22(1)
C(9)	2372(2)	5083(2)	1019(1)	26(1)
C(10)	2021(2)	5299(2)	1441(1)	32(1)
C(11)	1852(2)	4691(2)	1787(2)	37(1)
C(12)	2009(2)	3892(2)	1698(1)	32(1)
C(13)	2612(1)	1155(2)	-122(1)	18(1)
C(14)	3188(2)	878(2)	106(1)	24(1)
C(15)	3359(2)	64(2)	46(2)	30(1)
C(16)	2975(2)	-470(2)	-233(2)	33(1)
C(17)	2412(2)	-185(2)	-467(1)	30(1)
C(18)	2233(2)	611(2)	-410(1)	23(1)
C(19)	2142(1)	2355(2)	-494(1)	16(1)
C(20)	1601(1)	2851(2)	-468(1)	19(1)
C(21)	1374(2)	3255(2)	-913(1)	24(1)

C(22)	1673(2)	3173(2)	-1380(1)	28(1)
C(23)	2195(2)	2676(2)	-1410(1)	26(1)
C(24)	2434(2)	2273(2)	-974(1)	22(1)
C(25)	1159(2)	1043(2)	1522(1)	25(1)
C(26)	832(2)	1834(2)	1678(1)	27(1)
C(27)	1041(2)	2110(2)	2220(2)	35(1)
C(28)	111(2)	1716(3)	1650(2)	37(1)
C(29)	2157(2)	154(2)	1008(1)	29(1)
C(30)	1874(3)	-610(3)	1225(2)	70(2)
C(31)	2048(3)	-834(3)	1750(2)	60(1)
C(32)	1967(3)	-1309(3)	849(3)	72(2)
C(33)	2712(2)	4683(2)	-132(1)	32(1)
C(34)	2869(2)	4477(2)	-693(1)	32(1)
C(35)	2465(2)	5017(2)	-1062(2)	39(1)
C(36)	3567(2)	4582(3)	-806(2)	44(1)
C(37)	3750(3)	4687(5)	514(3)	28(2)
C(38)	4301(3)	4277(5)	818(3)	40(2)
C(39)	4106(4)	4014(9)	1350(4)	78(4)
C(40)	4873(4)	4851(9)	843(4)	65(3)
C(41)	3879(3)	4274(6)	590(3)	24(2)
C(42)	4008(3)	5071(4)	871(3)	23(2)
C(43)	3958(4)	4957(5)	1461(3)	32(2)
C(44)	4672(4)	5362(6)	750(4)	30(2)
C(45)	4418(2)	1510(2)	14(1)	31(1)
C(46)	4308(2)	1652(3)	-571(2)	34(1)
C(47)	4177(2)	2537(3)	-693(2)	47(1)
C(48)	4874(2)	1339(3)	-862(2)	47(1)
C(49)	3996(2)	1136(3)	1026(2)	35(1)
C(50)	4638(2)	1446(4)	1249(2)	54(1)
C(51)	4656(3)	2295(4)	1343(3)	75(2)
C(52)	5204(9)	1105(11)	1101(9)	54(6)
C(53)	4772(3)	921(5)	1767(3)	64(2)
C(54)	429(1)	2375(2)	-66(2)	26(1)
C(55)	469(2)	1531(2)	-311(1)	25(1)
C(56)	686(2)	885(2)	79(2)	31(1)
C(57)	-179(2)	1291(2)	-549(2)	35(1)

C(58)	960(2)	3931(2)	223(1)	26(1)
C(60)	730(3)	4145(4)	754(3)	26(2)
C(59)	387(4)	4138(5)	525(4)	31(3)
C(61)	249(3)	3659(3)	986(2)	53(1)
C(62)	475(3)	5062(3)	709(2)	71(2)
C(63)	1709(2)	7684(2)	2872(1)	21(1)
C(64)	1343(2)	7300(2)	2479(1)	20(1)
C(65)	812(2)	7656(2)	2241(1)	22(1)
C(66)	625(2)	8431(2)	2383(1)	29(1)
C(67)	983(2)	8828(2)	2764(1)	33(1)
C(68)	1514(2)	8468(2)	3001(1)	29(1)
C(69)	457(2)	7193(2)	1827(1)	26(1)
C(70)	833(3)	9684(3)	2921(2)	53(1)
C(71)	2476(1)	7541(2)	3738(1)	18(1)
C(72)	1981(1)	7718(2)	4066(1)	20(1)
C(73)	2089(1)	7912(2)	4590(1)	21(1)
C(74)	2696(1)	7936(2)	4807(1)	21(1)
C(75)	3194(1)	7750(2)	4489(1)	20(1)
C(76)	3086(1)	7552(2)	3972(1)	20(1)
C(77)	1540(2)	8154(3)	4904(2)	33(1)
C(78)	3854(2)	7767(2)	4713(1)	31(1)
C(79)	2924(2)	7606(2)	2761(1)	27(1)
C(80)	3306(2)	8270(2)	2885(2)	35(1)
C(81)	3786(2)	8535(3)	2571(2)	51(1)
C(82)	3869(3)	8164(4)	2094(2)	66(2)
C(83)	3481(3)	7536(4)	1954(2)	73(2)
C(84)	3023(2)	7247(3)	2282(2)	45(1)
C(85)	4202(4)	9226(4)	2734(3)	92(3)
C(86)	3502(4)	7355(6)	1388(3)	42(2)
C(87)	3677(7)	6851(10)	1499(4)	60(4)
C(88)	2322(1)	6291(2)	3135(1)	20(1)
C(89)	1760(2)	5868(2)	3211(1)	22(1)
C(90)	1745(2)	5024(2)	3245(1)	22(1)
C(91)	2291(2)	4566(2)	3211(1)	24(1)
C(92)	2855(2)	4973(2)	3151(1)	22(1)
C(93)	2870(2)	5813(2)	3108(1)	22(1)

C(94)	3465(2)	4519(2)	3120(2)	32(1)
C(95)	1123(2)	4619(2)	3328(2)	32(1)
F(3)	805(1)	7082(1)	1404(1)	34(1)
F(6)	862(1)	9813(1)	3416(1)	37(1)
F(2)	-78(1)	7556(2)	1667(1)	40(1)
F(1)	303(1)	6447(2)	1987(1)	44(1)
F(9)	1681(1)	8216(2)	5409(1)	50(1)
F(22)	3419(1)	3745(1)	3275(1)	43(1)
F(24)	848(1)	4907(2)	3760(1)	55(1)
F(20)	3921(1)	4837(2)	3423(1)	60(1)
F(23)	1164(1)	3830(1)	3400(1)	52(1)
F(7)	1058(1)	7637(2)	4850(1)	57(1)
F(12)	4272(1)	8029(2)	4388(1)	68(1)
F(25)	705(1)	4764(2)	2945(1)	64(1)
F(21)	3680(2)	4492(2)	2642(1)	69(1)
F(8)	1306(1)	8883(2)	4763(1)	57(1)
F(11)	4050(1)	7054(2)	4864(2)	98(2)
F(10)	3925(1)	8232(3)	5123(1)	99(2)
F(17)	4131(2)	7029(2)	1314(1)	80(1)
F(18)	3088(2)	6863(2)	1211(1)	90(1)
F(16)	3495(2)	7945(4)	1050(2)	58(2)
F(19)	3681(4)	6084(4)	1590(3)	76(3)
F(13)	4756(1)	9227(2)	2563(1)	64(1)
F(15)	3943(2)	9862(2)	2842(3)	126(2)
F(14)	4411(2)	9095(3)	3298(2)	112(2)
F(4)	332(3)	9947(3)	2724(2)	202(4)
F(5)	1327(2)	10212(2)	2766(1)	82(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for $[(\text{PNP})\text{Cu}]_2[\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$.

Cu(1)-N(1)	2.052(3)
Cu(1)-N(2)	2.061(2)
Cu(1)-P(1)	2.2484(9)
Cu(1)-P(4)	2.2654(9)
Cu(2)-N(2)	2.095(3)
Cu(2)-P(2)	2.2227(10)
Cu(2)-P(3)	2.2541(9)
Cu(2)-N(1)	2.358(3)
N(1)-C(1)	1.419(4)
N(1)-C(7)	1.426(4)
N(2)-C(19)	1.424(4)
N(2)-C(13)	1.430(4)
P(1)-C(2)	1.817(3)
P(1)-C(25)	1.842(3)
P(1)-C(29)	1.844(3)
P(2)-C(8)	1.824(3)
P(2)-C(33)	1.842(4)
P(2)-C(41)	1.864(7)
P(2)-C(37)	1.864(6)
P(3)-C(14)	1.820(4)
P(3)-C(49)	1.845(4)
P(3)-C(45)	1.846(3)
P(4)-C(20)	1.816(3)
P(4)-C(58)	1.847(3)
P(4)-C(54)	1.852(3)
B-C(63)	1.634(5)
B-C(88)	1.639(5)
B-C(79)	1.641(5)
B-C(71)	1.645(5)
C(1)-C(6)	1.401(5)
C(1)-C(2)	1.403(5)
C(2)-C(3)	1.400(5)
C(3)-C(4)	1.363(5)
C(3)-H(3)	0.9500

C(4)-C(5)	1.383(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.384(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.406(5)
C(7)-C(8)	1.407(5)
C(8)-C(9)	1.400(5)
C(9)-C(10)	1.385(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.397(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.382(5)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(18)	1.399(4)
C(13)-C(14)	1.411(4)
C(14)-C(15)	1.400(5)
C(15)-C(16)	1.382(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.397(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.376(5)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(20)	1.408(4)
C(19)-C(24)	1.408(4)
C(20)-C(21)	1.398(4)
C(21)-C(22)	1.386(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.381(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.388(5)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.537(5)

C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.523(5)
C(26)-C(28)	1.535(5)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.512(6)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(31)	1.442(8)
C(30)-C(32)	1.523(8)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.535(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(36)	1.523(6)
C(34)-C(35)	1.542(5)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.538(12)

C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(37)-H(42)	1.4414
C(38)-C(39)	1.510(12)
C(38)-C(40)	1.534(11)
C(38)-H(38)	0.9945
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(42)	1.522(11)
C(41)-H(38)	1.4031
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(44)	1.525(10)
C(42)-C(43)	1.542(11)
C(42)-H(42)	0.9918
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(46)	1.536(5)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.517(6)
C(46)-C(48)	1.525(5)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800

C(48)-H(48C)	0.9800
C(49)-C(50)	1.544(6)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(52)	1.387(19)
C(50)-C(51)	1.421(9)
C(50)-C(53)	1.610(8)
C(50)-H(50A)	1.0133
C(50)-H(50B)	0.9842
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(52)-H(50B)	0.6489
C(53)-H(50A)	0.7037
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-C(55)	1.533(5)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.525(5)
C(55)-C(57)	1.533(5)
C(55)-H(55)	1.0000
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-C(59)	1.501(8)
C(58)-C(60)	1.512(7)
C(58)-H(58A)	1.0043
C(58)-H(58B)	0.9970

C(58)-H(58C)	0.9944
C(58)-H(58D)	1.0063
C(60)-C(61)	1.441(8)
C(60)-C(62)	1.610(8)
C(60)-H(60)	0.9929
C(59)-C(61)	1.467(9)
C(59)-C(62)	1.607(10)
C(59)-H(58B)	1.5815
C(59)-H(59)	0.9980
C(59)-H(61A)	1.5584
C(61)-H(61A)	0.9972
C(61)-H(61B)	0.9927
C(61)-H(61C)	0.9807
C(62)-H(62A)	0.9835
C(62)-H(62B)	0.9850
C(62)-H(62C)	0.9898
C(63)-C(68)	1.402(5)
C(63)-C(64)	1.407(4)
C(64)-C(65)	1.390(4)
C(64)-H(64)	0.9500
C(65)-C(66)	1.391(5)
C(65)-C(69)	1.495(5)
C(66)-C(67)	1.384(5)
C(66)-H(66)	0.9500
C(67)-C(68)	1.391(5)
C(67)-C(70)	1.507(5)
C(68)-H(68)	0.9500
C(69)-F(2)	1.331(4)
C(69)-F(1)	1.342(4)
C(69)-F(3)	1.349(4)
C(70)-F(4)	1.236(6)
C(70)-F(6)	1.295(5)
C(70)-F(5)	1.427(7)
C(71)-C(72)	1.401(4)
C(71)-C(76)	1.405(4)
C(72)-C(73)	1.400(4)

C(72)-H(72)	0.9500
C(73)-C(74)	1.383(4)
C(73)-C(77)	1.491(4)
C(74)-C(75)	1.391(4)
C(74)-H(74)	0.9500
C(75)-C(76)	1.385(4)
C(75)-C(78)	1.491(4)
C(76)-H(76)	0.9500
C(77)-F(9)	1.330(4)
C(77)-F(7)	1.332(5)
C(77)-F(8)	1.346(5)
C(78)-F(11)	1.302(5)
C(78)-F(10)	1.312(5)
C(78)-F(12)	1.312(4)
C(79)-C(80)	1.391(5)
C(79)-C(84)	1.394(5)
C(80)-C(81)	1.391(5)
C(80)-H(80)	0.9500
C(81)-C(82)	1.391(7)
C(81)-C(85)	1.492(7)
C(82)-C(83)	1.363(7)
C(82)-H(82)	0.9500
C(83)-C(84)	1.391(6)
C(83)-C(86)	1.491(10)
C(83)-C(87)	1.692(15)
C(84)-H(84)	0.9500
C(85)-F(15)	1.219(7)
C(85)-F(13)	1.266(6)
C(85)-F(14)	1.521(10)
C(86)-F(18)	1.267(10)
C(86)-F(16)	1.308(11)
C(86)-F(17)	1.452(9)
C(87)-F(17)	1.125(12)
C(87)-F(19)	1.287(18)
C(87)-F(18)	1.427(16)
C(88)-C(89)	1.396(4)

C(88)-C(93)	1.405(4)
C(89)-C(90)	1.396(4)
C(89)-H(89)	0.9500
C(90)-C(91)	1.384(5)
C(90)-C(95)	1.498(5)
C(91)-C(92)	1.382(5)
C(91)-H(91)	0.9500
C(92)-C(93)	1.391(4)
C(92)-C(94)	1.495(5)
C(93)-H(93)	0.9500
C(94)-F(20)	1.327(5)
C(94)-F(21)	1.330(5)
C(94)-F(22)	1.343(4)
C(95)-F(23)	1.317(4)
C(95)-F(25)	1.325(4)
C(95)-F(24)	1.360(5)

N(1)-Cu(1)-N(2)	113.45(11)
N(1)-Cu(1)-P(1)	87.84(8)
N(2)-Cu(1)-P(1)	114.84(8)
N(1)-Cu(1)-P(4)	121.12(8)
N(2)-Cu(1)-P(4)	88.04(7)
P(1)-Cu(1)-P(4)	133.30(3)
N(2)-Cu(2)-P(2)	123.51(7)
N(2)-Cu(2)-P(3)	88.37(7)
P(2)-Cu(2)-P(3)	140.73(4)
N(2)-Cu(2)-N(1)	100.94(10)
P(2)-Cu(2)-N(1)	84.58(7)
P(3)-Cu(2)-N(1)	113.66(7)
C(1)-N(1)-C(7)	114.6(3)
C(1)-N(1)-Cu(1)	115.0(2)
C(7)-N(1)-Cu(1)	119.5(2)
C(1)-N(1)-Cu(2)	119.8(2)
C(7)-N(1)-Cu(2)	110.9(2)
Cu(1)-N(1)-Cu(2)	69.95(9)
C(19)-N(2)-C(13)	114.5(2)

C(19)-N(2)-Cu(1)	114.66(18)
C(13)-N(2)-Cu(1)	117.69(18)
C(19)-N(2)-Cu(2)	114.90(18)
C(13)-N(2)-Cu(2)	114.02(18)
Cu(1)-N(2)-Cu(2)	75.36(9)
C(2)-P(1)-C(25)	106.69(15)
C(2)-P(1)-C(29)	108.97(16)
C(25)-P(1)-C(29)	105.01(16)
C(2)-P(1)-Cu(1)	98.38(11)
C(25)-P(1)-Cu(1)	115.80(11)
C(29)-P(1)-Cu(1)	120.94(12)
C(8)-P(2)-C(33)	101.71(16)
C(8)-P(2)-C(41)	107.0(3)
C(33)-P(2)-C(41)	114.2(3)
C(8)-P(2)-C(37)	101.7(2)
C(33)-P(2)-C(37)	93.9(3)
C(41)-P(2)-C(37)	23.4(3)
C(8)-P(2)-Cu(2)	102.56(11)
C(33)-P(2)-Cu(2)	126.82(12)
C(41)-P(2)-Cu(2)	102.7(3)
C(37)-P(2)-Cu(2)	125.8(3)
C(14)-P(3)-C(49)	104.95(18)
C(14)-P(3)-C(45)	100.46(16)
C(49)-P(3)-C(45)	101.52(16)
C(14)-P(3)-Cu(2)	97.78(11)
C(49)-P(3)-Cu(2)	122.23(13)
C(45)-P(3)-Cu(2)	125.63(13)
C(20)-P(4)-C(58)	104.25(15)
C(20)-P(4)-C(54)	100.94(15)
C(58)-P(4)-C(54)	102.70(16)
C(20)-P(4)-Cu(1)	97.43(10)
C(58)-P(4)-Cu(1)	124.22(12)
C(54)-P(4)-Cu(1)	122.78(12)
C(63)-B-C(88)	111.9(3)
C(63)-B-C(79)	104.9(3)
C(88)-B-C(79)	111.4(3)

C(63)-B-C(71)	112.4(3)
C(88)-B-C(71)	104.5(2)
C(79)-B-C(71)	112.0(3)
C(6)-C(1)-C(2)	118.0(3)
C(6)-C(1)-N(1)	120.5(3)
C(2)-C(1)-N(1)	121.5(3)
C(3)-C(2)-C(1)	119.3(3)
C(3)-C(2)-P(1)	124.2(3)
C(1)-C(2)-P(1)	116.5(2)
C(4)-C(3)-C(2)	122.1(3)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	119.0(3)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	120.5(4)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	121.2(4)
C(5)-C(6)-H(6)	119.4
C(1)-C(6)-H(6)	119.4
C(12)-C(7)-C(8)	118.4(3)
C(12)-C(7)-N(1)	120.0(3)
C(8)-C(7)-N(1)	121.5(3)
C(9)-C(8)-C(7)	119.2(3)
C(9)-C(8)-P(2)	121.0(2)
C(7)-C(8)-P(2)	119.8(2)
C(10)-C(9)-C(8)	122.1(3)
C(10)-C(9)-H(9)	118.9
C(8)-C(9)-H(9)	118.9
C(9)-C(10)-C(11)	118.3(3)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-H(10)	120.8
C(12)-C(11)-C(10)	120.7(3)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7

C(11)-C(12)-C(7)	121.2(3)
C(11)-C(12)-H(12)	119.4
C(7)-C(12)-H(12)	119.4
C(18)-C(13)-C(14)	118.9(3)
C(18)-C(13)-N(2)	120.4(3)
C(14)-C(13)-N(2)	120.6(3)
C(15)-C(14)-C(13)	119.1(3)
C(15)-C(14)-P(3)	122.4(3)
C(13)-C(14)-P(3)	118.2(2)
C(16)-C(15)-C(14)	121.4(3)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(15)-C(16)-C(17)	119.1(3)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	120.6(3)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(13)	121.0(3)
C(17)-C(18)-H(18)	119.5
C(13)-C(18)-H(18)	119.5
C(20)-C(19)-C(24)	118.6(3)
C(20)-C(19)-N(2)	121.0(3)
C(24)-C(19)-N(2)	120.4(3)
C(21)-C(20)-C(19)	119.6(3)
C(21)-C(20)-P(4)	122.8(2)
C(19)-C(20)-P(4)	117.4(2)
C(22)-C(21)-C(20)	120.9(3)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	119.7(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.5(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7

C(23)-C(24)-C(19)	120.6(3)
C(23)-C(24)-H(24)	119.7
C(19)-C(24)-H(24)	119.7
C(26)-C(25)-P(1)	114.6(2)
C(26)-C(25)-H(25A)	108.6
P(1)-C(25)-H(25A)	108.6
C(26)-C(25)-H(25B)	108.6
P(1)-C(25)-H(25B)	108.6
H(25A)-C(25)-H(25B)	107.6
C(27)-C(26)-C(28)	109.7(3)
C(27)-C(26)-C(25)	112.1(3)
C(28)-C(26)-C(25)	109.5(3)
C(27)-C(26)-H(26)	108.5
C(28)-C(26)-H(26)	108.5
C(25)-C(26)-H(26)	108.5
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-P(1)	123.5(3)
C(30)-C(29)-H(29A)	106.4
P(1)-C(29)-H(29A)	106.4
C(30)-C(29)-H(29B)	106.4
P(1)-C(29)-H(29B)	106.4
H(29A)-C(29)-H(29B)	106.5
C(31)-C(30)-C(29)	118.1(6)
C(31)-C(30)-C(32)	111.7(5)
C(29)-C(30)-C(32)	109.5(4)

C(31)-C(30)-H(30)	105.5
C(29)-C(30)-H(30)	105.5
C(32)-C(30)-H(30)	105.5
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-P(2)	117.6(3)
C(34)-C(33)-H(33A)	107.9
P(2)-C(33)-H(33A)	107.9
C(34)-C(33)-H(33B)	107.9
P(2)-C(33)-H(33B)	107.9
H(33A)-C(33)-H(33B)	107.2
C(36)-C(34)-C(33)	113.5(3)
C(36)-C(34)-C(35)	109.6(3)
C(33)-C(34)-C(35)	108.8(3)
C(36)-C(34)-H(34)	108.3
C(33)-C(34)-H(34)	108.3
C(35)-C(34)-H(34)	108.3
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5

C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-P(2)	114.8(6)
C(38)-C(37)-H(37A)	108.6
P(2)-C(37)-H(37A)	108.6
C(38)-C(37)-H(37B)	108.6
P(2)-C(37)-H(37B)	108.6
H(37A)-C(37)-H(37B)	107.6
C(38)-C(37)-H(42)	105.1
P(2)-C(37)-H(42)	121.4
H(37A)-C(37)-H(42)	96.5
H(37B)-C(37)-H(42)	14.1
C(39)-C(38)-C(40)	112.2(7)
C(39)-C(38)-C(37)	111.3(7)
C(40)-C(38)-C(37)	109.4(8)
C(39)-C(38)-H(38)	107.6
C(40)-C(38)-H(38)	108.5
C(37)-C(38)-H(38)	107.7
C(42)-C(41)-P(2)	118.5(6)
C(42)-C(41)-H(38)	109.7
P(2)-C(41)-H(38)	130.5
C(42)-C(41)-H(41A)	107.7
P(2)-C(41)-H(41A)	107.7
H(38)-C(41)-H(41A)	43.5
C(42)-C(41)-H(41B)	107.7
P(2)-C(41)-H(41B)	107.7
H(38)-C(41)-H(41B)	65.1
H(41A)-C(41)-H(41B)	107.1
C(41)-C(42)-C(44)	109.0(6)
C(41)-C(42)-C(43)	110.3(6)
C(44)-C(42)-C(43)	109.6(6)
C(41)-C(42)-H(42)	108.6
C(44)-C(42)-H(42)	110.1
C(43)-C(42)-H(42)	109.3
C(46)-C(45)-P(3)	116.1(2)

C(46)-C(45)-H(45A)	108.3
P(3)-C(45)-H(45A)	108.3
C(46)-C(45)-H(45B)	108.3
P(3)-C(45)-H(45B)	108.3
H(45A)-C(45)-H(45B)	107.4
C(47)-C(46)-C(48)	111.3(4)
C(47)-C(46)-C(45)	111.8(3)
C(48)-C(46)-C(45)	109.8(3)
C(47)-C(46)-H(46)	107.9
C(48)-C(46)-H(46)	107.9
C(45)-C(46)-H(46)	107.9
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-P(3)	115.2(3)
C(50)-C(49)-H(49A)	108.5
P(3)-C(49)-H(49A)	108.5
C(50)-C(49)-H(49B)	108.5
P(3)-C(49)-H(49B)	108.5
H(49A)-C(49)-H(49B)	107.5
C(52)-C(50)-C(51)	115.4(9)
C(52)-C(50)-C(49)	121.3(10)
C(51)-C(50)-C(49)	114.1(4)
C(52)-C(50)-C(53)	83.2(10)
C(51)-C(50)-C(53)	112.6(5)
C(49)-C(50)-C(53)	104.9(5)
C(52)-C(50)-H(50A)	99.3

C(51)-C(50)-H(50A)	101.2
C(49)-C(50)-H(50A)	100.0
C(53)-C(50)-H(50A)	16.8
C(52)-C(50)-H(50B)	25.2
C(51)-C(50)-H(50B)	107.6
C(49)-C(50)-H(50B)	109.5
C(53)-C(50)-H(50B)	108.0
H(50A)-C(50)-H(50B)	124.4
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
C(50)-C(52)-H(50B)	40.2
H(52A)-C(52)-H(50B)	72.1
H(52B)-C(52)-H(50B)	137.5
H(52C)-C(52)-H(50B)	109.5
C(50)-C(53)-H(50A)	24.6
C(50)-C(53)-H(53A)	109.5
C(50)-C(53)-H(53B)	109.5
C(50)-C(53)-H(53C)	109.5
C(55)-C(54)-P(4)	116.7(2)
C(55)-C(54)-H(54A)	108.1
P(4)-C(54)-H(54A)	108.1
C(55)-C(54)-H(54B)	108.1
P(4)-C(54)-H(54B)	108.1
H(54A)-C(54)-H(54B)	107.3
C(56)-C(55)-C(54)	112.5(3)
C(56)-C(55)-C(57)	109.1(3)
C(54)-C(55)-C(57)	109.7(3)
C(56)-C(55)-H(55)	108.5
C(54)-C(55)-H(55)	108.5

C(57)-C(55)-H(55)	108.5
C(55)-C(56)-H(56A)	109.5
C(55)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(55)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(55)-C(57)-H(57A)	109.5
C(55)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(55)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(59)-C(58)-C(60)	35.6(4)
C(59)-C(58)-P(4)	119.9(4)
C(60)-C(58)-P(4)	115.1(3)
C(59)-C(58)-H(58A)	128.8
C(60)-C(58)-H(58A)	108.7
P(4)-C(58)-H(58A)	108.2
C(59)-C(58)-H(58B)	75.6
C(60)-C(58)-H(58B)	109.8
P(4)-C(58)-H(58B)	108.6
H(58A)-C(58)-H(58B)	105.9
C(59)-C(58)-H(58C)	108.3
C(60)-C(58)-H(58C)	77.7
P(4)-C(58)-H(58C)	107.7
H(58A)-C(58)-H(58C)	35.5
H(58B)-C(58)-H(58C)	134.4
C(59)-C(58)-H(58D)	107.5
C(60)-C(58)-H(58D)	134.5
P(4)-C(58)-H(58D)	107.1
H(58A)-C(58)-H(58D)	71.4
H(58B)-C(58)-H(58D)	37.1
H(58C)-C(58)-H(58D)	105.4
C(61)-C(60)-C(58)	120.0(5)
C(61)-C(60)-C(62)	108.3(5)

C(58)-C(60)-C(62)	105.7(5)
C(61)-C(60)-H(60)	107.8
C(58)-C(60)-H(60)	107.9
C(62)-C(60)-H(60)	106.3
C(61)-C(59)-C(58)	119.0(6)
C(61)-C(59)-C(62)	107.2(7)
C(58)-C(59)-C(62)	106.4(6)
C(61)-C(59)-H(58B)	143.1
C(58)-C(59)-H(58B)	37.6
C(62)-C(59)-H(58B)	107.7
C(61)-C(59)-H(59)	108.9
C(58)-C(59)-H(59)	107.3
C(62)-C(59)-H(59)	107.5
H(58B)-C(59)-H(59)	71.2
C(61)-C(59)-H(61A)	38.3
C(58)-C(59)-H(61A)	143.0
C(62)-C(59)-H(61A)	108.9
H(58B)-C(59)-H(61A)	134.1
H(59)-C(59)-H(61A)	72.2
C(60)-C(61)-C(59)	36.9(4)
C(60)-C(61)-H(61A)	111.2
C(59)-C(61)-H(61A)	75.8
C(60)-C(61)-H(61B)	111.2
C(59)-C(61)-H(61B)	133.9
H(61A)-C(61)-H(61B)	107.1
C(60)-C(61)-H(61C)	110.8
C(59)-C(61)-H(61C)	114.3
H(61A)-C(61)-H(61C)	108.0
H(61B)-C(61)-H(61C)	108.4
C(59)-C(62)-C(60)	33.2(4)
C(59)-C(62)-H(62A)	81.4
C(60)-C(62)-H(62A)	110.6
C(59)-C(62)-H(62B)	137.5
C(60)-C(62)-H(62B)	110.2
H(62A)-C(62)-H(62B)	108.8
C(59)-C(62)-H(62C)	107.0

C(60)-C(62)-H(62C)	110.5
H(62A)-C(62)-H(62C)	108.4
H(62B)-C(62)-H(62C)	108.3
C(68)-C(63)-C(64)	115.3(3)
C(68)-C(63)-B	121.8(3)
C(64)-C(63)-B	122.7(3)
C(65)-C(64)-C(63)	123.0(3)
C(65)-C(64)-H(64)	118.5
C(63)-C(64)-H(64)	118.5
C(64)-C(65)-C(66)	120.3(3)
C(64)-C(65)-C(69)	118.5(3)
C(66)-C(65)-C(69)	121.2(3)
C(67)-C(66)-C(65)	118.0(3)
C(67)-C(66)-H(66)	121.0
C(65)-C(66)-H(66)	121.0
C(66)-C(67)-C(68)	121.5(3)
C(66)-C(67)-C(70)	121.3(3)
C(68)-C(67)-C(70)	117.1(4)
C(67)-C(68)-C(63)	122.0(3)
C(67)-C(68)-H(68)	119.0
C(63)-C(68)-H(68)	119.0
F(2)-C(69)-F(1)	107.2(3)
F(2)-C(69)-F(3)	107.0(3)
F(1)-C(69)-F(3)	105.6(3)
F(2)-C(69)-C(65)	113.0(3)
F(1)-C(69)-C(65)	111.7(3)
F(3)-C(69)-C(65)	111.9(3)
F(4)-C(70)-F(6)	110.9(5)
F(4)-C(70)-F(5)	107.2(5)
F(6)-C(70)-F(5)	99.6(4)
F(4)-C(70)-C(67)	113.8(4)
F(6)-C(70)-C(67)	114.6(3)
F(5)-C(70)-C(67)	109.5(4)
C(72)-C(71)-C(76)	115.5(3)
C(72)-C(71)-B	122.7(3)
C(76)-C(71)-B	121.7(3)

C(73)-C(72)-C(71)	122.2(3)
C(73)-C(72)-H(72)	118.9
C(71)-C(72)-H(72)	118.9
C(74)-C(73)-C(72)	121.0(3)
C(74)-C(73)-C(77)	120.0(3)
C(72)-C(73)-C(77)	118.8(3)
C(73)-C(74)-C(75)	117.7(3)
C(73)-C(74)-H(74)	121.1
C(75)-C(74)-H(74)	121.1
C(76)-C(75)-C(74)	121.2(3)
C(76)-C(75)-C(78)	119.9(3)
C(74)-C(75)-C(78)	118.9(3)
C(75)-C(76)-C(71)	122.4(3)
C(75)-C(76)-H(76)	118.8
C(71)-C(76)-H(76)	118.8
F(9)-C(77)-F(7)	107.3(3)
F(9)-C(77)-F(8)	105.3(3)
F(7)-C(77)-F(8)	105.7(3)
F(9)-C(77)-C(73)	113.6(3)
F(7)-C(77)-C(73)	112.2(3)
F(8)-C(77)-C(73)	112.1(3)
F(11)-C(78)-F(10)	105.1(4)
F(11)-C(78)-F(12)	106.0(4)
F(10)-C(78)-F(12)	105.2(4)
F(11)-C(78)-C(75)	112.6(3)
F(10)-C(78)-C(75)	113.7(3)
F(12)-C(78)-C(75)	113.6(3)
C(80)-C(79)-C(84)	115.7(3)
C(80)-C(79)-B	123.6(3)
C(84)-C(79)-B	120.5(3)
C(79)-C(80)-C(81)	122.9(4)
C(79)-C(80)-H(80)	118.6
C(81)-C(80)-H(80)	118.6
C(82)-C(81)-C(80)	119.6(4)
C(82)-C(81)-C(85)	119.8(4)
C(80)-C(81)-C(85)	120.6(4)

C(83)-C(82)-C(81)	118.5(4)
C(83)-C(82)-H(82)	120.8
C(81)-C(82)-H(82)	120.8
C(82)-C(83)-C(84)	121.5(4)
C(82)-C(83)-C(86)	112.0(5)
C(84)-C(83)-C(86)	124.9(5)
C(82)-C(83)-C(87)	122.2(6)
C(84)-C(83)-C(87)	112.7(6)
C(86)-C(83)-C(87)	34.0(5)
C(83)-C(84)-C(79)	121.6(4)
C(83)-C(84)-H(84)	119.2
C(79)-C(84)-H(84)	119.2
F(15)-C(85)-F(13)	120.4(5)
F(15)-C(85)-C(81)	117.3(6)
F(13)-C(85)-C(81)	116.3(4)
F(15)-C(85)-F(14)	91.4(6)
F(13)-C(85)-F(14)	95.3(7)
C(81)-C(85)-F(14)	108.1(5)
F(18)-C(86)-F(16)	104.1(7)
F(18)-C(86)-F(17)	109.8(7)
F(16)-C(86)-F(17)	100.2(6)
F(18)-C(86)-C(83)	116.0(7)
F(16)-C(86)-C(83)	120.3(8)
F(17)-C(86)-C(83)	105.2(7)
F(17)-C(87)-F(19)	109.4(15)
F(17)-C(87)-F(18)	121.1(10)
F(19)-C(87)-F(18)	96.3(9)
F(17)-C(87)-C(83)	110.7(10)
F(19)-C(87)-C(83)	122.0(8)
F(18)-C(87)-C(83)	97.0(10)
C(89)-C(88)-C(93)	115.7(3)
C(89)-C(88)-B	122.6(3)
C(93)-C(88)-B	121.6(3)
C(90)-C(89)-C(88)	121.9(3)
C(90)-C(89)-H(89)	119.0
C(88)-C(89)-H(89)	119.0

C(91)-C(90)-C(89)	121.4(3)
C(91)-C(90)-C(95)	120.1(3)
C(89)-C(90)-C(95)	118.5(3)
C(92)-C(91)-C(90)	117.7(3)
C(92)-C(91)-H(91)	121.1
C(90)-C(91)-H(91)	121.1
C(91)-C(92)-C(93)	121.0(3)
C(91)-C(92)-C(94)	120.8(3)
C(93)-C(92)-C(94)	118.2(3)
C(92)-C(93)-C(88)	122.3(3)
C(92)-C(93)-H(93)	118.9
C(88)-C(93)-H(93)	118.9
F(20)-C(94)-F(21)	107.1(3)
F(20)-C(94)-F(22)	105.0(3)
F(21)-C(94)-F(22)	106.0(3)
F(20)-C(94)-C(92)	112.4(3)
F(21)-C(94)-C(92)	112.9(3)
F(22)-C(94)-C(92)	112.9(3)
F(23)-C(95)-F(25)	108.8(3)
F(23)-C(95)-F(24)	104.9(3)
F(25)-C(95)-F(24)	104.9(3)
F(23)-C(95)-C(90)	114.1(3)
F(25)-C(95)-C(90)	112.2(3)
F(24)-C(95)-C(90)	111.2(3)
C(87)-F(17)-C(86)	40.8(9)
C(86)-F(18)-C(87)	40.7(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(\text{PNP})\text{Cu}]_2[\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$. The anisotropic

displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

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

C(22)	46(2)	20(2)	16(2)	3(1)	-6(1)	-5(1)
C(23)	40(2)	24(2)	15(2)	-2(1)	3(1)	-9(1)
C(24)	26(2)	24(2)	17(2)	-3(1)	5(1)	-6(1)
C(25)	23(2)	31(2)	22(2)	3(1)	3(1)	-3(1)
C(26)	24(2)	32(2)	27(2)	9(1)	9(1)	3(1)
C(27)	31(2)	40(2)	34(2)	-4(2)	10(2)	3(2)
C(28)	24(2)	54(2)	33(2)	7(2)	8(1)	5(2)
C(29)	40(2)	23(2)	26(2)	4(1)	6(1)	4(1)
C(30)	102(4)	32(2)	80(4)	18(2)	59(4)	10(3)
C(31)	68(3)	46(3)	65(3)	11(2)	8(3)	-7(2)
C(32)	71(4)	36(3)	110(5)	-2(3)	-5(3)	-10(2)
C(33)	53(2)	21(2)	23(2)	4(1)	7(2)	3(2)
C(34)	54(2)	21(2)	20(2)	1(1)	4(2)	0(2)
C(35)	64(3)	26(2)	25(2)	4(1)	0(2)	2(2)
C(36)	61(3)	46(2)	26(2)	6(2)	12(2)	1(2)
C(37)	23(3)	25(4)	38(4)	-3(3)	4(3)	-7(3)
C(38)	21(3)	63(5)	35(4)	-1(3)	-3(3)	-15(3)
C(39)	36(5)	154(13)	43(5)	38(6)	-11(4)	-31(6)
C(40)	32(5)	114(10)	49(6)	-9(6)	0(4)	-38(6)
C(41)	19(3)	30(4)	22(4)	-2(3)	0(3)	0(3)
C(42)	16(3)	23(3)	30(4)	-1(3)	-1(3)	-4(2)
C(43)	32(4)	41(5)	23(4)	1(3)	-3(3)	-8(3)
C(44)	19(4)	33(4)	39(5)	-3(4)	3(3)	-8(3)
C(45)	18(2)	43(2)	31(2)	-3(2)	1(1)	2(1)
C(46)	22(2)	49(2)	31(2)	-2(2)	3(1)	-8(2)
C(47)	42(2)	57(3)	43(3)	12(2)	5(2)	-9(2)
C(48)	29(2)	72(3)	40(2)	-11(2)	10(2)	-9(2)
C(49)	23(2)	54(2)	28(2)	5(2)	3(1)	15(2)
C(50)	30(2)	101(4)	32(2)	-8(2)	-3(2)	21(2)
C(51)	48(3)	105(5)	72(4)	-20(4)	-1(3)	-5(3)
C(52)	48(10)	37(9)	76(14)	5(9)	-3(9)	9(8)
C(53)	58(4)	101(6)	33(3)	10(3)	-9(3)	38(4)
C(54)	12(1)	30(2)	37(2)	0(1)	0(1)	-1(1)
C(55)	20(1)	30(2)	26(2)	1(1)	2(1)	-6(1)
C(56)	30(2)	29(2)	33(2)	2(1)	-2(1)	-6(1)
C(57)	28(2)	38(2)	38(2)	5(2)	-6(2)	-8(2)

C(58)	26(2)	25(2)	29(2)	4(1)	6(1)	6(1)
C(60)	23(4)	28(3)	29(4)	-2(2)	1(3)	3(2)
C(59)	23(5)	30(4)	42(6)	11(4)	13(4)	9(3)
C(61)	71(3)	39(2)	50(3)	7(2)	33(2)	13(2)
C(62)	115(5)	25(2)	75(4)	-4(2)	65(4)	3(2)
C(63)	26(2)	21(1)	18(2)	5(1)	0(1)	-4(1)
C(64)	23(1)	20(1)	17(1)	3(1)	2(1)	0(1)
C(65)	25(2)	24(2)	19(2)	6(1)	-1(1)	0(1)
C(66)	36(2)	30(2)	23(2)	7(1)	-1(1)	9(1)
C(67)	50(2)	21(2)	27(2)	2(1)	-6(2)	10(2)
C(68)	42(2)	20(2)	24(2)	3(1)	-8(1)	-1(1)
C(69)	25(2)	30(2)	24(2)	5(1)	-1(1)	-2(1)
C(70)	92(4)	26(2)	39(2)	-2(2)	-14(2)	21(2)
C(71)	18(1)	17(1)	20(2)	3(1)	2(1)	0(1)
C(72)	14(1)	23(1)	22(2)	3(1)	0(1)	0(1)
C(73)	19(1)	24(2)	21(2)	2(1)	8(1)	2(1)
C(74)	20(1)	24(2)	18(2)	2(1)	2(1)	2(1)
C(75)	15(1)	24(1)	19(2)	-1(1)	-1(1)	1(1)
C(76)	13(1)	26(2)	22(2)	-2(1)	4(1)	1(1)
C(77)	20(2)	48(2)	29(2)	-2(2)	7(1)	1(2)
C(78)	18(1)	46(2)	29(2)	-2(2)	-2(1)	2(1)
C(79)	28(2)	30(2)	22(2)	4(1)	2(1)	-4(1)
C(80)	41(2)	25(2)	41(2)	-3(2)	17(2)	-9(2)
C(81)	55(3)	39(2)	60(3)	-3(2)	32(2)	-20(2)
C(82)	67(3)	89(4)	43(3)	1(3)	31(2)	-35(3)
C(83)	73(4)	117(5)	30(2)	-26(3)	31(2)	-49(4)
C(84)	45(2)	67(3)	23(2)	-11(2)	11(2)	-25(2)
C(85)	99(5)	50(3)	131(6)	-42(4)	79(5)	-43(3)
C(86)	39(4)	51(5)	36(4)	6(4)	13(3)	6(4)
C(87)	75(9)	80(10)	28(6)	-2(6)	17(6)	-31(8)
C(88)	22(1)	22(1)	15(1)	-1(1)	-1(1)	-1(1)
C(89)	21(1)	23(2)	20(2)	5(1)	-3(1)	1(1)
C(90)	22(1)	24(2)	20(2)	4(1)	-6(1)	-4(1)
C(91)	28(2)	23(2)	19(2)	3(1)	-4(1)	0(1)
C(92)	25(2)	22(1)	18(2)	-1(1)	-2(1)	1(1)
C(93)	21(1)	26(2)	20(2)	-3(1)	1(1)	-2(1)

C(94)	31(2)	27(2)	37(2)	2(2)	4(2)	5(1)
C(95)	24(2)	29(2)	41(2)	13(2)	-7(1)	-5(1)
F(3)	32(1)	46(1)	23(1)	-6(1)	1(1)	-2(1)
F(6)	40(1)	30(1)	43(1)	-6(1)	10(1)	3(1)
F(2)	26(1)	56(2)	39(1)	-1(1)	-10(1)	5(1)
F(1)	55(2)	39(1)	37(1)	8(1)	-12(1)	-22(1)
F(9)	40(1)	84(2)	26(1)	-8(1)	14(1)	5(1)
F(22)	39(1)	29(1)	61(2)	5(1)	12(1)	11(1)
F(24)	36(1)	58(2)	71(2)	11(1)	20(1)	-11(1)
F(20)	30(1)	43(1)	106(2)	-8(2)	-23(1)	11(1)
F(23)	36(1)	27(1)	92(2)	16(1)	-3(1)	-9(1)
F(7)	28(1)	84(2)	60(2)	-16(2)	21(1)	-18(1)
F(12)	23(1)	129(3)	51(2)	24(2)	-4(1)	-24(2)
F(25)	40(1)	79(2)	71(2)	40(2)	-33(1)	-29(1)
F(21)	66(2)	89(2)	53(2)	25(2)	37(2)	38(2)
F(8)	48(2)	61(2)	64(2)	3(1)	22(1)	31(1)
F(11)	39(2)	70(2)	179(4)	50(2)	-55(2)	-5(2)
F(10)	30(1)	187(4)	79(2)	-88(3)	-16(1)	9(2)
F(17)	110(3)	77(2)	56(2)	-25(2)	25(2)	-6(2)
F(18)	135(4)	86(3)	49(2)	-24(2)	7(2)	-20(3)
F(16)	50(3)	95(4)	29(3)	22(3)	5(2)	-10(3)
F(19)	105(6)	57(4)	68(5)	-39(4)	41(4)	-15(4)
F(13)	48(2)	55(2)	89(2)	-7(2)	4(2)	-14(1)
F(15)	65(2)	44(2)	269(7)	-32(3)	-20(3)	3(2)
F(14)	108(3)	113(3)	115(4)	-38(3)	30(3)	-57(3)
F(4)	252(6)	110(3)	228(6)	-132(4)	-215(5)	151(4)
F(5)	170(4)	31(1)	48(2)	2(1)	31(2)	-10(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for [(PNP)Cu]₂[B(3,5-(CF₃)₂-C₆H₃)₄].

	x	y	z	U(eq)
H(3)	2571	589	2151	36
H(4)	3245	1160	2770	39
H(5)	3582	2498	2669	45
H(6)	3205	3267	1971	45
H(9)	2494	5494	784	31
H(10)	1899	5846	1495	38
H(11)	1626	4829	2087	44
H(12)	1878	3485	1932	39
H(15)	3746	-125	199	35
H(16)	3093	-1023	-266	40
H(17)	2150	-544	-666	35
H(18)	1846	793	-568	28
H(21)	1010	3590	-895	29
H(22)	1518	3459	-1678	33
H(23)	2394	2609	-1732	31
H(24)	2797	1938	-998	26
H(25A)	866	734	1288	30
H(25B)	1239	711	1837	30
H(26)	944	2266	1425	33
H(27A)	892	1722	2476	52
H(27B)	862	2646	2288	52
H(27C)	1504	2141	2245	52
H(28A)	-6	1287	1891	55
H(28B)	-24	1562	1296	55
H(28C)	-97	2223	1744	55
H(29A)	2096	122	626	35
H(29B)	2619	121	1082	35
H(30)	1406	-513	1222	84
H(31A)	1868	-1366	1828	89
H(31B)	1883	-430	1989	89

H(31C)	2510	-858	1791	89
H(32A)	2421	-1424	827	108
H(32B)	1792	-1161	506	108
H(32C)	1750	-1792	974	108
H(33A)	2246	4679	-107	38
H(33B)	2857	5244	-60	38
H(34)	2751	3899	-760	38
H(35A)	2017	4964	-980	58
H(35B)	2523	4846	-1421	58
H(35C)	2596	5583	-1021	58
H(36A)	3634	4457	-1171	66
H(36B)	3821	4213	-585	66
H(36C)	3695	5142	-733	66
H(37A)	3906	4879	178	34
H(37B)	3615	5168	710	34
H(38)	4420	3782	624	48
H(39A)	3963	4487	1543	117
H(39B)	4468	3765	1536	117
H(39C)	3761	3620	1315	117
H(40A)	4870	5163	1166	98
H(40B)	4849	5222	547	98
H(40C)	5264	4533	832	98
H(41A)	4038	3831	817	28
H(41B)	4135	4269	276	28
H(42)	3689	5475	747	28
H(43A)	3535	4754	1536	48
H(43B)	4029	5477	1636	48
H(43C)	4278	4566	1585	48
H(44A)	4972	4912	793	45
H(44B)	4796	5802	987	45
H(44C)	4675	5559	392	45
H(45A)	4745	1897	143	37
H(45B)	4590	957	65	37
H(46)	3927	1331	-687	41
H(47A)	4553	2860	-601	71
H(47B)	3820	2725	-493	71

H(47C)	4074	2597	-1064	71
H(48A)	4783	1380	-1236	70
H(48B)	4953	771	-769	70
H(48C)	5248	1664	-769	70
H(49A)	3672	1221	1289	42
H(49B)	4029	544	968	42
H(51A)	5079	2448	1478	112
H(51B)	4341	2435	1598	112
H(51C)	4561	2587	1019	112
H(50A)	4625	1226	1614	90
H(52A)	5196	1037	724	81
H(52B)	5260	575	1268	81
H(52C)	5556	1461	1208	81
H(50B)	4972	1321	1004	65
H(53A)	4768	343	1680	97
H(53B)	4442	1033	2015	97
H(53C)	5186	1068	1921	97
H(54A)	163	2335	241	32
H(54B)	206	2738	-318	32
H(55)	780	1552	-595	30
H(56A)	1106	1026	223	46
H(56B)	705	358	-96	46
H(56C)	385	856	359	46
H(57A)	-141	778	-737	52
H(57B)	-329	1715	-789	52
H(57C)	-482	1226	-272	52
H(58A)	1336	4279	148	32
H(58B)	628	4071	-47	32
H(60)	1104	4158	998	32
H(58C)	1331	4221	381	32
H(58D)	896	4170	-134	32
H(59)	13	4119	279	38
H(61A)	-174	3757	816	79
H(61B)	212	3792	1359	79
H(61C)	347	3080	956	79
H(62A)	282	5163	363	106

H(62B)	827	5447	769	106
H(62C)	154	5167	971	106
H(64)	1463	6773	2371	24
H(66)	263	8680	2224	35
H(68)	1750	8763	3257	35
H(72)	1558	7706	3929	24
H(74)	2770	8075	5161	25
H(76)	3438	7418	3769	24
H(80)	3235	8555	3197	42
H(82)	4189	8344	1872	79
H(84)	2772	6795	2177	54
H(89)	1377	6164	3241	26
H(91)	2277	3991	3228	28
H(93)	3265	6072	3058	27
