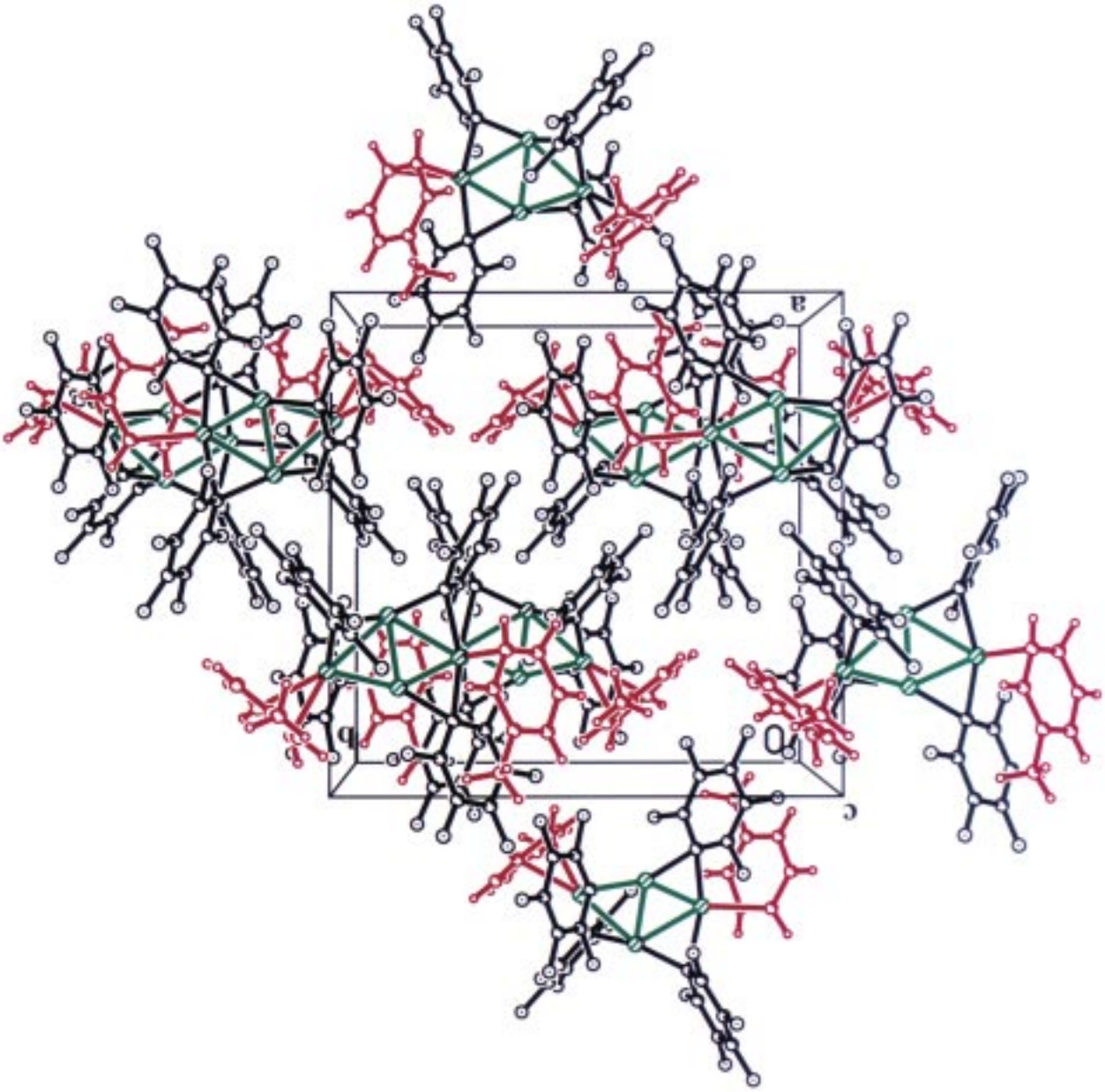
Figure S1. View of a part of the crystal packing of **2**; color code: red for the toluene molecules; green for the Cu_4 core.



Structural Diversity of Pentafluorophenylcopper Complexes. First Evidence of π-Coordination of Unsupported Arenes to Organocopper Aggregates

Anand Sundararaman[†], Roger A. Lalancette[†], Lev N. Zakharov[‡], Arnold L Rheingold[‡], and Frieder Jäkle[†]*

Department of Chemistry, Rutgers University-Newark, 73 Warren Street, Newark, NJ 07079, USA, and Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093, USA.

Supplementary Material

Table S1. Crystal data and structure refinement for **1**.

Identification code	fjak07	
Empirical formula	C25 H2 Cl Cu4 F20	
Formula weight	971.88	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.3875(6) Å	α= 86.9080(10)°.
	b = 10.8497(6) Å	β= 88.6850(10)°.
	c = 12.1005(6) Å	γ = 79.9220(10)°.
Volume	1340.62(13) $Å^3$	
Z	2	
Density (calculated)	2.408 Mg/m^3	
Absorption coefficient	3.389 mm^{-1}	
F(000)	930	
Crystal size	0.33 x 0.29 x 0.15 mm^3	
Theta range for data collection	1.69 to 27.52°.	
Index ranges	-13<=h<=13, -14<=k<=6, -15<=l<=15	
Reflections collected	8428	
Independent reflections	5871 [R(int) = 0.0173]	
Completeness to theta = 27.52°	95.2 %	
Absorption correction	Empirical	
Max. and min. transmission	0.6304 and 0.4009	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5871 / 0 / 459	
Goodness-of-fit on F^2	0.405	
Final R indices [I>2sigma(I)]	R1 = 0.0238, wR2 = 0.0652	
R indices (all data)	R1 = 0.0259, wR2 = 0.0681	
Largest diff. peak and hole	0.814 and -0.515 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for fjak07. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2656(1)	-5135(1)	2706(1)	16(1)
Cu(2)	3876(1)	-7218(1)	3203(1)	16(1)
Cu(3)	5734(1)	-6165(1)	3392(1)	15(1)
Cu(4)	4496(1)	-4068(1)	2926(1)	16(1)
C(1)	2164(2)	-6800(2)	2454(2)	16(1)
C(2)	968(2)	-6875(2)	2976(2)	15(1)
C(3)	-47(2)	-7280(2)	2465(2)	16(1)
C(4)	122(2)	-7665(2)	1396(2)	18(1)
C(5)	1294(2)	-7634(2)	845(2)	18(1)
C(6)	2273(2)	-7196(2)	1375(2)	17(1)
C(7)	5683(2)	-7982(2)	3666(2)	15(1)
C(8)	5829(2)	-8555(2)	4726(2)	16(1)
C(9)	6579(2)	-9717(2)	4947(2)	19(1)
C(10)	7217(2)	-10365(2)	4090(2)	23(1)
C(11)	7119(2)	-9850(2)	3022(2)	22(1)
C(12)	6378(2)	-8677(2)	2838(2)	18(1)
C(13)	6386(2)	-4639(2)	2753(2)	16(1)
C(14)	6801(2)	-4875(2)	1670(2)	17(1)
C(15)	8009(2)	-4727(2)	1255(2)	18(1)
C(16)	8865(2)	-4309(2)	1946(2)	18(1)
C(17)	8523(2)	-4070(2)	3029(2)	17(1)
C(18)	7299(2)	-4230(2)	3412(2)	15(1)
C(19)	2621(2)	-3309(2)	2880(2)	16(1)
C(20)	2257(2)	-2525(2)	1945(2)	17(1)
C(21)	1409(2)	-1394(2)	1985(2)	18(1)
C(22)	885(2)	-1015(2)	2992(2)	18(1)
C(23)	1205(2)	-1749(2)	3950(2)	17(1)
C(24)	2058(2)	-2866(2)	3870(2)	16(1)
F(1)	751(1)	-6507(1)	4017(1)	22(1)
F(2)	-1196(1)	-7300(1)	2986(1)	21(1)
F(3)	-848(1)	-8064(1)	906(1)	27(1)

F(4)	1460(1)	-8010(1)	-193(1)	28(1)
F(5)	3383(1)	-7151(1)	787(1)	25(1)
F(6)	5204(1)	-7974(1)	5596(1)	22(1)
F(7)	6704(1)	-10233(1)	5983(1)	27(1)
F(8)	7935(2)	-11494(1)	4293(1)	35(1)
F(9)	7735(1)	-10484(1)	2190(1)	33(1)
F(10)	6329(1)	-8189(1)	1791(1)	25(1)
F(11)	5988(1)	-5274(1)	969(1)	25(1)
F(12)	8385(1)	-4990(1)	218(1)	26(1)
F(13)	10050(1)	-4157(1)	1563(1)	26(1)
F(14)	9392(1)	-3708(1)	3686(1)	24(1)
F(15)	6996(1)	-3980(1)	4472(1)	19(1)
F(16)	2765(1)	-2855(1)	953(1)	25(1)
F(17)	1118(1)	-650(1)	1076(1)	27(1)
F(18)	80(1)	83(1)	3058(1)	25(1)
F(19)	696(1)	-1352(1)	4918(1)	24(1)
F(20)	2355(1)	-3548(1)	4828(1)	22(1)
Cl(1S)	5656(1)	-9634(1)	8336(1)	34(1)
C(1S)	5529(3)	-9646(3)	9812(2)	29(1)

Table S3. Bond lengths [Å] and angles [°] for fjak07.

Cu(1)-C(19)	1.998(2)	C(13)-C(14)	1.393(3)
Cu(1)-C(1)	2.002(2)	C(13)-C(18)	1.397(3)
Cu(1)-Cu(4)	2.4286(3)	C(14)-F(11)	1.350(2)
Cu(1)-Cu(2)	2.4413(3)	C(14)-C(15)	1.373(3)
Cu(2)-C(1)	1.984(2)	C(15)-F(12)	1.336(2)
Cu(2)-C(7)	1.9947(19)	C(15)-C(16)	1.382(3)
Cu(2)-Cu(3)	2.4301(3)	C(16)-F(13)	1.340(2)
Cu(3)-C(7)	1.991(2)	C(16)-C(17)	1.376(3)
Cu(3)-C(13)	2.0067(19)	C(17)-F(14)	1.339(2)
Cu(3)-Cu(4)	2.4534(3)	C(17)-C(18)	1.379(3)
Cu(4)-C(13)	1.9624(19)	C(18)-F(15)	1.344(2)
Cu(4)-C(19)	1.979(2)	C(19)-C(24)	1.392(3)
C(1)-C(6)	1.393(3)	C(19)-C(20)	1.396(3)
C(1)-C(2)	1.393(3)	C(20)-F(16)	1.341(2)
C(2)-F(1)	1.344(2)	C(20)-C(21)	1.382(3)
C(2)-C(3)	1.381(3)	C(21)-F(17)	1.337(2)
C(3)-F(2)	1.340(2)	C(21)-C(22)	1.377(3)
C(3)-C(4)	1.379(3)	C(22)-F(18)	1.335(2)
C(4)-F(3)	1.328(2)	C(22)-C(23)	1.383(3)
C(4)-C(5)	1.379(3)	C(23)-F(19)	1.336(2)
C(5)-F(4)	1.340(2)	C(23)-C(24)	1.377(3)
C(5)-C(6)	1.379(3)	C(24)-F(20)	1.353(2)
C(6)-F(5)	1.348(2)	Cl(1S)-C(1S)	1.788(2)
C(7)-C(8)	1.394(3)	C(1S)-C(1S)#1	1.497(5)
C(7)-C(12)	1.396(3)	C(1S)-H(1SB)	0.93(3)
C(8)-F(6)	1.351(2)	C(1S)-H(1SA)	0.96(3)
C(8)-C(9)	1.378(3)		
C(9)-F(7)	1.345(2)	C(19)-Cu(1)-C(1)	164.09(8)
C(9)-C(10)	1.376(3)	C(19)-Cu(1)-Cu(4)	52.01(6)
C(10)-F(8)	1.332(3)	C(1)-Cu(1)-Cu(4)	143.71(6)
C(10)-C(11)	1.379(3)	C(19)-Cu(1)-Cu(2)	143.09(6)
C(11)-F(9)	1.337(2)	C(1)-Cu(1)-Cu(2)	51.90(6)
C(11)-C(12)	1.377(3)	Cu(4)-Cu(1)-Cu(2)	94.777(12)
C(12)-F(10)	1.345(2)	C(1)-Cu(2)-C(7)	165.02(8)

C(1)-Cu(2)-Cu(3)	135.26(6)	F(5)-C(6)-C(1)	119.64(18)
C(7)-Cu(2)-Cu(3)	52.36(6)	C(5)-C(6)-C(1)	123.88(18)
C(1)-Cu(2)-Cu(1)	52.55(6)	C(8)-C(7)-C(12)	114.43(18)
C(7)-Cu(2)-Cu(1)	137.83(6)	C(8)-C(7)-Cu(3)	121.44(15)
Cu(3)-Cu(2)-Cu(1)	85.505(12)	C(12)-C(7)-Cu(3)	110.49(15)
C(7)-Cu(3)-C(13)	157.34(8)	C(8)-C(7)-Cu(2)	117.24(14)
C(7)-Cu(3)-Cu(2)	52.50(6)	C(12)-C(7)-Cu(2)	112.27(14)
C(13)-Cu(3)-Cu(2)	138.61(6)	Cu(3)-C(7)-Cu(2)	75.14(7)
C(7)-Cu(3)-Cu(4)	146.84(6)	F(6)-C(8)-C(9)	116.71(18)
C(13)-Cu(3)-Cu(4)	51.01(6)	F(6)-C(8)-C(7)	119.98(18)
Cu(2)-Cu(3)-Cu(4)	94.429(12)	C(9)-C(8)-C(7)	123.30(19)
C(13)-Cu(4)-C(19)	170.52(8)	F(7)-C(9)-C(10)	119.14(19)
C(13)-Cu(4)-Cu(1)	131.41(6)	F(7)-C(9)-C(8)	121.5(2)
C(19)-Cu(4)-Cu(1)	52.72(6)	C(10)-C(9)-C(8)	119.4(2)
C(13)-Cu(4)-Cu(3)	52.64(6)	F(8)-C(10)-C(9)	119.9(2)
C(19)-Cu(4)-Cu(3)	135.20(6)	F(8)-C(10)-C(11)	119.8(2)
Cu(1)-Cu(4)-Cu(3)	85.272(12)	C(9)-C(10)-C(11)	120.3(2)
C(6)-C(1)-C(2)	114.60(18)	F(9)-C(11)-C(12)	121.3(2)
C(6)-C(1)-Cu(2)	110.54(14)	F(9)-C(11)-C(10)	120.2(2)
C(2)-C(1)-Cu(2)	124.00(15)	C(12)-C(11)-C(10)	118.5(2)
C(6)-C(1)-Cu(1)	117.09(15)	F(10)-C(12)-C(11)	117.01(19)
C(2)-C(1)-Cu(1)	109.48(14)	F(10)-C(12)-C(7)	118.94(18)
Cu(2)-C(1)-Cu(1)	75.55(7)	C(11)-C(12)-C(7)	124.1(2)
F(1)-C(2)-C(3)	117.00(18)	C(14)-C(13)-C(18)	114.98(18)
F(1)-C(2)-C(1)	119.71(17)	C(14)-C(13)-Cu(4)	114.39(14)
C(3)-C(2)-C(1)	123.27(19)	C(18)-C(13)-Cu(4)	122.41(15)
F(2)-C(3)-C(4)	119.28(18)	C(14)-C(13)-Cu(3)	107.50(14)
F(2)-C(3)-C(2)	121.32(18)	C(18)-C(13)-Cu(3)	113.93(14)
C(4)-C(3)-C(2)	119.40(18)	Cu(4)-C(13)-Cu(3)	76.35(7)
F(3)-C(4)-C(3)	119.57(19)	F(11)-C(14)-C(15)	116.68(19)
F(3)-C(4)-C(5)	120.53(19)	F(11)-C(14)-C(13)	119.43(18)
C(3)-C(4)-C(5)	119.90(18)	C(15)-C(14)-C(13)	123.90(19)
F(4)-C(5)-C(6)	121.14(19)	F(12)-C(15)-C(14)	122.3(2)
F(4)-C(5)-C(4)	119.94(19)	F(12)-C(15)-C(16)	119.39(19)
C(6)-C(5)-C(4)	118.92(19)	C(14)-C(15)-C(16)	118.35(19)
F(5)-C(6)-C(5)	116.47(18)	F(13)-C(16)-C(17)	119.60(19)

F(13)-C(16)-C(15)	119.63(19)	F(17)-C(21)-C(20)	121.50(19)
C(17)-C(16)-C(15)	120.76(19)	C(22)-C(21)-C(20)	118.89(19)
F(14)-C(17)-C(16)	119.20(18)	F(18)-C(22)-C(21)	120.17(19)
F(14)-C(17)-C(18)	121.79(19)	F(18)-C(22)-C(23)	119.14(19)
C(16)-C(17)-C(18)	119.01(19)	C(21)-C(22)-C(23)	120.67(19)
F(15)-C(18)-C(17)	117.34(18)	F(19)-C(23)-C(24)	122.14(19)
F(15)-C(18)-C(13)	119.67(17)	F(19)-C(23)-C(22)	119.47(18)
C(17)-C(18)-C(13)	122.99(19)	C(24)-C(23)-C(22)	118.38(19)
C(24)-C(19)-C(20)	114.78(18)	F(20)-C(24)-C(23)	116.45(18)
C(24)-C(19)-Cu(4)	116.25(14)	F(20)-C(24)-C(19)	119.55(18)
C(20)-C(19)-Cu(4)	114.63(15)	C(23)-C(24)-C(19)	124.00(19)
C(24)-C(19)-Cu(1)	114.42(14)	C(1S)#1-C(1S)-Cl(1S)	108.9(2)
C(20)-C(19)-Cu(1)	115.76(15)	C(1S)#1-C(1S)-H(1SB)	111.9(19)
Cu(4)-C(19)-Cu(1)	75.27(7)	Cl(1S)-C(1S)-H(1SB)	107.7(18)
F(16)-C(20)-C(21)	117.27(18)	C(1S)#1-C(1S)-H(1SA)	108(2)
F(16)-C(20)-C(19)	119.45(18)	Cl(1S)-C(1S)-H(1SA)	109(2)
C(21)-C(20)-C(19)	123.27(19)	H(1SB)-C(1S)-H(1SA)	111(3)
F(17)-C(21)-C(22)	119.58(18)		

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($Å^2 x 10^3$) for fjak07. 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)	13(1)	12(1)	24(1)	-1(1)	-1(1)	-3(1)
Cu(2)	11(1)	14(1)	22(1)	1(1)	-3(1)	-3(1)
Cu(3)	13(1)	12(1)	21(1)	1(1)	0(1)	-4(1)
Cu(4)	10(1)	14(1)	23(1)	0(1)	0(1)	-3(1)
C(1)	14(1)	14(1)	21(1)	1(1)	-3(1)	-3(1)
C(2)	16(1)	12(1)	17(1)	0(1)	-2(1)	-3(1)
C(3)	11(1)	15(1)	22(1)	3(1)	-1(1)	-3(1)
C(4)	17(1)	15(1)	22(1)	1(1)	-7(1)	-5(1)
C(5)	23(1)	16(1)	15(1)	-1(1)	-1(1)	-3(1)
C(6)	13(1)	15(1)	22(1)	2(1)	4(1)	-2(1)
C(7)	12(1)	14(1)	20(1)	0(1)	-1(1)	-3(1)
C(8)	14(1)	16(1)	21(1)	-3(1)	-1(1)	-6(1)
C(9)	18(1)	16(1)	25(1)	5(1)	-6(1)	-7(1)
C(10)	16(1)	15(1)	37(1)	-2(1)	-6(1)	-1(1)
C(11)	15(1)	22(1)	28(1)	-11(1)	1(1)	-3(1)
C(12)	15(1)	20(1)	19(1)	-2(1)	-1(1)	-6(1)
C(13)	12(1)	13(1)	22(1)	2(1)	0(1)	-4(1)
C(14)	16(1)	14(1)	21(1)	1(1)	-4(1)	-4(1)
C(15)	19(1)	16(1)	18(1)	2(1)	4(1)	-1(1)
C(16)	11(1)	15(1)	28(1)	3(1)	4(1)	-2(1)
C(17)	13(1)	14(1)	25(1)	-1(1)	-2(1)	-3(1)
C(18)	15(1)	11(1)	20(1)	-1(1)	0(1)	-1(1)
C(19)	12(1)	14(1)	23(1)	-1(1)	-2(1)	-3(1)
C(20)	15(1)	17(1)	19(1)	-2(1)	0(1)	-4(1)
C(21)	19(1)	14(1)	22(1)	2(1)	-6(1)	-4(1)
C(22)	14(1)	12(1)	26(1)	0(1)	-1(1)	-2(1)
C(23)	15(1)	15(1)	21(1)	-2(1)	2(1)	-5(1)
C(24)	13(1)	14(1)	21(1)	3(1)	-2(1)	-6(1)
F(1)	23(1)	27(1)	17(1)	-5(1)	2(1)	-6(1)
F(2)	13(1)	24(1)	28(1)	2(1)	3(1)	-7(1)
F(3)	22(1)	31(1)	31(1)	-5(1)	-9(1)	-12(1)

F(4)	35(1)	33(1)	18(1)	-8(1)	1(1)	-6(1)
F(5)	17(1)	29(1)	27(1)	-1(1)	8(1)	-5(1)
F(6)	21(1)	25(1)	21(1)	-4(1)	3(1)	-3(1)
F(7)	30(1)	23(1)	28(1)	11(1)	-8(1)	-7(1)
F(8)	31(1)	15(1)	55(1)	-2(1)	-10(1)	7(1)
F(9)	27(1)	34(1)	37(1)	-19(1)	3(1)	4(1)
F(10)	27(1)	31(1)	18(1)	-1(1)	1(1)	-8(1)
F(11)	22(1)	33(1)	22(1)	-4(1)	-4(1)	-10(1)
F(12)	27(1)	31(1)	19(1)	0(1)	7(1)	-4(1)
F(13)	13(1)	29(1)	35(1)	1(1)	8(1)	-6(1)
F(14)	14(1)	26(1)	34(1)	-8(1)	-3(1)	-8(1)
F(15)	19(1)	19(1)	19(1)	-3(1)	2(1)	-5(1)
F(16)	31(1)	23(1)	20(1)	-3(1)	1(1)	0(1)
F(17)	37(1)	19(1)	23(1)	4(1)	-7(1)	1(1)
F(18)	25(1)	13(1)	33(1)	0(1)	1(1)	4(1)
F(19)	26(1)	21(1)	23(1)	-4(1)	6(1)	-1(1)
F(20)	25(1)	19(1)	21(1)	4(1)	-1(1)	-1(1)
Cl(1S)	37(1)	51(1)	22(1)	-7(1)	5(1)	-25(1)
C(1S)	30(1)	38(1)	22(1)	-7(1)	3(1)	-14(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for fjak07.

	x	y	z	U(eq)
H(1SB)	5350(30)	-8820(30)	10010(20)	29(7)
H(1SA)	6340(30)	-10070(30)	10130(30)	40(9)

Table S6. Crystal data and structure refinement for **2**.

Identification code	fjak01	
Empirical formula	C38 H16 Cu4 F20	
Formula weight	1106.67	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.2253(9) Å	α= 90°.
	b = 15.3381(9) Å	β= 91.7160(10)°.
	c = 15.8026(9) Å	γ = 90°.
Volume	3688.7(4) $Å^3$	
Z	4	
Density (calculated)	1.993 Mg/m^3	
Absorption coefficient	2.407 mm^{-1}	
F(000)	2160	
Crystal size	0.40 x 0.30 x 0.30 mm^3	
Theta range for data collection	1.89 to 28.26°.	
Index ranges	-15<=h<=20, -18<=k<=20, -21<=l<=20	
Reflections collected	23498	
Independent reflections	8720 [R(int) = 0.0212]	
Completeness to theta = 28.26°	95.3 %	
Absorption correction	None	
Max. and min. transmission	0.5321 and 0.4460	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8720 / 0 / 559	
Goodness-of-fit on F^2	1.115	
Final R indices [I>2sigma(I)]	R1 = 0.0306, wR2 = 0.0831	
R indices (all data)	R1 = 0.0372, wR2 = 0.0869	
Largest diff. peak and hole	0.410 and -0.445 e.$Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for fjak01. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	3597(1)	8850(1)	621(1)	25(1)
Cu(2)	2150(1)	8676(1)	-271(1)	25(1)
Cu(3)	2783(1)	7459(1)	549(1)	25(1)
Cu(4)	2517(1)	10024(1)	521(1)	24(1)
F(12)	4831(1)	7731(1)	1593(1)	44(1)
F(13)	6251(1)	6926(1)	1019(1)	60(1)
F(14)	6313(1)	6444(1)	-626(1)	64(1)
F(15)	4969(1)	6854(1)	-1719(1)	50(1)
F(16)	3572(1)	7720(1)	-1180(1)	36(1)
F(22)	3829(1)	9777(1)	-912(1)	41(1)
F(23)	3796(1)	10692(1)	-2348(1)	59(1)
F(24)	2243(1)	11248(1)	-3048(1)	58(1)
F(25)	719(1)	10880(1)	-2285(1)	55(1)
F(26)	728(1)	9983(1)	-835(1)	43(1)
F(32)	929(1)	8432(1)	1174(1)	37(1)
F(33)	-688(1)	7758(1)	947(1)	43(1)
F(34)	-999(1)	6536(1)	-269(1)	49(1)
F(35)	323(1)	5988(1)	-1254(1)	52(1)
F(36)	1929(1)	6682(1)	-1063(1)	41(1)
F(42)	2636(1)	8893(1)	2292(1)	37(1)
F(43)	3557(1)	9330(1)	3709(1)	41(1)
F(44)	4909(1)	10470(1)	3631(1)	47(1)
F(45)	5278(1)	11257(1)	2148(1)	46(1)
F(46)	4356(1)	10848(1)	722(1)	36(1)
C(11)	4115(1)	7754(1)	244(1)	24(1)
C(12)	4835(2)	7529(2)	761(1)	30(1)
C(13)	5571(2)	7110(2)	487(2)	38(1)
C(14)	5609(2)	6873(2)	-350(2)	39(1)
C(15)	4926(2)	7078(2)	-902(1)	33(1)
C(16)	4209(1)	7519(1)	-605(1)	25(1)
C(21)	2280(1)	9838(1)	-795(1)	25(1)

C(22)	3035(2)	10046(1)	-1222(1)	29(1)
C(23)	3043(2)	10514(2)	-1968(2)	37(1)
C(24)	2257(2)	10801(2)	-2320(1)	37(1)
C(25)	1479(2)	10617(2)	-1930(1)	36(1)
C(26)	1515(2)	10151(1)	-1189(1)	29(1)
C(31)	1512(1)	7594(1)	64(1)	25(1)
C(32)	805(2)	7833(1)	555(1)	27(1)
C(33)	-28(1)	7499(2)	452(1)	29(1)
C(34)	-194(2)	6878(2)	-163(2)	34(1)
C(35)	476(2)	6608(2)	-664(1)	33(1)
C(36)	1299(1)	6973(1)	-548(1)	28(1)
C(41)	3464(1)	9839(1)	1439(1)	24(1)
C(42)	3294(1)	9483(1)	2225(1)	26(1)
C(43)	3753(2)	9692(1)	2964(1)	29(1)
C(44)	4431(2)	10283(2)	2925(1)	31(1)
C(45)	4624(1)	10670(1)	2170(1)	30(1)
C(46)	4145(1)	10442(1)	1454(1)	26(1)
C(51)	1283(2)	10673(2)	1040(2)	51(1)
C(52)	1291(2)	10470(2)	1901(2)	47(1)
C(53)	1798(2)	10944(2)	2480(2)	36(1)
C(54)	2313(2)	11617(2)	2187(2)	39(1)
C(55)	2319(2)	11820(2)	1332(2)	47(1)
C(56)	1799(2)	11347(2)	757(2)	51(1)
C(57)	1792(2)	10735(2)	3414(2)	54(1)
C(61)	2890(2)	5947(2)	1049(2)	60(1)
C(62)	2079(3)	5545(2)	882(2)	58(1)
C(63)	1368(2)	5773(2)	1350(2)	45(1)
C(64)	1432(2)	6403(2)	1976(2)	38(1)
C(65)	2241(2)	6796(2)	2137(2)	42(1)
C(66)	2963(2)	6559(2)	1681(2)	52(1)
C(67)	649(2)	6656(2)	2485(2)	66(1)

Table S8. Bond lengths [Å] and angles [°] for fjak01.

Cu(1)-C(11)	1.957(2)	F(44)-C(44)	1.344(2)
Cu(1)-C(41)	2.006(2)	F(45)-C(45)	1.343(2)
Cu(1)-Cu(4)	2.4404(4)	F(46)-C(46)	1.361(2)
Cu(1)-Cu(3)	2.4672(4)	C(11)-C(12)	1.392(3)
Cu(1)-Cu(2)	2.5935(4)	C(11)-C(16)	1.401(3)
Cu(2)-C(21)	1.978(2)	C(12)-C(13)	1.373(3)
Cu(2)-C(31)	2.001(2)	C(13)-C(14)	1.374(4)
Cu(2)-Cu(3)	2.4522(4)	C(14)-C(15)	1.373(4)
Cu(2)-Cu(4)	2.4729(4)	C(15)-C(16)	1.378(3)
Cu(3)-C(31)	2.070(2)	C(21)-C(22)	1.388(3)
Cu(3)-C(11)	2.145(2)	C(21)-C(26)	1.389(3)
Cu(3)-C(66)	2.271(2)	C(22)-C(23)	1.380(3)
Cu(3)-C(61)	2.455(3)	C(23)-C(24)	1.376(4)
Cu(4)-C(41)	2.034(2)	C(24)-C(25)	1.380(4)
Cu(4)-C(21)	2.119(2)	C(25)-C(26)	1.372(3)
Cu(4)-C(51)	2.298(2)	C(31)-C(36)	1.389(3)
Cu(4)-C(56)	2.339(2)	C(31)-C(32)	1.395(3)
F(12)-C(12)	1.351(2)	C(32)-C(33)	1.373(3)
F(13)-C(13)	1.344(3)	C(33)-C(34)	1.378(3)
F(14)-C(14)	1.343(3)	C(34)-C(35)	1.373(3)
F(15)-C(15)	1.340(3)	C(35)-C(36)	1.380(3)
F(16)-C(16)	1.346(2)	C(41)-C(46)	1.389(3)
F(22)-C(22)	1.356(3)	C(41)-C(42)	1.389(3)
F(23)-C(23)	1.338(3)	C(42)-C(43)	1.380(3)
F(24)-C(24)	1.339(2)	C(43)-C(44)	1.376(3)
F(25)-C(25)	1.334(3)	C(44)-C(45)	1.373(3)
F(26)-C(26)	1.362(3)	C(45)-C(46)	1.372(3)
F(32)-C(32)	1.351(2)	C(51)-C(56)	1.380(5)
F(33)-C(33)	1.351(2)	C(51)-C(52)	1.396(4)
F(34)-C(34)	1.339(3)	C(52)-C(53)	1.385(4)
F(35)-C(35)	1.348(3)	C(53)-C(54)	1.384(3)
F(36)-C(36)	1.352(2)	C(53)-C(57)	1.511(4)
F(42)-C(42)	1.357(2)	C(54)-C(55)	1.386(4)
F(43)-C(43)	1.344(2)	C(55)-C(56)	1.391(4)

C(61)-C(66)	1.373(5)	C(64)-C(65)	1.389(3)
C(61)-C(62)	1.398(5)	C(64)-C(67)	1.508(4)
C(62)-C(63)	1.374(4)	C(65)-C(66)	1.380(4)
C(63)-C(64)	1.385(4)		

C(11)-Cu(1)-C(41)	153.47(9)	C(11)-Cu(3)-Cu(1)	49.61(6)
C(11)-Cu(1)-Cu(4)	152.96(6)	C(66)-Cu(3)-Cu(1)	116.14(8)
C(41)-Cu(1)-Cu(4)	53.36(6)	Cu(2)-Cu(3)-Cu(1)	63.633(11)
C(11)-Cu(1)-Cu(3)	56.60(6)	C(61)-Cu(3)-Cu(1)	140.68(9)
C(41)-Cu(1)-Cu(3)	128.58(6)	C(41)-Cu(4)-C(21)	140.99(8)
Cu(4)-Cu(1)-Cu(3)	107.378(14)	C(41)-Cu(4)-C(51)	112.08(9)
C(11)-Cu(1)-Cu(2)	95.11(6)	C(21)-Cu(4)-C(51)	106.91(9)
C(41)-Cu(1)-Cu(2)	109.13(6)	C(41)-Cu(4)-C(56)	109.39(9)
Cu(4)-Cu(1)-Cu(2)	58.750(10)	C(21)-Cu(4)-C(56)	101.91(9)
Cu(3)-Cu(1)-Cu(2)	57.901(10)	C(51)-Cu(4)-C(56)	34.62(11)
C(21)-Cu(2)-C(31)	155.94(9)	C(41)-Cu(4)-Cu(1)	52.32(6)
C(21)-Cu(2)-Cu(3)	149.78(6)	C(21)-Cu(4)-Cu(1)	93.39(6)
C(31)-Cu(2)-Cu(3)	54.26(6)	C(51)-Cu(4)-Cu(1)	148.49(9)
C(21)-Cu(2)-Cu(4)	55.53(6)	C(56)-Cu(4)-Cu(1)	161.18(8)
C(31)-Cu(2)-Cu(4)	131.55(6)	C(41)-Cu(4)-Cu(2)	112.87(6)
Cu(3)-Cu(2)-Cu(4)	106.828(13)	C(21)-Cu(4)-Cu(2)	50.32(6)
C(21)-Cu(2)-Cu(1)	92.33(6)	C(51)-Cu(4)-Cu(2)	111.59(8)
C(31)-Cu(2)-Cu(1)	110.64(6)	C(56)-Cu(4)-Cu(2)	134.95(8)
Cu(3)-Cu(2)-Cu(1)	58.466(10)	Cu(1)-Cu(4)-Cu(2)	63.719(11)
Cu(4)-Cu(2)-Cu(1)	57.531(10)	C(12)-C(11)-C(16)	113.35(19)
C(31)-Cu(3)-C(11)	140.79(8)	C(12)-C(11)-Cu(1)	110.58(15)
C(31)-Cu(3)-C(66)	116.21(9)	C(16)-C(11)-Cu(1)	124.57(16)
C(11)-Cu(3)-C(66)	102.28(9)	C(12)-C(11)-Cu(3)	123.33(15)
C(31)-Cu(3)-Cu(2)	51.69(6)	C(16)-C(11)-Cu(3)	106.59(15)
C(11)-Cu(3)-Cu(2)	94.61(6)	Cu(1)-C(11)-Cu(3)	73.78(7)
C(66)-Cu(3)-Cu(2)	156.24(9)	F(12)-C(12)-C(13)	116.3(2)
C(31)-Cu(3)-C(61)	105.41(10)	F(12)-C(12)-C(11)	119.2(2)
C(11)-Cu(3)-C(61)	102.56(9)	C(13)-C(12)-C(11)	124.5(2)
C(66)-Cu(3)-C(61)	33.50(11)	F(13)-C(13)-C(14)	119.5(2)
Cu(2)-Cu(3)-C(61)	155.55(9)	F(13)-C(13)-C(12)	121.4(2)
C(31)-Cu(3)-Cu(1)	113.15(6)	C(14)-C(13)-C(12)	119.1(2)

F(14)-C(14)-C(15)	120.2(2)	F(32)-C(32)-C(33)	116.64(19)
F(14)-C(14)-C(13)	120.0(2)	F(32)-C(32)-C(31)	119.20(19)
C(15)-C(14)-C(13)	119.9(2)	C(33)-C(32)-C(31)	124.2(2)
F(15)-C(15)-C(14)	119.7(2)	F(33)-C(33)-C(32)	121.4(2)
F(15)-C(15)-C(16)	121.1(2)	F(33)-C(33)-C(34)	119.2(2)
C(14)-C(15)-C(16)	119.2(2)	C(32)-C(33)-C(34)	119.4(2)
F(16)-C(16)-C(15)	116.42(18)	F(34)-C(34)-C(35)	120.1(2)
F(16)-C(16)-C(11)	119.64(19)	F(34)-C(34)-C(33)	120.5(2)
C(15)-C(16)-C(11)	123.9(2)	C(35)-C(34)-C(33)	119.4(2)
C(22)-C(21)-C(26)	113.45(19)	F(35)-C(35)-C(34)	119.7(2)
C(22)-C(21)-Cu(2)	120.34(16)	F(35)-C(35)-C(36)	121.0(2)
C(26)-C(21)-Cu(2)	113.93(16)	C(34)-C(35)-C(36)	119.3(2)
C(22)-C(21)-Cu(4)	109.13(15)	F(36)-C(36)-C(35)	116.4(2)
C(26)-C(21)-Cu(4)	120.60(15)	F(36)-C(36)-C(31)	119.32(19)
Cu(2)-C(21)-Cu(4)	74.15(7)	C(35)-C(36)-C(31)	124.3(2)
F(22)-C(22)-C(23)	115.9(2)	C(46)-C(41)-C(42)	113.88(19)
F(22)-C(22)-C(21)	119.76(19)	C(46)-C(41)-Cu(1)	115.18(15)
C(23)-C(22)-C(21)	124.3(2)	C(42)-C(41)-Cu(1)	107.72(14)
F(23)-C(23)-C(24)	119.9(2)	C(46)-C(41)-Cu(4)	115.61(15)
F(23)-C(23)-C(22)	121.3(2)	C(42)-C(41)-Cu(4)	123.07(16)
C(24)-C(23)-C(22)	118.8(2)	Cu(1)-C(41)-Cu(4)	74.32(7)
F(24)-C(24)-C(23)	120.2(2)	F(42)-C(42)-C(43)	116.51(18)
F(24)-C(24)-C(25)	119.7(2)	F(42)-C(42)-C(41)	119.27(19)
C(23)-C(24)-C(25)	120.1(2)	C(43)-C(42)-C(41)	124.2(2)
F(25)-C(25)-C(26)	121.9(2)	F(43)-C(43)-C(44)	119.9(2)
F(25)-C(25)-C(24)	119.8(2)	F(43)-C(43)-C(42)	121.7(2)
C(26)-C(25)-C(24)	118.4(2)	C(44)-C(43)-C(42)	118.49(19)
F(26)-C(26)-C(25)	115.9(2)	F(44)-C(44)-C(45)	120.3(2)
F(26)-C(26)-C(21)	119.10(19)	F(44)-C(44)-C(43)	119.4(2)
C(25)-C(26)-C(21)	125.0(2)	C(45)-C(44)-C(43)	120.2(2)
C(36)-C(31)-C(32)	113.51(19)	F(45)-C(45)-C(46)	121.8(2)
C(36)-C(31)-Cu(2)	119.34(15)	F(45)-C(45)-C(44)	119.3(2)
C(32)-C(31)-Cu(2)	108.57(15)	C(46)-C(45)-C(44)	119.0(2)
C(36)-C(31)-Cu(3)	112.68(15)	F(46)-C(46)-C(45)	116.77(19)
C(32)-C(31)-Cu(3)	123.28(15)	F(46)-C(46)-C(41)	119.02(18)
Cu(2)-C(31)-Cu(3)	74.05(7)	C(45)-C(46)-C(41)	124.2(2)

C(56)-C(51)-C(52)	119.6(3)	C(66)-C(61)-C(62)	119.3(3)
C(56)-C(51)-Cu(4)	74.32(16)	C(66)-C(61)-Cu(3)	65.90(16)
C(52)-C(51)-Cu(4)	105.55(19)	C(62)-C(61)-Cu(3)	107.83(19)
C(53)-C(52)-C(51)	121.0(3)	C(63)-C(62)-C(61)	119.5(3)
C(52)-C(53)-C(54)	118.8(2)	C(62)-C(63)-C(64)	121.5(3)
C(52)-C(53)-C(57)	120.9(3)	C(63)-C(64)-C(65)	118.5(3)
C(54)-C(53)-C(57)	120.4(2)	C(63)-C(64)-C(67)	121.4(3)
C(53)-C(54)-C(55)	120.9(2)	C(65)-C(64)-C(67)	120.1(3)
C(54)-C(55)-C(56)	120.0(3)	C(66)-C(65)-C(64)	120.4(3)
C(51)-C(56)-C(55)	119.8(3)	C(61)-C(66)-C(65)	120.8(3)
C(51)-C(56)-Cu(4)	71.05(15)	C(61)-C(66)-Cu(3)	80.60(17)
C(55)-C(56)-Cu(4)	107.29(18)	C(65)-C(66)-Cu(3)	99.88(17)

Table S9. Anisotropic displacement parameters ($Å^2 x 10^3$) for fjak01. 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)	23(1)	23(1)	29(1)	-4(1)	1(1)	0(1)
Cu(2)	27(1)	23(1)	25(1)	2(1)	-1(1)	-4(1)
Cu(3)	22(1)	24(1)	28(1)	2(1)	-1(1)	-1(1)
Cu(4)	23(1)	25(1)	25(1)	-2(1)	-2(1)	1(1)
F(12)	43(1)	64(1)	25(1)	-2(1)	-8(1)	0(1)
F(13)	30(1)	83(1)	67(1)	24(1)	-10(1)	13(1)
F(14)	47(1)	64(1)	83(1)	11(1)	31(1)	27(1)
F(15)	69(1)	50(1)	34(1)	-10(1)	23(1)	-1(1)
F(16)	36(1)	48(1)	24(1)	5(1)	-5(1)	-6(1)
F(22)	24(1)	59(1)	42(1)	7(1)	5(1)	2(1)
F(23)	60(1)	64(1)	55(1)	16(1)	25(1)	-13(1)
F(24)	99(2)	38(1)	36(1)	17(1)	2(1)	6(1)
F(25)	61(1)	62(1)	40(1)	-1(1)	-21(1)	26(1)
F(26)	23(1)	65(1)	40(1)	1(1)	-1(1)	1(1)
F(32)	40(1)	34(1)	39(1)	-13(1)	6(1)	-5(1)
F(33)	27(1)	54(1)	48(1)	-3(1)	9(1)	2(1)
F(34)	30(1)	63(1)	55(1)	1(1)	-7(1)	-18(1)
F(35)	49(1)	55(1)	52(1)	-25(1)	-7(1)	-17(1)
F(36)	37(1)	46(1)	39(1)	-16(1)	8(1)	-3(1)
F(42)	38(1)	36(1)	37(1)	2(1)	4(1)	-15(1)
F(43)	52(1)	45(1)	27(1)	7(1)	1(1)	3(1)
F(44)	46(1)	57(1)	37(1)	-10(1)	-16(1)	-4(1)
F(45)	40(1)	48(1)	50(1)	-6(1)	-5(1)	-24(1)
F(46)	37(1)	36(1)	34(1)	5(1)	2(1)	-12(1)
C(11)	23(1)	25(1)	23(1)	0(1)	1(1)	2(1)
C(12)	30(1)	33(1)	26(1)	2(1)	-1(1)	-2(1)
C(13)	23(1)	42(1)	48(1)	14(1)	-2(1)	4(1)
C(14)	32(1)	36(1)	50(1)	6(1)	17(1)	9(1)
C(15)	39(1)	28(1)	33(1)	-2(1)	14(1)	-3(1)
C(16)	27(1)	24(1)	25(1)	2(1)	0(1)	-3(1)
C(21)	26(1)	25(1)	24(1)	1(1)	2(1)	-2(1)

C(22)	30(1)	28(1)	30(1)	-1(1)	2(1)	-2(1)
C(23)	48(2)	30(1)	34(1)	4(1)	13(1)	-9(1)
C(24)	61(2)	25(1)	26(1)	6(1)	1(1)	0(1)
C(25)	45(2)	31(1)	30(1)	-4(1)	-11(1)	9(1)
C(26)	30(1)	29(1)	28(1)	-4(1)	-2(1)	-1(1)
C(31)	24(1)	23(1)	27(1)	3(1)	-1(1)	-3(1)
C(32)	31(1)	23(1)	27(1)	0(1)	-2(1)	-2(1)
C(33)	23(1)	33(1)	33(1)	5(1)	2(1)	1(1)
C(34)	25(1)	36(1)	40(1)	6(1)	-7(1)	-9(1)
C(35)	36(1)	33(1)	29(1)	-3(1)	-8(1)	-5(1)
C(36)	25(1)	30(1)	27(1)	0(1)	0(1)	0(1)
C(41)	24(1)	21(1)	27(1)	-2(1)	-1(1)	0(1)
C(42)	25(1)	21(1)	33(1)	-2(1)	2(1)	-2(1)
C(43)	32(1)	28(1)	26(1)	1(1)	0(1)	5(1)
C(44)	29(1)	34(1)	30(1)	-8(1)	-9(1)	3(1)
C(45)	25(1)	27(1)	39(1)	-6(1)	-4(1)	-4(1)
C(46)	25(1)	25(1)	27(1)	-2(1)	1(1)	0(1)
C(51)	26(1)	69(2)	57(2)	-28(2)	-5(1)	16(1)
C(52)	29(1)	49(2)	63(2)	-24(1)	10(1)	-2(1)
C(53)	31(1)	36(1)	40(1)	-9(1)	6(1)	8(1)
C(54)	41(1)	32(1)	45(1)	-12(1)	-1(1)	3(1)
C(55)	59(2)	29(1)	55(2)	0(1)	10(1)	10(1)
C(56)	60(2)	51(2)	41(1)	-6(1)	-6(1)	35(2)
C(57)	56(2)	59(2)	46(2)	-2(1)	14(1)	8(1)
C(61)	54(2)	64(2)	62(2)	34(2)	13(2)	27(2)
C(62)	97(3)	31(1)	45(2)	7(1)	-1(2)	7(2)
C(63)	50(2)	40(2)	45(1)	18(1)	-15(1)	-17(1)
C(64)	37(1)	41(1)	35(1)	15(1)	-3(1)	-7(1)
C(65)	47(2)	41(2)	38(1)	14(1)	-12(1)	-11(1)
C(66)	37(2)	63(2)	57(2)	37(2)	-14(1)	-6(1)
C(67)	58(2)	86(2)	53(2)	26(2)	12(2)	6(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for fjak01.

	x	y	z	U(eq)
H(51A)	719	10566	716	61
H(52A)	944	10000	2094	56
H(54A)	2668	11944	2577	47
H(55A)	2678	12281	1139	57
H(56A)	1575	11667	244	61
H(57A)	1398	10241	3507	81
H(57B)	1586	11244	3726	81
H(57C)	2388	10583	3614	81
H(61A)	3431	5612	910	72
H(62A)	2020	5118	449	69
H(63A)	820	5491	1242	54
H(65A)	2299	7231	2563	51
H(66A)	3545	6590	1991	63
H(67A)	135	6320	2289	99
H(67B)	531	7279	2412	99
H(67C)	774	6531	3085	99

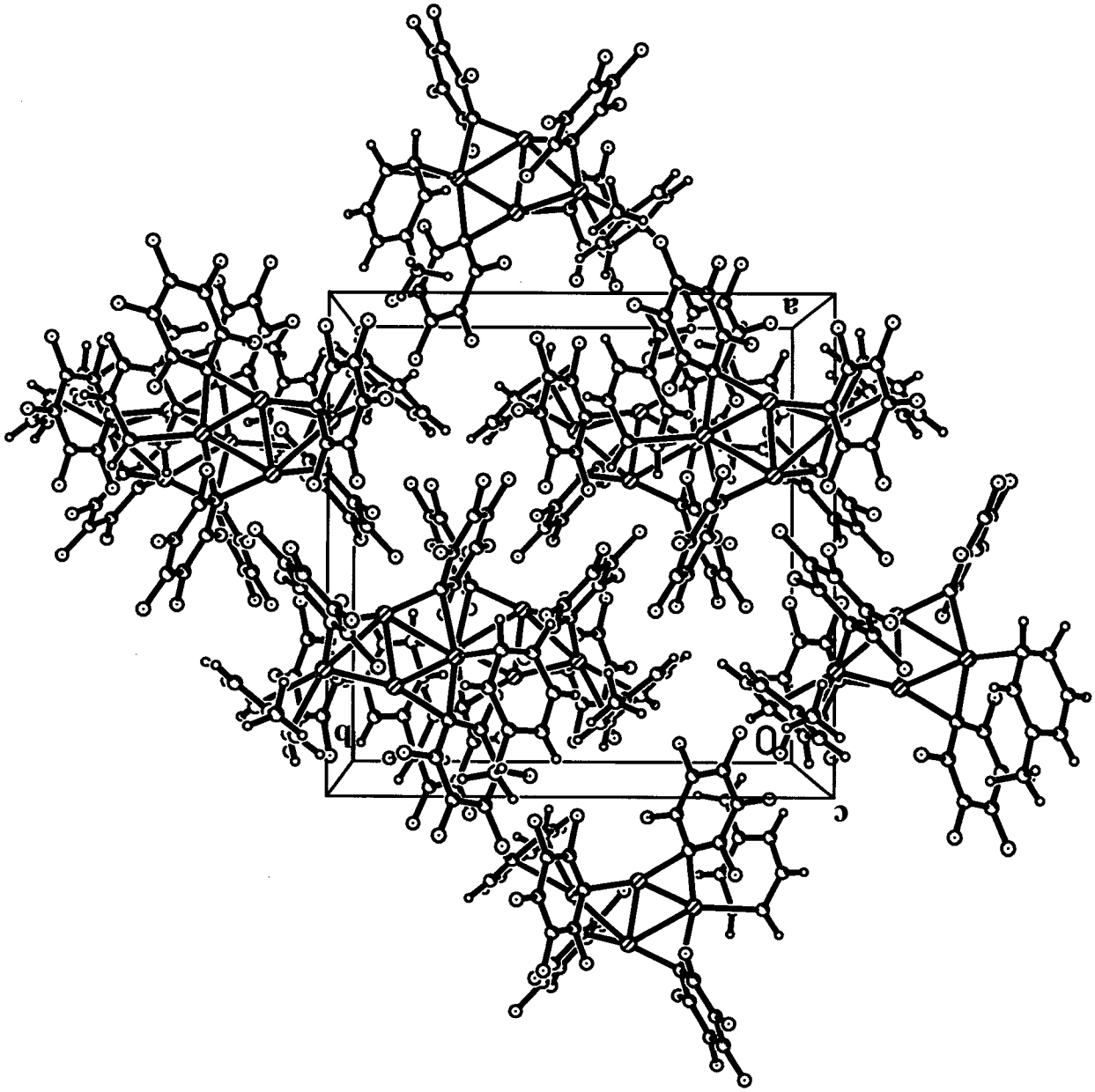



Figure S1. View of a part of the crystal packing of **2**; color code: red for the toluene molecules; green for the Cu_4 core.