Supporting Information

CFA-2 and CFA-3 (Coordination Framework Augsburg University-2 and -3); Novel MOFs Assembled from Trinuclear Cu(I)/Ag(I) Secondary Building Units and 3,3',5,5'-Tetraphenyl-bipyrazolate Ligands

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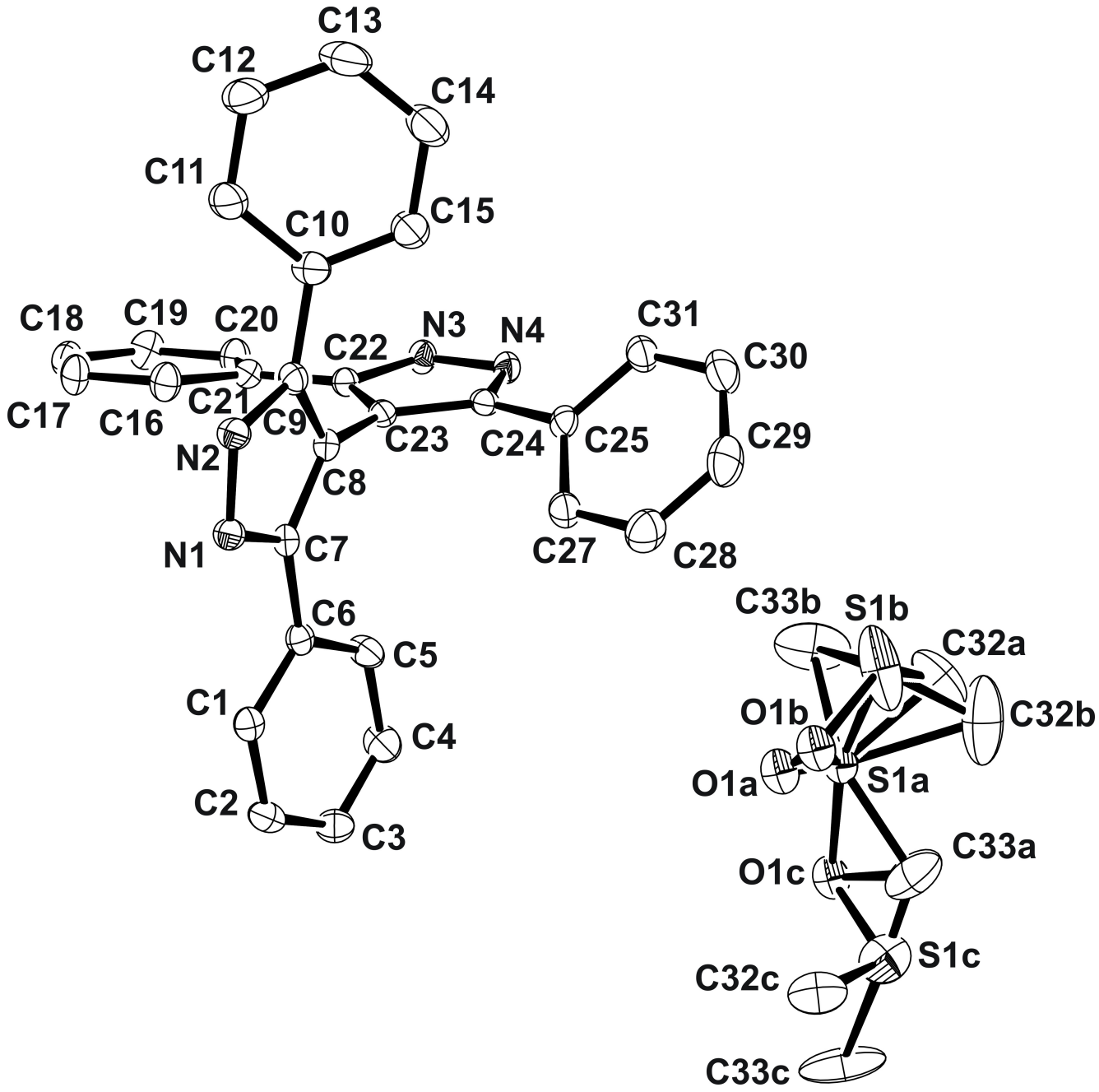

Fig. **S1**. View of the asymmetric unit of **1** showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

ATOM	x	y	z	U(eq)
N(1)	8603(1)	322(1)	1144(1)	18(1)
N(2)	8209(1)	81(1)	1857(1)	19(1)

N(3)	5368(1)	3114(1)	2013(1)	20(1)
N(4)	6433(1)	3423(1)	2419(1)	20(1)
C(1)	9164(2)	1177(1)	-265(1)	19(1)
C(2)	9582(2)	1610(1)	-910(1)	23(1)
C(3)	9396(2)	2467(1)	-975(1)	27(1)
C(4)	8762(2)	2876(1)	-390(1)	28(1)
C(5)	8336(2)	2443(1)	259(1)	24(1)
C(6)	8547(2)	1584(1)	340(1)	17(1)
C(7)	8209(2)	1116(1)	1055(1)	16(1)
C(8)	7556(2)	1378(1)	1730(1)	16(1)
C(9)	7595(2)	695(1)	2233(1)	18(1)
C(10)	7130(2)	567(1)	3032(1)	23(1)
C(11)	6358(2)	-123(1)	3181(1)	35(1)
C(12)	6007(3)	-283(1)	3948(1)	44(1)
C(13)	6413(2)	244(1)	4569(1)	40(1)
C(14)	7133(2)	942(1)	4420(1)	38(1)
C(15)	7491(2)	1105(1)	3654(1)	29(1)
C(16)	4649(2)	1056(1)	1034(1)	24(1)
C(17)	3659(2)	642(1)	601(1)	26(1)
C(18)	2520(2)	1048(1)	365(1)	25(1)
C(19)	2369(2)	1878(1)	569(1)	26(1)
C(20)	3360(2)	2301(1)	998(1)	24(1)
C(21)	4520(2)	1899(1)	1235(1)	19(1)
C(22)	5569(2)	2354(1)	1689(1)	18(1)
C(23)	6859(2)	2160(1)	1890(1)	16(1)
C(24)	7347(2)	2844(1)	2346(1)	17(1)

C(25)	8653(2)	2963(1)	2737(1)	19(1)
C(27)	9758(2)	2776(1)	2342(1)	23(1)
C(28)	10978(2)	2923(1)	2711(1)	32(1)
C(29)	11105(2)	3243(1)	3479(1)	35(1)
C(30)	10016(2)	3417(1)	3881(1)	31(1)
C(31)	8795(2)	3283(1)	3512(1)	24(1)
S(1A)	12849(1)	5100(1)	1692(1)	22(1)
O(1A)	13231(2)	4203(1)	1675(1)	26(1)
C(33A)	14125(3)	5666(2)	1302(3)	53(1)
C(32A)	13102(5)	5424(3)	2701(2)	54(1)
S(1B)	12969(4)	4816(2)	2641(2)	61(1)
O(1B)	13522(8)	4223(5)	2041(5)	26(1)
C(33B)	11465(12)	5052(9)	2190(8)	59(4)
C(32B)	13586(19)	5813(12)	2582(14)	75(7)
S(1C)	14459(6)	5661(4)	627(4)	45(1)
O(1C)	13080(12)	5584(7)	741(8)	26(1)
C(32C)	15090(20)	4630(16)	501(14)	40(5)
C(33C)	14450(30)	5930(20)	-424(18)	70(10)

Table S2. Selected bond lengths [A] and angles [deg] for **1**.

N(1)-C(7)	1.341(2)	N(1)-N(2)	1.349(2)
N(2)-C(9)	1.352(2)	N(4)-C(24)	1.338(2)
N(4)-N(3)	1.349(2)	N(3)-C(22)	1.356(2)
C(6)-C(5)	1.398(2)	C(6)-C(1)	1.399(2)
C(6)-C(7)	1.478(2)	C(24)-C(23)	1.409(2)
C(24)-C(25)	1.475(2)	C(22)-C(23)	1.391(2)

C(22)-C(21)	1.475(2)	C(7)-C(8)	1.424(2)
C(1)-C(2)	1.382(2)	C(25)-C(27)	1.396(3)
C(25)-C(31)	1.396(2)	C(21)-C(20)	1.397(3)
C(21)-C(16)	1.400(2)	C(23)-C(8)	1.480(2)
C(8)-C(9)	1.379(2)	C(9)-C(10)	1.471(2)
C(20)-C(19)	1.387(3)	C(16)-C(17)	1.383(3)
C(10)-C(15)	1.384(3)	C(10)-C(11)	1.397(3)
C(27)-C(28)	1.388(3)	C(31)-C(30)	1.386(3)
C(18)-C(17)	1.382(3)	C(18)-C(19)	1.386(3)
C(5)-C(4)	1.389(3)	C(2)-C(3)	1.388(3)
C(3)-C(4)	1.385(3)	C(15)-C(14)	1.387(3)
C(30)-C(29)	1.385(3)	C(29)-C(28)	1.385(3)
C(14)-C(13)	1.378(3)	C(11)-C(12)	1.387(3)
C(13)-C(12)	1.382(3)	S(1A)-O(1A)	1.490(2)
S(1A)-C(33A)	1.768(3)	S(1A)-C(32A)	1.773(4)
S(1B)-O(1B)	1.526(9)	S(1B)-C(32B)	1.725(19)
S(1B)-C(33B)	1.726(12)	S(1C)-O(1C)	1.461(15)
S(1C)-C(32C)	1.79(3)	S(1C)-C(33C)	1.82(3)
S(1C)-C(32C)#1	2.04(2)	C(32C)-C(33C)#1	1.03(4)
C(32C)-S(1C)#1	2.04(2)	C(33C)-C(32C)#1	1.03(4)

C(7)-N(1)-N(2)	105.08(13)	N(1)-N(2)-C(9)	112.88(13)
C(24)-N(4)-N(3)	105.06(13)	N(4)-N(3)-C(22)	112.78(14)
C(5)-C(6)-C(1)	117.67(16)	C(5)-C(6)-C(7)	122.23(15)
C(1)-C(6)-C(7)	120.00(15)	N(4)-C(24)-C(23)	111.07(15)
N(4)-C(24)-C(25)	120.30(15)	C(23)-C(24)-C(25)	128.61(15)

N(3)-C(22)-C(23)	106.06(14)	N(3)-C(22)-C(21)	121.43(15)
C(23)-C(22)-C(21)	132.51(15)	N(1)-C(7)-C(8)	110.43(14)
N(1)-C(7)-C(6)	118.89(15)	C(8)-C(7)-C(6)	130.60(15)
C(2)-C(1)-C(6)	121.38(16)	C(27)-C(25)-C(31)	119.05(16)
C(27)-C(25)-C(24)	121.42(16)	C(31)-C(25)-C(24)	119.52(16)
C(20)-C(21)-C(16)	118.08(16)	C(20)-C(21)-C(22)	120.52(15)
C(16)-C(21)-C(22)	121.39(16)	C(22)-C(23)-C(24)	105.03(14)
C(22)-C(23)-C(8)	128.24(15)	C(24)-C(23)-C(8)	126.53(15)
C(9)-C(8)-C(7)	105.03(14)	C(9)-C(8)-C(23)	123.54(15)
C(7)-C(8)-C(23)	131.24(15)	N(2)-C(9)-C(8)	106.56(15)
N(2)-C(9)-C(10)	121.29(15)	C(8)-C(9)-C(10)	132.14(15)
C(19)-C(20)-C(21)	120.92(17)	C(17)-C(16)-C(21)	120.57(17)
C(15)-C(10)-C(11)	119.06(17)	C(15)-C(10)-C(9)	120.73(16)
C(11)-C(10)-C(9)	120.16(16)	C(28)-C(27)-C(25)	120.40(17)
C(30)-C(31)-C(25)	120.27(18)	C(17)-C(18)-C(19)	119.32(17)
C(4)-C(5)-C(6)	120.68(17)	C(1)-C(2)-C(3)	120.48(17)
C(18)-C(17)-C(16)	120.82(17)	C(4)-C(3)-C(2)	118.85(17)
C(10)-C(15)-C(14)	120.30(18)	C(18)-C(19)-C(20)	120.27(17)
C(3)-C(4)-C(5)	120.91(17)	C(29)-C(30)-C(31)	120.21(18)
C(30)-C(29)-C(28)	120.10(19)	C(29)-C(28)-C(27)	119.95(19)
C(13)-C(14)-C(15)	120.37(19)	C(12)-C(11)-C(10)	120.24(19)
C(14)-C(13)-C(12)	119.89(19)	C(13)-C(12)-C(11)	120.0(2)
O(1A)-S(1A)-C(33A)	106.27(15)	O(1A)-S(1A)-C(32A)	106.22(18)
C(33A)-S(1A)-C(32A)	98.0(2)	O(1B)-S(1B)-C(32B)	112.3(9)
O(1B)-S(1B)-C(33B)	102.6(6)	C(32B)-S(1B)-C(33B)	95.7(8)
O(1C)-S(1C)-C(32C)	107.7(9)	O(1C)-S(1C)-C(33C)	102.0(11)

C(32C)-S(1C)-C(33C)	94.6(14)	O(1C)-S(1C)-C(32C)#1	113.3(9)
C(32C)-S(1C)-C(32C)#1	64.5(12)	C(33C)-S(1C)-C(32C)#1	30.4(11)
C(33C)#1-C(32C)-S(1C)	173(3)	C(33C)#1-C(32C)-S(1C)#1	63(2)
S(1C)-C(32C)-S(1C)#1	115.5(12)	C(32C)#1-C(33C)-S(1C)	87(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,-y+1,-z

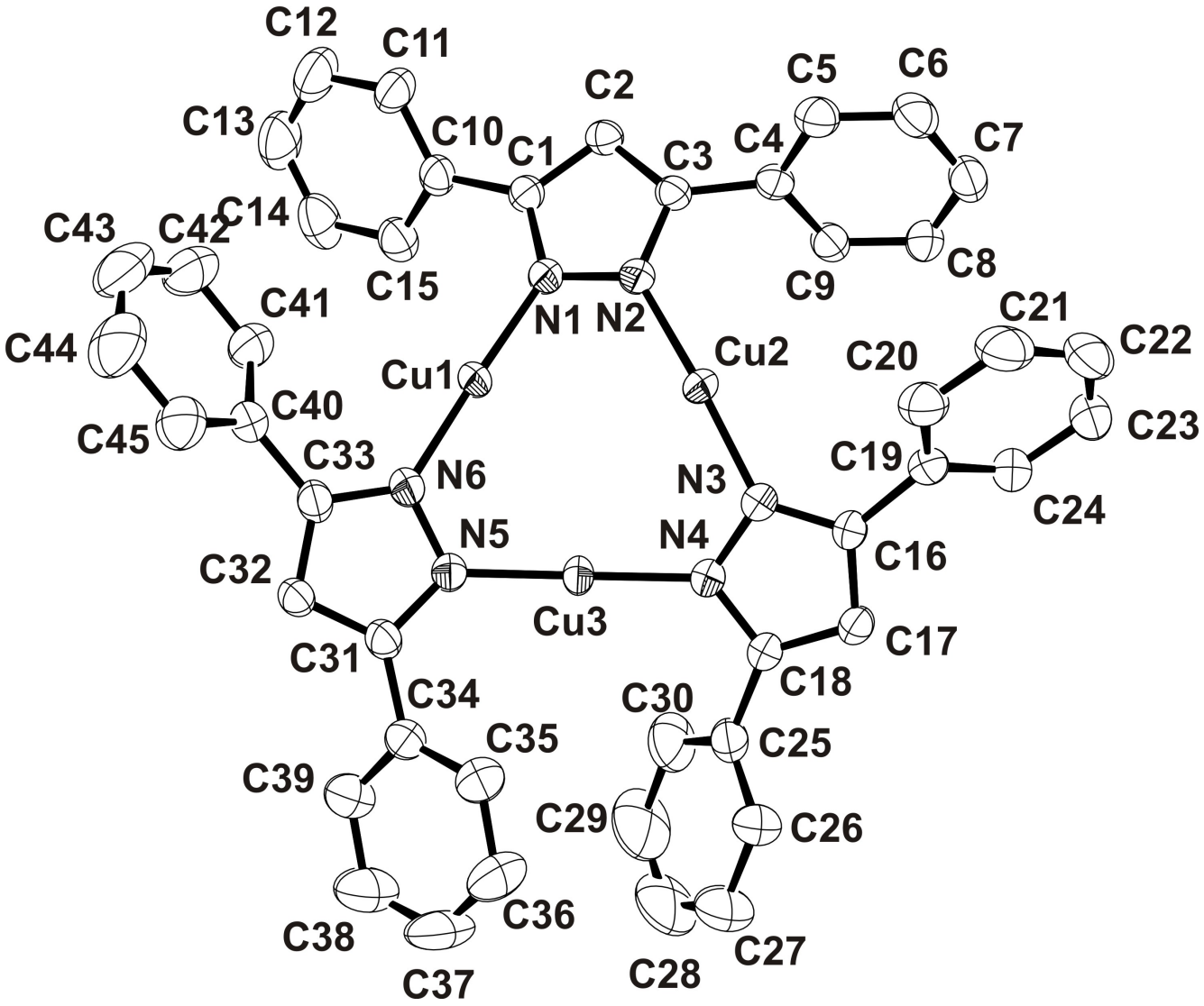

Fig. S2. View of the asymmetric unit of **CFA-2** showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **CFA-2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

ATOM	x	y	z	U(eq)
Cu(1)	766(1)	3804(1)	-215(1)	33(1)
Cu(2)	1285(1)	3237(1)	551(1)	32(1)
Cu(3)	1499(1)	4257(1)	388(1)	34(1)
N(1)	536(1)	3286(1)	-9(1)	32(1)
N(2)	791(1)	3028(1)	259(1)	33(1)
N(3)	1736(1)	3499(1)	873(1)	34(1)
N(4)	1753(1)	3944(1)	862(1)	35(1)
N(5)	1289(1)	4543(1)	-124(1)	37(1)
N(6)	1015(1)	4321(1)	-408(1)	37(1)
C(1)	162(1)	3074(1)	-89(1)	30(1)
C(2)	170(1)	2666(1)	125(1)	30(1)
C(3)	574(1)	2656(1)	346(1)	29(1)
C(4)	778(1)	2349(1)	669(1)	31(1)
C(5)	913(1)	1937(1)	545(1)	41(1)
C(6)	1133(1)	1681(1)	856(1)	47(1)
C(7)	1225(1)	1834(1)	1286(1)	45(1)
C(8)	1089(1)	2240(1)	1415(1)	41(1)
C(9)	865(1)	2498(1)	1111(1)	36(1)
C(10)	-196(1)	3282(1)	-341(1)	37(1)
C(11)	-447(1)	3048(1)	-653(1)	48(1)
C(12)	-797(1)	3245(1)	-865(1)	66(1)
C(13)	-901(1)	3670(1)	-772(1)	70(1)

C(14)	-660(1)	3903(1)	-469(1)	60(1)
C(15)	-307(1)	3711(1)	-251(1)	44(1)
C(16)	2015(1)	3362(1)	1197(1)	32(1)
C(17)	2219(1)	3719(1)	1395(1)	33(1)
C(18)	2041(1)	4080(1)	1176(1)	35(1)
C(19)	2084(1)	2901(1)	1309(1)	38(1)
C(20)	2154(1)	2593(1)	971(1)	49(1)
C(21)	2257(1)	2169(1)	1088(1)	62(1)
C(22)	2288(1)	2049(1)	1539(1)	65(1)
C23)	2210(1)	2349(1)	1878(1)	58(1)
C(24)	2109(1)	2770(1)	1763(1)	45(1)
C(25)	2121(1)	4544(1)	1247(1)	49(1)
C(26)	2546(1)	4698(1)	1292(1)	69(1)
C(27)	2619(2)	5139(1)	1367(2)	108(2)
C(28)	2271(2)	5421(1)	1395(2)	126(2)
C(29)	1863(2)	5273(1)	1350(2)	112(2)
C(30)	1782(1)	4832(1)	1275(1)	74(1)
C(31)	1404(1)	4915(1)	-336(1)	35(1)
C(32)	1204(1)	4934(1)	-762(1)	33(1)
C(33)	965(1)	4552(1)	-793(1)	35(1)
C(34)	1702(1)	5229(1)	-129(1)	42(1)
C(35)	2097(1)	5101(1)	54(1)	63(1)
C(36)	2375(1)	5410(1)	233(1)	92(1)
C(37)	2275(2)	5834(1)	221(2)	102(1)
C(38)	1883(1)	5969(1)	41(1)	82(1)
C(39)	1601(1)	5666(1)	-134(1)	57(1)

C(40)	702(1)	4391(1)	-1180(1)	40(1)
C(41)	296(1)	4215(1)	-1111(1)	56(1)
C(42)	54(1)	4058(1)	-1471(1)	79(1)
C(43)	220(1)	4083(1)	-1911(1)	88(1)
C(44)	615(1)	4263(1)	-1985(1)	83(1)
C(45)	862(1)	4419(1)	-1621(1)	58(1)

Table S4. Selected bond lengths [A] and angles [deg] for **CFA-2**.

Cu(1)-N(1)	1.8487(18)	C(16)-C(17)	1.397(3)
Cu(1)-N(6)	1.8565(19)	C(16)-C(19)	1.474(3)
Cu(2)-N(3)	1.8626(18)	C(17)-C(18)	1.395(3)
Cu(2)-N(2)	1.8631(18)	C(17)-C(32)#2	1.469(3)
Cu(3)-N(5)	1.8593(17)	C(18)-C(25)	1.468(3)
Cu(3)-N(4)	1.8628(17)	C(19)-C(20)	1.389(3)
N(1)-C(1)	1.347(3)	C(19)-C(24)	1.391(3)
N(1)-N(2)	1.366(2)	C(20)-C(21)	1.389(4)
N(2)-C(3)	1.351(3)	C(21)-C(22)	1.376(5)
N(3)-C(16)	1.351(3)	C(22)-C(23)	1.375(5)
N(3)-N(4)	1.373(3)	C(23)-C(24)	1.378(4)
N(4)-C(18)	1.347(3)	C(25)-C(30)	1.374(4)
N(5)-C(31)	1.350(3)	C(25)-C(26)	1.402(4)
N(5)-N(6)	1.368(3)	C(26)-C(27)	1.397(5)
N(6)-C(33)	1.345(3)	C(27)-C(28)	1.384(8)
C(1)-C(2)	1.405(3)	C(28)-C(29)	1.344(8)
C(1)-C(10)	1.475(3)	C(29)-C(30)	1.400(5)
C(2)-C(3)	1.406(3)	C(31)-C(32)	1.394(3)
C(2)-C(2)#1	1.466(4)	C(31)-C(34)	1.468(3)

C(3)-C(4)	1.478(3)	C(32)-C(33)	1.391(3)
C(4)-C(5)	1.388(3)	C(32)-C(17)#3	1.469(3)
C(4)-C(9)	1.398(3)	C(33)-C(40)	1.482(3)
C(5)-C(6)	1.383(3)	C(34)-C(39)	1.383(4)
C(6)-C(7)	1.378(4)	C(34)-C(35)	1.386(4)
C(7)-C(8)	1.374(4)	C(35)-C(36)	1.385(5)
C(8)-C(9)	1.379(3)	C(11)-C(12)	1.387(4)
C(10)-C(15)	1.391(3)	C(12)-C(13)	1.376(5)
C(10)-C(11)	1.396(3)	C(13)-C(14)	1.364(5)
C(14)-C(15)	1.393(4)	C(36)-C(37)	1.344(6)
C(37)-C(38)	1.383(6)	C(41)-C(42)	1.380(4)
C(38)-C(39)	1.375(4)	C(42)-C(43)	1.390(5)
C(40)-C(41)	1.380(4)	C(43)-C(44)	1.357(5)
C(40)-C(45)	1.384(4)	C(44)-C(45)	1.395(4)

N(1)-Cu(1)-N(6)	177.78(8)	C(13)-C(14)-C(15)	120.0(3)
N(3)-Cu(2)-N(2)	173.04(8)	C(10)-C(15)-C(14)	120.8(2)
N(5)-Cu(3)-N(4)	174.02(8)	N(3)-C(16)-C(17)	109.45(17)
C(1)-N(1)-N(2)	108.02(15)	N(3)-C(16)-C(19)	123.37(18)
C(1)-N(1)-Cu(1)	133.64(13)	C(17)-C(16)-C(19)	127.18(18)
N(2)-N(1)-Cu(1)	118.15(12)	C(16)-C(17)-C(18)	105.09(17)
C(3)-N(2)-N(1)	108.63(15)	C(16)-C(17)-C(32)#2	125.96(18)
C(3)-N(2)-Cu(2)	127.73(14)	C(18)-C(17)-C(32)#2	128.83(19)
N(1)-N(2)-Cu(2)	122.10(12)	N(4)-C(18)-C(17)	109.04(18)
C(16)-N(3)-N(4)	107.70(16)	N(4)-C(18)-C(25)	120.71(18)
C(16)-N(3)-Cu(2)	134.13(14)	C(17)-C(18)-C(25)	130.25(19)

N(4)-N(3)-Cu(2)	116.72(12)	C(20)-C(19)-C(24)	118.4(2)
C(18)-N(4)-N(3)	108.72(16)	C(20)-C(19)-C(16)	121.6(2)
C(18)-N(4)-Cu(3)	128.71(14)	C(24)-C(19)-C(16)	119.9(2)
N(3)-N(4)-Cu(3)	121.24(13)	C(21)-C(20)-C(19)	120.2(3)
C(31)-N(5)-N(6)	107.98(16)	C(22)-C(21)-C(20)	120.3(3)
C(31)-N(5)-Cu(3)	132.95(15)	C(23)-C(22)-C(21)	120.1(2)
N(6)-N(5)-Cu(3)	117.97(13)	C(22)-C(23)-C(24)	119.7(3)
C(33)-N(6)-N(5)	108.29(16)	C(23)-C(24)-C(19)	121.3(3)
C(33)-N(6)-Cu(1)	131.66(15)	C(30)-C(25)-C(26)	119.2(3)
N(5)-N(6)-Cu(1)	119.99(13)	C(30)-C(25)-C(18)	120.8(3)
N(1)-C(1)-C(2)	110.00(17)	C(26)-C(25)-C(18)	119.9(2)
N(1)-C(1)-C(10)	121.18(17)	C(27)-C(26)-C(25)	119.7(4)
C(2)-C(1)-C(10)	128.67(18)	C(28)-C(27)-C(26)	119.7(4)
C(1)-C(2)-C(3)	103.97(17)	C(29)-C(28)-C(27)	120.5(3)
C(1)-C(2)-C(2)#1	127.9(2)	C(28)-C(29)-C(30)	120.8(4)
C(3)-C(2)-C(2)#1	128.1(2)	C(25)-C(30)-C(29)	120.0(4)
N(2)-C(3)-C(2)	109.37(17)	N(5)-C(31)-C(32)	109.34(18)
N(2)-C(3)-C(4)	116.96(17)	N(5)-C(31)-C(34)	122.44(18)
C(2)-C(3)-C(4)	133.41(18)	C(32)-C(31)-C(34)	128.21(18)
C(5)-C(4)-C(9)	119.07(19)	C(33)-C(32)-C(31)	104.85(17)
C(5)-C(4)-C(3)	123.01(18)	C(33)-C(32)-C(17)#3	126.07(19)
C(9)-C(4)-C(3)	117.76(18)	C(31)-C(32)-C(17)#3	129.05(19)
C(6)-C(5)-C(4)	119.9(2)	N(6)-C(33)-C(32)	109.54(18)
C(7)-C(6)-C(5)	120.6(2)	N(6)-C(33)-C(40)	121.77(19)
C(8)-C(7)-C(6)	120.1(2)	C(32)-C(33)-C(40)	128.66(18)
C(7)-C(8)-C(9)	120.0(2)	C(39)-C(34)-C(35)	118.7(2)

C(8)-C(9)-C(4)	120.4(2)	C(39)-C(34)-C(31)	119.8(2)
C(15)-C(10)-C(11)	118.5(2)	C(35)-C(34)-C(31)	121.4(2)
C(15)-C(10)-C(1)	120.2(2)	C(36)-C(35)-C(34)	119.7(3)
C(11)-C(10)-C(1)	121.2(2)	C(37)-C(36)-C(35)	121.0(3)
C(12)-C(11)-C(10)	119.9(3)	C(36)-C(37)-C(38)	120.3(3)
C(13)-C(12)-C(11)	120.7(3)	C(14)-C(13)-C(12)	120.2(3)
C(39)-C(38)-C(37)	119.4(3)	C(42)-C(41)-C(40)	121.1(3)
C(38)-C(39)-C(34)	120.9(3)	C(41)-C(42)-C(43)	119.3(3)
C(41)-C(40)-C(45)	119.0(2)	C(44)-C(43)-C(42)	120.2(3)
C(41)-C(40)-C(33)	121.1(2)	C(43)-C(44)-C(45)	120.5(3)
C(45)-C(40)-C(33)	119.9(2)	C(40)-C(45)-C(44)	119.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+0,-y+1/2,z+0; #2 -y+3/4,x+1/4,z+1/4; #3 y-1/4,-x+3/4,z-1/4

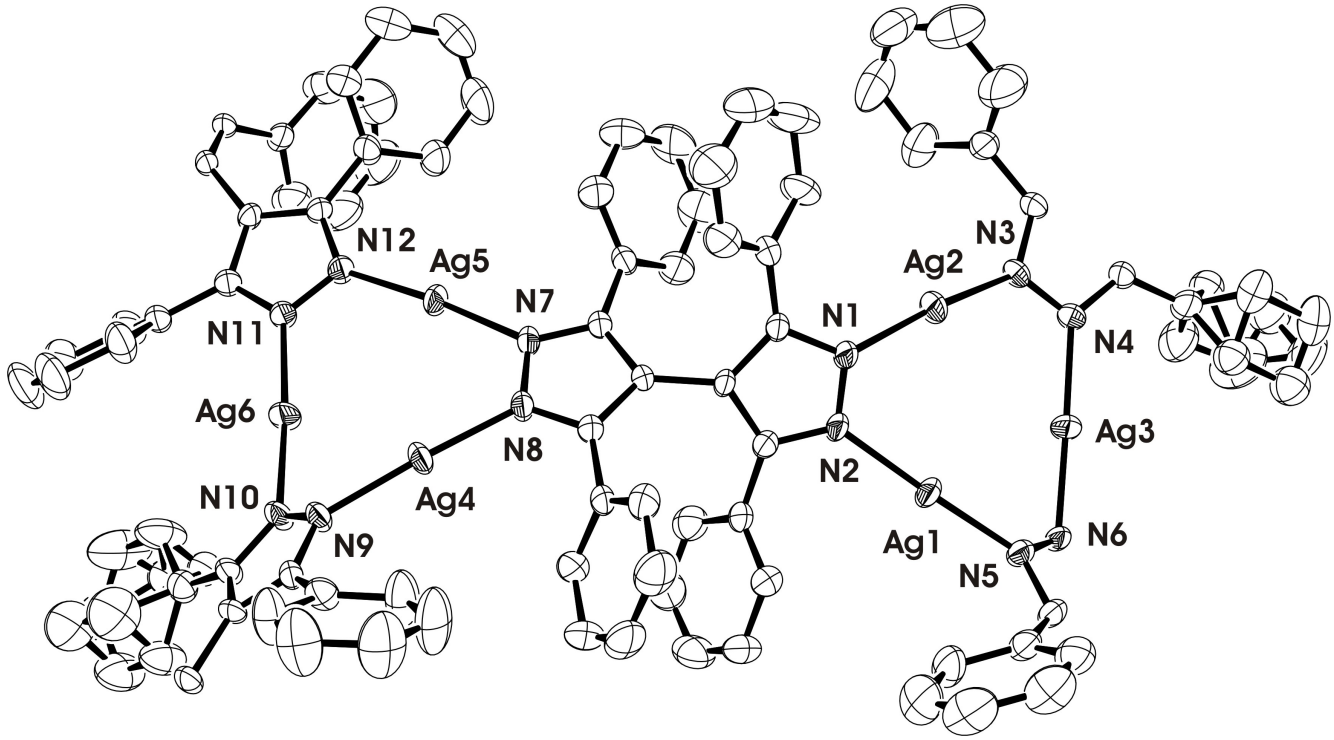

Fig. S3. View of the asymmetric unit of **CFA-3** showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **CFA-3.**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

ATOM	x	y	z	U(eq)
Ag(1)	7649(1)	1905(1)	9973(1)	37(1)
Ag(2)	6599(1)	2853(1)	9482(1)	38(1)
Ag(3)	8702(1)	2850(1)	10384(1)	40(1)
Ag(4)	3064(1)	664(1)	6103(1)	42(1)
Ag(5)	2714(1)	1532(1)	4914(1)	42(1)
Ag(6)	2196(1)	664(1)	3723(1)	40(1)
N(1)	6033(3)	2311(1)	8930(3)	30(1)
N(2)	6389(3)	1932(1)	9156(3)	31(1)
N(3)	7225(3)	3399(1)	9934(3)	35(1)
N(4)	8075(3)	3404(1)	9982(3)	35(1)
N(5)	8913(3)	1936(2)	10771(3)	34(1)
N(6)	9295(3)	2313(2)	10937(3)	35(1)
N(7)	3518(3)	1514(2)	6171(3)	37(1)
N(8)	3407(4)	1222(1)	6731(3)	38(1)

N(9)	2787(4)	139(1)	5344(3)	37(1)
N(10)	2331(3)	145(1)	4488(3)	36(1)
N(11)	1974(3)	1233(1)	3090(3)	33(1)
N(12)	1905(3)	1526(1)	3668(3)	34(1)
C(1)	5281(4)	2265(2)	8327(4)	29(1)
C(2)	5138(4)	1848(2)	8133(4)	28(1)
C(3)	5859(4)	1654(2)	8672(4)	29(1)
C(4)	6067(4)	1212(2)	8743(4)	37(2)
C(5)	6311(5)	1018(2)	9528(5)	58(2)
C(6)	6453(6)	600(3)	9578(7)	77(3)
C(7)	6397(7)	377(2)	8843(7)	82(3)
C(8)	6170(6)	571(2)	8061(6)	70(3)
C(9)	6003(5)	986(2)	8007(5)	48(2)
C(10)	4734(4)	2623(2)	7967(4)	31(2)
C(11)	3896(5)	2647(2)	7987(5)	47(2)
C(12)	3405(5)	2986(3)	7650(5)	61(2)
C(13)	3737(6)	3294(2)	7286(6)	64(3)
C(14)	4557(6)	3274(2)	7263(5)	60(2)
C(15)	5071(5)	2942(2)	7600(4)	42(2)
C(16)	4421(4)	1657(2)	7464(4)	28(1)
C(17)	4121(4)	1775(2)	6598(4)	32(1)
C(18)	3947(4)	1308(2)	7522(4)	32(2)
C(19)	3926(4)	1074(2)	8289(4)	38(2)
C(20)	3879(5)	1283(2)	9010(5)	54(2)
C(21)	3832(7)	1075(3)	9732(6)	80(3)
C(22)	3838(8)	660(3)	9746(6)	91(4)
C(23)	3905(8)	447(3)	9039(7)	99(4)
C(24)	3957(6)	653(2)	8313(5)	63(2)
C(25)	4376(4)	2119(2)	6156(4)	36(2)
C(26)	3785(5)	2403(2)	5708(4)	43(2)
C(27)	4040(6)	2731(2)	5300(5)	57(2)
C(28)	4862(7)	2774(2)	5328(5)	62(2)
C(29)	5482(6)	2500(3)	5778(5)	60(2)
C(30)	5235(5)	2170(2)	6183(5)	48(2)
C(31)	9464(4)	1663(2)	11264(4)	30(1)
C(32)	10203(4)	1858(2)	11740(4)	29(1)
C(33)	10069(4)	2271(2)	11521(4)	32(2)

C(34)	9223(4)	1228(2)	11279(4)	37(2)
C(35)	9343(5)	1029(2)	12068(5)	52(2)
C(36)	9119(7)	622(3)	12091(7)	77(3)
C(37)	8778(8)	415(3)	11334(8)	93(4)
C(38)	8661(7)	600(3)	10566(7)	85(3)
C(39)	8864(6)	1008(2)	10532(5)	60(2)
C(40)	10946(4)	1672(2)	12395(4)	30(1)
C(41)	11399(4)	1319(2)	12319(4)	33(2)
C(42)	11385(4)	1087(2)	11544(4)	38(2)
C(43)	11251(8)	671(2)	11473(6)	81(3)
C(44)	11270(10)	465(3)	10724(8)	117(5)
C(45)	11411(9)	675(4)	10051(7)	103(4)
C(46)	11476(8)	1082(3)	10098(6)	86(3)
C(47)	11473(6)	1283(3)	10844(5)	66(2)
C(48)	10619(4)	2633(2)	11834(4)	39(2)
C(49)	10315(5)	2953(2)	12199(5)	56(2)
C(50)	10834(7)	3293(2)	12512(7)	81(3)
C(51)	11659(6)	3311(3)	12439(7)	82(3)
C(52)	11959(5)	2986(3)	12091(6)	72(3)
C(53)	11451(5)	2649(2)	11779(5)	53(2)
C(54)	8334(4)	3795(2)	10022(4)	30(1)
C(55)	7652(4)	4051(2)	10022(4)	31(1)
C(56)	6956(4)	3790(2)	9968(4)	32(2)
C(57)	9219(4)	3905(2)	10028(4)	39(2)
C(60)	10862(6)	4125(3)	10023(6)	78(3)
C(63)	7614(4)	4499(2)	10042(4)	31(2)
C(64)	6078(4)	3894(2)	9939(4)	34(2)
C(65)	5380(5)	3721(3)	9353(6)	64(2)
C(66)	4559(5)	3838(3)	9311(7)	81(3)
C(67)	4437(6)	4144(3)	9827(7)	81(3)
C(68)	5111(6)	4323(3)	10399(7)	76(3)
C(69)	5940(5)	4201(3)	10462(5)	59(2)
C(70)	1284(4)	1791(2)	3252(4)	34(2)
C(71)	1036(5)	2139(2)	3701(4)	38(2)
C(72)	194(5)	2190(2)	3700(5)	52(2)
C(73)	-47(6)	2520(3)	4100(6)	66(2)
C(74)	560(7)	2804(3)	4532(6)	73(3)

C(75)	1392(7)	2760(3)	4542(6)	73(3)
C(76)	1644(5)	2426(2)	4130(5)	56(2)
C(77)	2825(4)	-248(2)	5630(4)	29(1)
C(78)	3314(5)	-365(2)	6518(4)	43(2)
C(79)	4169(6)	-302(3)	6815(6)	85(3)
C(80)	4626(8)	-435(4)	7666(8)	117(5)
C(81)	4224(10)	-617(4)	8165(7)	104(5)
C(82)	3401(12)	-673(5)	7881(8)	140(6)
C(83)	2925(8)	-549(4)	7047(7)	109(5)
C(84)	2087(4)	-241(2)	4250(4)	31(1)
C(85)	1601(5)	-344(2)	3350(5)	47(2)
C(88)	709(9)	-571(4)	1683(8)	104(4)
C(86A)	750(8)	-474(4)	3183(8)	79(4)
C(87A)	318(10)	-573(5)	2321(10)	103(6)
C(89A)	1552(13)	-451(6)	1911(8)	110(6)
C(90A)	2003(8)	-328(4)	2743(7)	70(4)
C(86B)	920(19)	-146(10)	2800(20)	48(9)
C(87B)	480(20)	-236(12)	1960(20)	59(11)
C(89B)	1370(30)	-788(15)	2020(30)	75(13)
C(90B)	1870(20)	-671(11)	2870(20)	47(9)
C(58A)	9359(6)	4268(3)	9631(7)	60(3)
C(59A)	10183(7)	4385(3)	9645(8)	75(4)
C(61A)	10732(7)	3776(4)	10376(11)	100(6)
C(62A)	9925(6)	3663(3)	10372(8)	72(4)
C(58B)	9580(50)	4240(20)	10470(40)	100(30)
C(59B)	10410(50)	4350(20)	10520(40)	90(20)
C(61B)	10470(40)	3747(16)	9720(30)	45(14)
C(62B)	9640(30)	3677(15)	9690(30)	43(14)

Table S6. Selected bond lengths [A] and angles [deg] for **CFA-3**.

Ag(1)-N(5)	2.087(5)	C(34)-C(35)	1.401(10)
Ag(1)-N(2)	2.093(5)	C(35)-C(36)	1.385(11)
Ag(2)-N(1)	2.079(5)	C(36)-C(37)	1.369(14)
Ag(2)-N(3)	2.080(5)	C(37)-C(38)	1.349(14)
Ag(2)-Ag(3)	3.3087(7)	C(38)-C(39)	1.383(11)
Ag(3)-N(6)	2.079(5)	C(40)-C(70)#2	1.393(8)

Ag(3)-N(4)	2.091(5)	C(40)-C(41)	1.397(8)
Ag(4)-N(9)	2.085(5)	C(41)-N(11)#2	1.354(7)
Ag(4)-N(8)	2.089(5)	C(41)-C(42)	1.465(9)
Ag(5)-N(12)	2.062(5)	C(42)-C(47)	1.351(10)
Ag(5)-N(7)	2.075(5)	C(42)-C(43)	1.380(10)
Ag(6)-N(10)	2.080(5)	C(43)-C(44)	1.400(13)
Ag(6)-N(11)	2.106(5)	C(44)-C(45)	1.367(16)
N(1)-C(1)	1.332(7)	C(45)-C(46)	1.337(14)
N(1)-N(2)	1.373(7)	C(46)-C(47)	1.382(12)
N(2)-C(3)	1.339(7)	C(48)-C(49)	1.371(10)
N(3)-C(56)	1.361(7)	C(48)-C(53)	1.390(10)
N(3)-N(4)	1.369(7)	C(49)-C(50)	1.401(11)
N(4)-C(54)	1.343(7)	C(50)-C(51)	1.389(14)
N(5)-C(31)	1.350(7)	C(51)-C(52)	1.365(13)
N(5)-N(6)	1.374(7)	C(52)-C(53)	1.383(11)
N(6)-C(33)	1.342(7)	C(54)-C(55)	1.395(8)
N(7)-C(17)	1.333(7)	C(54)-C(57)	1.487(9)
N(7)-N(8)	1.368(7)	C(55)-C(56)	1.403(9)
N(8)-C(18)	1.354(7)	C(55)-C(63)	1.470(8)
N(9)-C(77)	1.346(7)	C(56)-C(64)	1.462(9)
N(9)-N(10)	1.368(7)	C(57)-C(62B)	1.25(5)
N(10)-C(84)	1.347(7)	C(57)-C(58B)	1.34(9)
N(11)-C(41)#1	1.354(7)	C(57)-C(62A)	1.375(11)
N(11)-N(12)	1.373(7)	C(57)-C(58A)	1.403(11)
N(12)-C(70)	1.353(7)	C(60)-C(61A)	1.325(15)
C(1)-C(2)	1.405(8)	C(60)-C(59A)	1.386(14)
C(1)-C(10)	1.486(8)	C(60)-C(61B)	1.41(5)
C(2)-C(3)	1.394(8)	C(60)-C(59B)	1.44(8)
C(2)-C(16)	1.479(7)	C(63)-C(77)#3	1.388(8)
C(3)-C(4)	1.483(8)	C(63)-C(84)#3	1.397(8)
C(4)-C(5)	1.373(10)	C(64)-C(65)	1.372(9)
C(4)-C(9)	1.385(10)	C(64)-C(69)	1.378(10)
C(5)-C(6)	1.387(11)	C(65)-C(66)	1.376(11)
C(6)-C(7)	1.380(14)	C(66)-C(67)	1.360(13)
C(7)-C(8)	1.370(13)	C(67)-C(68)	1.345(12)
C(8)-C(9)	1.382(10)	C(68)-C(69)	1.387(12)
C(10)-C(11)	1.383(10)	C(70)-C(40)#1	1.393(8)

C(10)-C(15)	1.394(9)	C(70)-C(71)	1.476(9)
C(11)-C(12)	1.383(10)	C(71)-C(72)	1.385(11)
C(12)-C(13)	1.362(12)	C(71)-C(76)	1.392(10)
C(13)-C(14)	1.353(12)	C(72)-C(73)	1.379(11)
C(14)-C(15)	1.385(10)	C(73)-C(74)	1.388(13)
C(16)-C(18)	1.399(8)	C(74)-C(75)	1.361(14)
C(16)-C(17)	1.401(8)	C(75)-C(76)	1.408(11)
C(17)-C(25)	1.461(9)	C(77)-C(63)#4	1.388(8)
C(18)-C(19)	1.472(9)	C(77)-C(78)	1.477(9)
C(19)-C(20)	1.381(10)	C(78)-C(79)	1.351(11)
C(19)-C(24)	1.382(9)	C(78)-C(83)	1.353(12)
C(20)-C(21)	1.379(11)	C(79)-C(80)	1.431(14)
C(21)-C(22)	1.361(13)	C(80)-C(81)	1.328(18)
C(22)-C(23)	1.377(15)	C(81)-C(82)	1.298(19)
C(23)-C(24)	1.384(12)	C(82)-C(83)	1.408(15)
C(25)-C(26)	1.380(9)	C(84)-C(63)#4	1.397(8)
C(25)-C(30)	1.401(10)	C(84)-C(85)	1.480(9)
C(26)-C(27)	1.392(10)	C(85)-C(90A)	1.340(14)
C(27)-C(28)	1.338(12)	C(85)-C(86B)	1.36(3)
C(28)-C(29)	1.387(12)	C(85)-C(86A)	1.401(14)
C(29)-C(30)	1.387(11)	C(85)-C(90B)	1.47(4)
C(31)-C(32)	1.381(8)	C(88)-C(89B)	1.27(5)
C(31)-C(34)	1.480(8)	C(88)-C(87B)	1.28(4)
C(32)-C(33)	1.397(8)	C(88)-C(87A)	1.37(2)
C(32)-C(40)	1.486(8)	C(88)-C(89A)	1.37(2)
C(33)-C(48)	1.484(8)	C(86A)-C(87A)	1.406(18)
C(34)-C(39)	1.383(9)	C(89A)-C(90A)	1.394(17)
C(86B)-C(87B)	1.38(5)	C(61A)-C(62A)	1.368(14)
C(89B)-C(90B)	1.44(6)	C(58B)-C(59B)	1.38(10)
C(58A)-C(59A)	1.394(14)	C(61B)-C(62B)	1.36(7)

N(5)-Ag(1)-N(2)	174.66(19)	C(31)-N(5)-Ag(1)	134.2(4)
N(1)-Ag(2)-N(3)	174.1(2)	N(6)-N(5)-Ag(1)	118.3(3)
N(1)-Ag(2)-Ag(3)	117.20(14)	C(33)-N(6)-N(5)	108.9(5)
N(3)-Ag(2)-Ag(3)	60.65(14)	C(33)-N(6)-Ag(3)	127.8(4)
N(6)-Ag(3)-N(4)	172.5(2)	N(5)-N(6)-Ag(3)	123.3(3)
N(6)-Ag(3)-Ag(2)	118.90(14)	C(17)-N(7)-N(8)	109.0(5)

N(4)-Ag(3)-Ag(2)	60.78(14)	C(17)-N(7)-Ag(5)	130.3(4)
N(9)-Ag(4)-N(8)	172.1(2)	N(8)-N(7)-Ag(5)	120.4(4)
N(12)-Ag(5)-N(7)	177.66(19)	C(18)-N(8)-N(7)	108.1(5)
N(10)-Ag(6)-N(11)	170.9(2)	C(18)-N(8)-Ag(4)	130.4(4)
C(1)-N(1)-N(2)	108.6(4)	N(7)-N(8)-Ag(4)	110.8(4)
C(1)-N(1)-Ag(2)	127.4(4)	C(77)-N(9)-N(10)	108.6(5)
N(2)-N(1)-Ag(2)	124.0(3)	C(77)-N(9)-Ag(4)	126.3(4)
C(3)-N(2)-N(1)	108.0(4)	N(10)-N(9)-Ag(4)	123.2(4)
C(3)-N(2)-Ag(1)	133.3(4)	C(84)-N(10)-N(9)	107.8(5)
N(1)-N(2)-Ag(1)	117.8(3)	C(84)-N(10)-Ag(6)	128.7(4)
C(56)-N(3)-N(4)	108.6(5)	N(9)-N(10)-Ag(6)	123.2(4)
C(56)-N(3)-Ag(2)	133.8(4)	C(41)#1-N(11)-N(12)	108.1(5)
N(4)-N(3)-Ag(2)	114.6(4)	C(41)#1-N(11)-Ag(6)	127.5(4)
C(54)-N(4)-N(3)	108.4(5)	N(12)-N(11)-Ag(6)	108.8(4)
C(54)-N(4)-Ag(3)	134.0(4)	C(70)-N(12)-N(11)	108.0(5)
N(3)-N(4)-Ag(3)	113.5(4)	C(70)-N(12)-Ag(5)	130.5(4)
C(31)-N(5)-N(6)	107.1(5)	N(11)-N(12)-Ag(5)	121.3(4)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z-1; #2 x+1,y,z+1; #3 -x+1,y+1/2,-z+3/2; #4 -x+1,y-1/2,-z+3/2

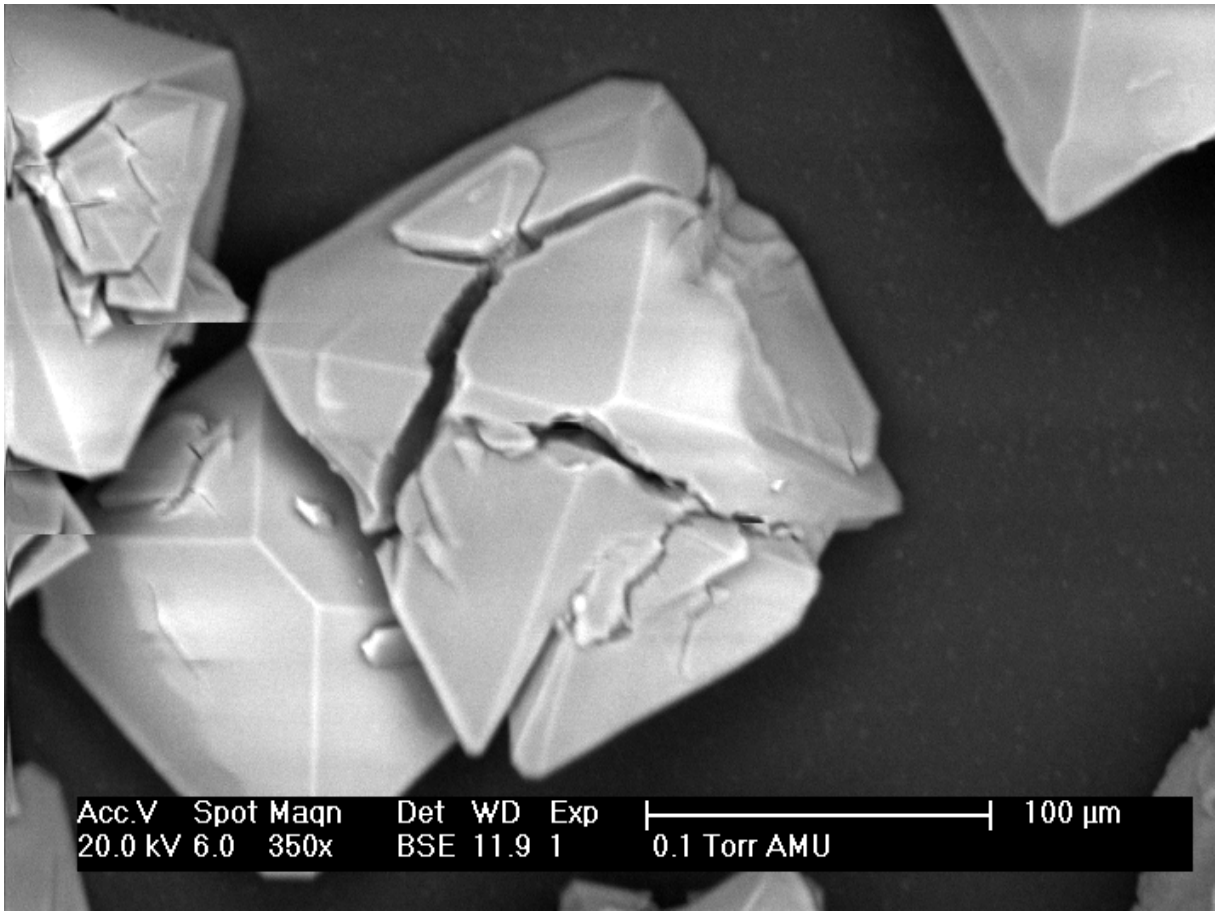

Fig. S4. Single crystal of **CFA-2** after solvent removal.

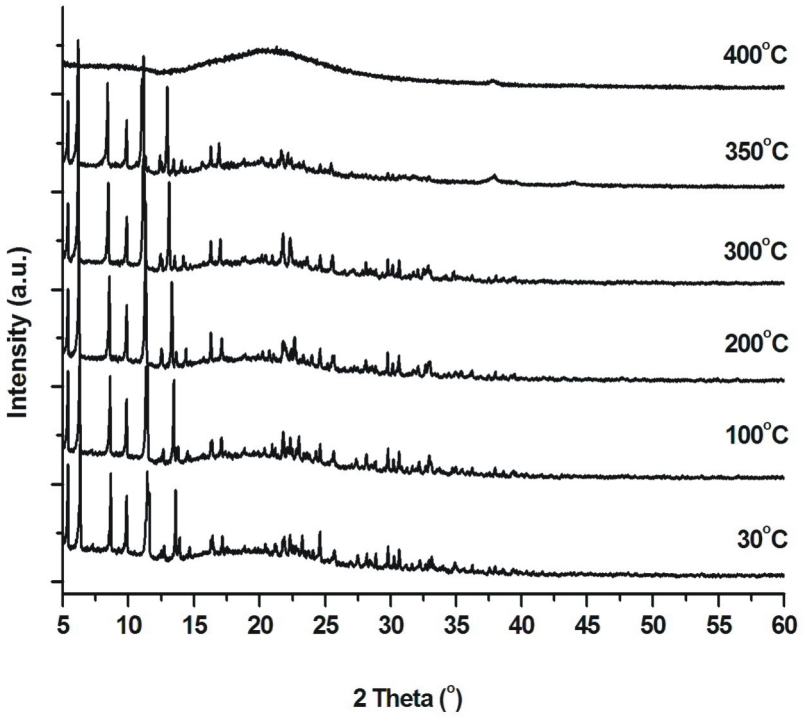

Fig. S5. VTXRPD plots of **CFA-3** under air.

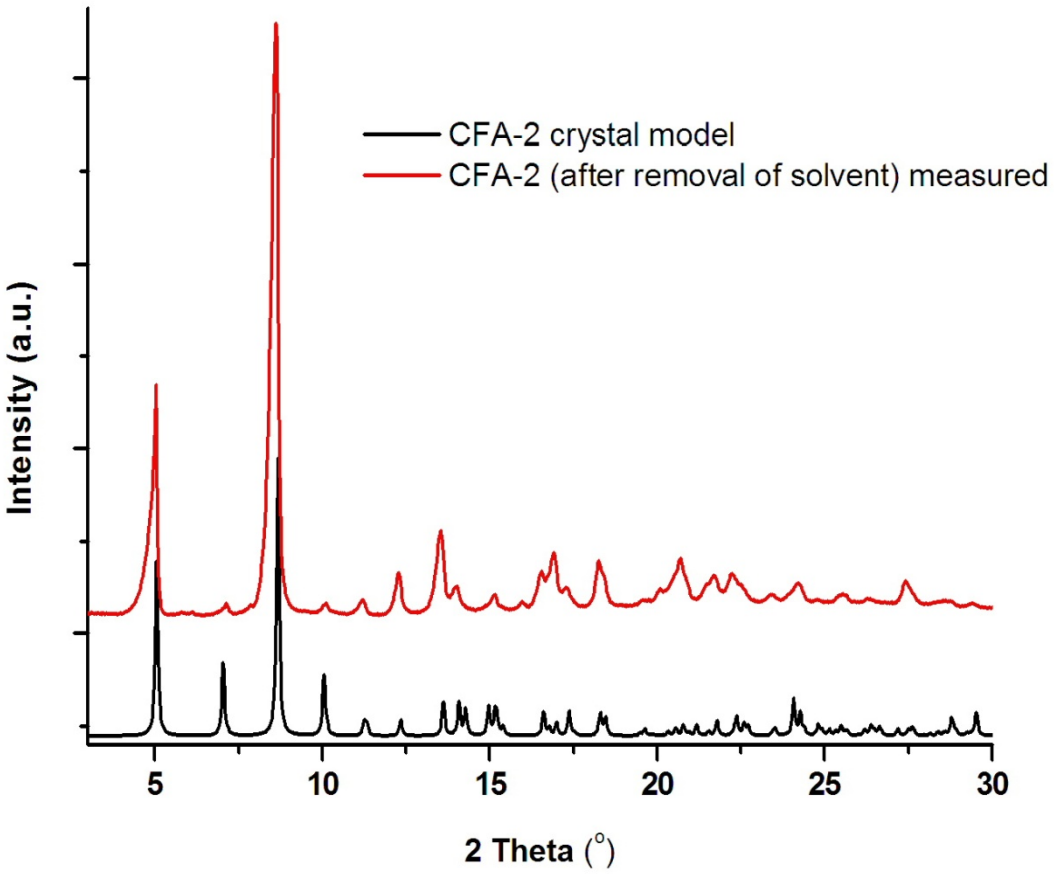

Fig. S6. Comparison of XRPD patterns for **CFA-2** model and **CFA-2** sample after removal of the solvent.

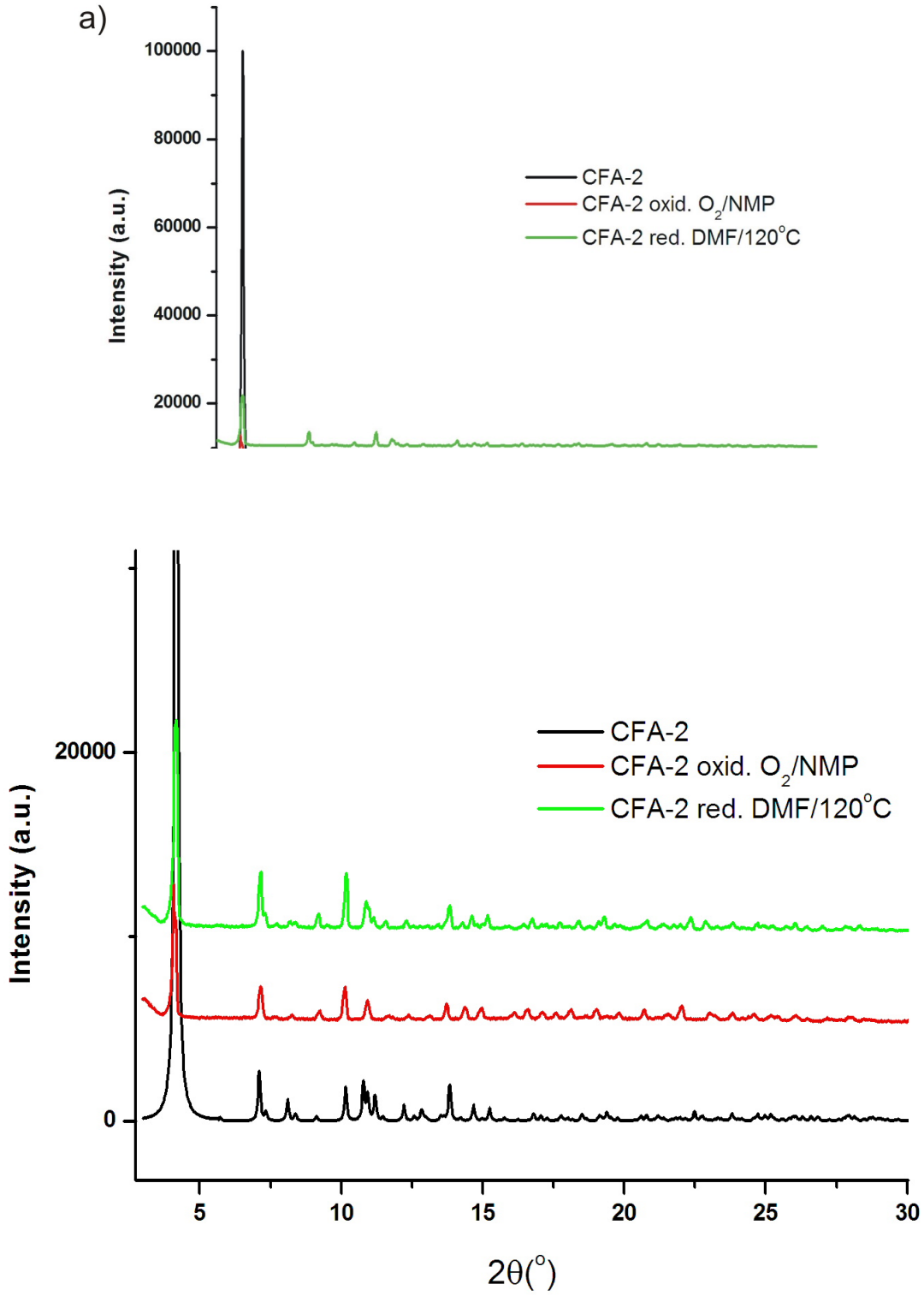

Fig. S7. XRPD patterns of **CFA-2**: black line – calculated pattern, red – **CFA-2** oxidized by oxygen in NMP, green – reduced by heating in DMF at 120 °C during 3-4 hours..

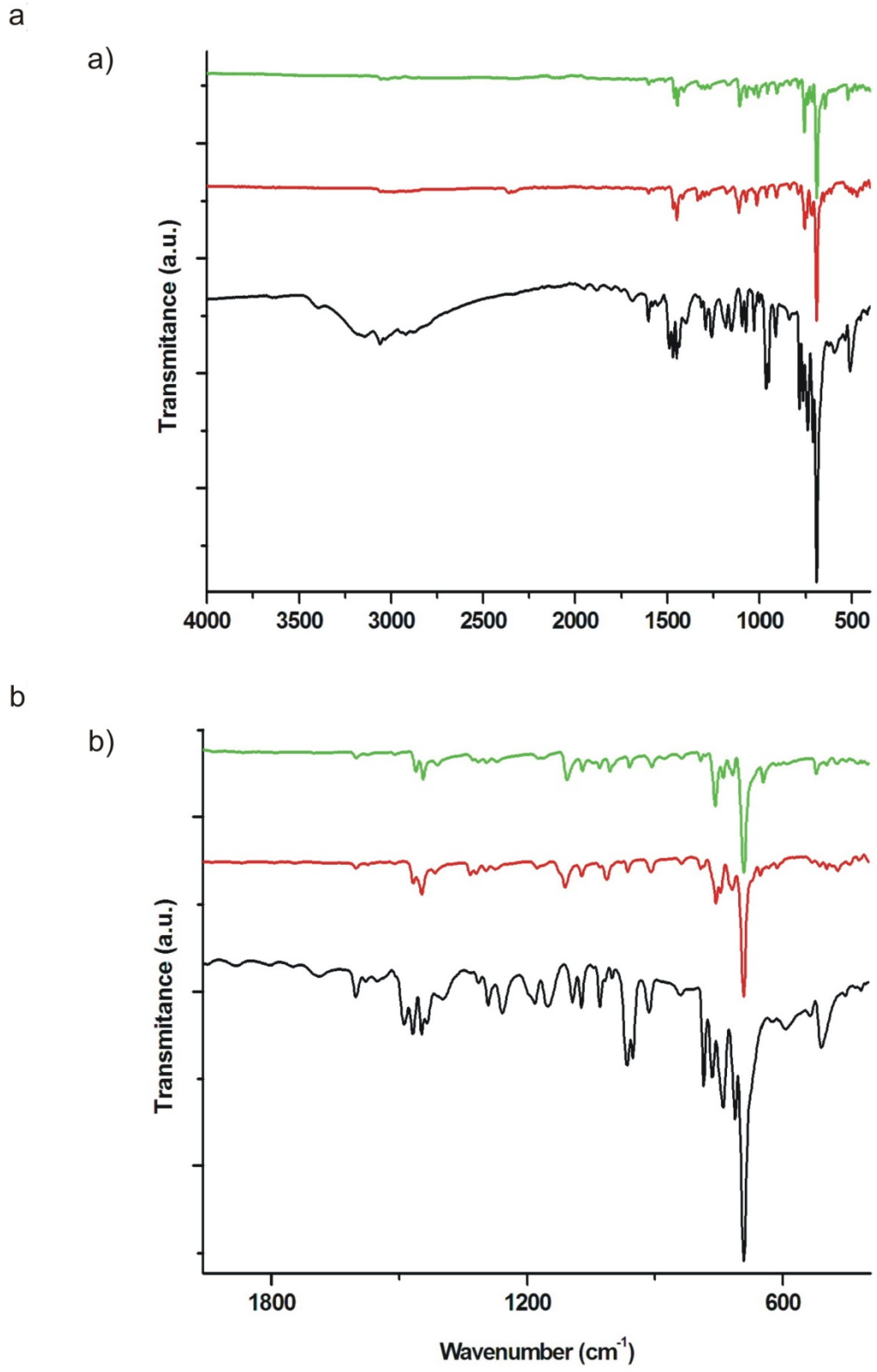

Fig. S8. IR spectra for **1** (black), **2** (red) and **3** (green).

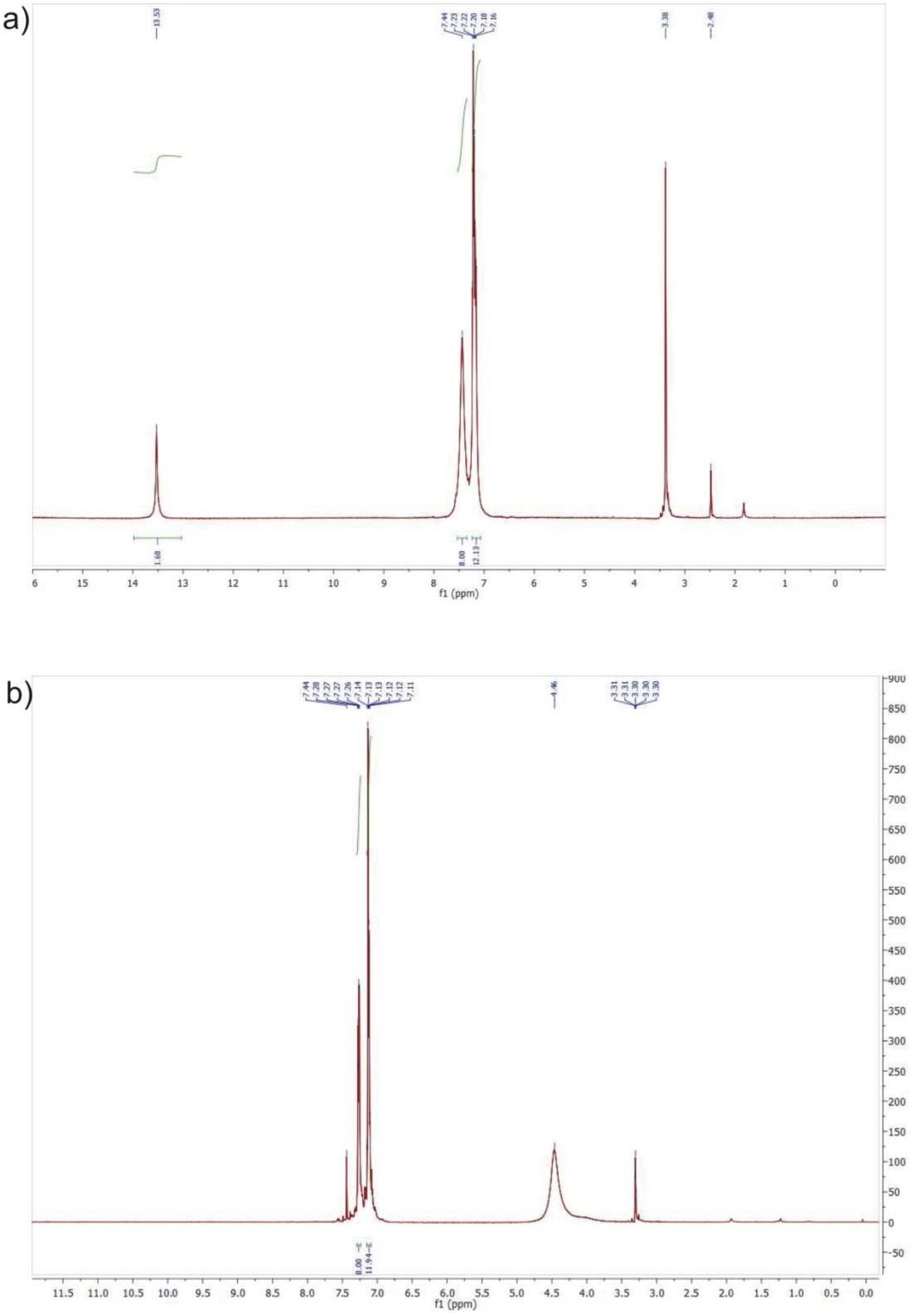

Fig. S9. ^{1}H NMR spectra DMSO–d_6 (**a**) and $CDCl_3$/MeOH–d_4 4:1 (**b**) for **1**.

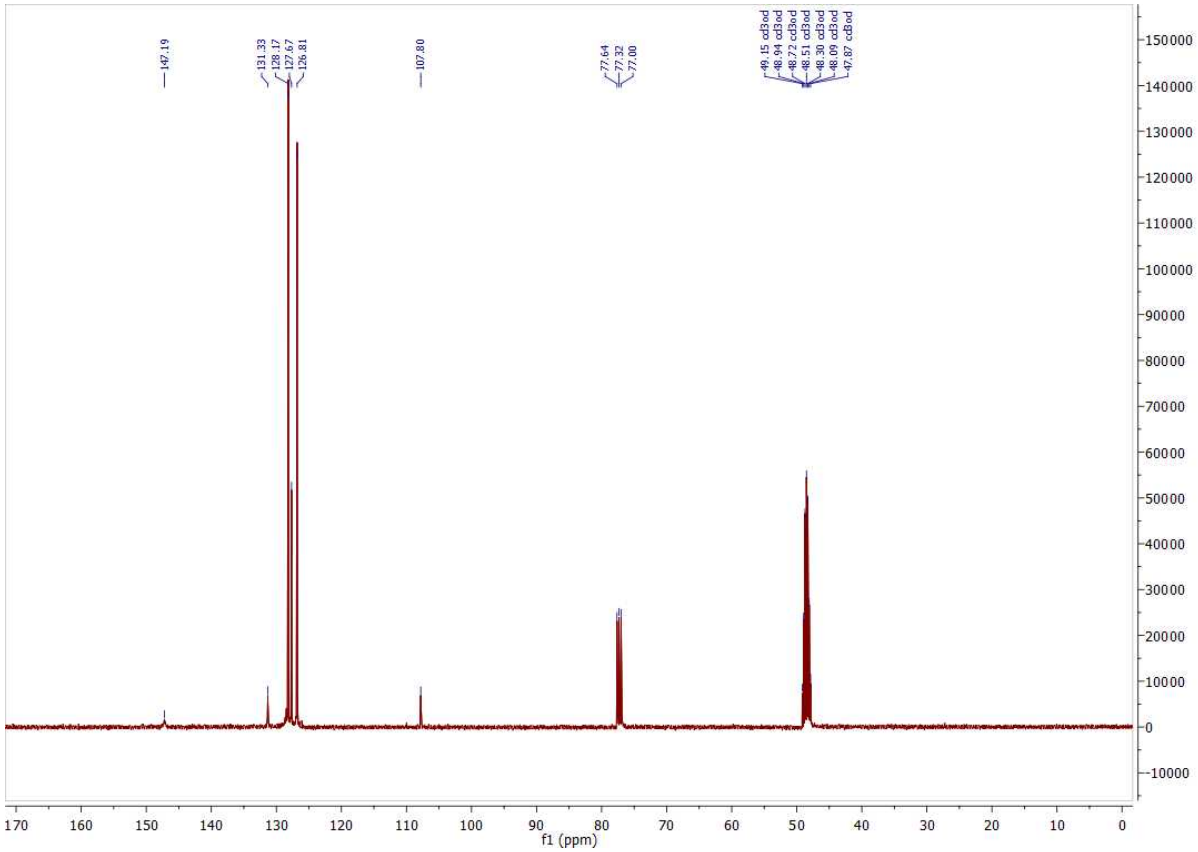

Fig. S10. ^{13}C NMR spectrum $CDCl_3$/MeOH–d_4 4:1 for **1**.