Supporting Information

for

Origin of a Counterintuitive Yellow Light-Emitting Electrochemical Cell Based on a Blue-Emitting Heteroleptic Copper(I) Complex

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*Note on crystal data analysis and checkcif results of for compound **1***

Compound **1** grows in very thin and most often aggregated laminae. To find a suitable single crystal a very thin but rather large lamina was chosen. In this way it was possible to have sufficient diffracting materials. With such a crystal, it was possible to have atomic resolution data to solve and refine the structure. However the weak diffracting power, the elongated shape of the peaks giving some superposition during data reduction and the problem of the absorption in such a large lamina with an heavy atom (as a note face adsorption correction was attempted but it resulted impossible because of the irregularity of the lamina edges) resulted in poor data at high angles and in some violation of the systematic extinctions. Visual inspection of CCD images and a test of data collection suggested to run a very long data collection limited at 0.9 Å resolution, with a redundant full sphere and a frame time of 120 sec. In this way, the data show an agreement factor rather high as highlighted by the checkcif, but the inspection of the structure, the possibility of refining anisotropically all the non-H atoms without unexpected, negative or too large values and absence of correlation matrix elements larger than 0.5 confirmed the validity of the structure. Artificially better agreement factors could be obtained just by cutting more the data resolution (a test at 1.0Å was done) but this resulted in a more unstable refinements, and of course this strategy was not chosen. Twinning was also tested, but no indication emerged in this direction. As a consequence the precision on C-C bond lengths is not high (as again highlighted by checkcif) but sufficient to characterize the molecular structure and its connectivity, and to serve as starting point for DFT calculations.

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

Empirical formula	C55 H43 Cu F6 N3 O2 P3
Formula weight	1048.37
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 14.356(3) Å b = 18.063(2) Å c = 19.496(3) Å = 92.90(2)°
Volume	5059.7(4) $Å^3$
Z	5049.1(14) $Å^3$
Density (calculated)	4
Absorption coefficient	1.379 Mg/m^3
F(000)	0.594 mm^{-1}
Crystal size	0,400 x 0,100 x 0,020 mm^3
Theta range for data collection	2.888 to 20.814°
Index ranges	-14<=h<=14 -18<=k<=18 -19<=l<=19
Reflections collected	48407
Independent reflections	5268 [R(int) = 0.1879]
Completeness to theta = 20.814°	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5268 / 0 / 631
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.1235, wR2 = 0.2487
Largest diff. peak and hole	1.558 and -0.659 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for compound **1**. The equivalent isotropic displacement factor U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	3152(1)	1008(1)	8325(1)	67(1)
P(1)	2985(3)	-116(2)	8831(2)	63(1)
P(2)	1800(3)	1354(2)	7750(2)	72(1)
P(3)	2294(4)	-1487(3)	4713(3)	99(2)
F(4)	1258(10)	-1445(8)	4881(8)	169(6)
F(5)	2021(11)	-1482(13)	3958(7)	228(9)
F(6)	2310(13)	-2321(8)	4747(12)	231(9)
O(2)	6200(9)	44(6)	6991(6)	84(3)
N(4)	3513(10)	1853(7)	9029(6)	66(4)
O(3)	1296(8)	633(7)	9069(5)	85(3)
N(2)	5883(8)	1519(7)	7615(6)	61(3)
N(1)	4434(9)	1305(6)	7991(6)	70(4)
C(1)	5783(11)	1945(9)	8253(7)	61(4)
C(68)	5385(13)	168(8)	6633(9)	70(5)
C(2)	4872(11)	1802(8)	8422(8)	64(4)
C(3)	4390(11)	2112(8)	8989(7)	56(4)
C(4)	3294(15)	2729(10)	9926(8)	91(6)
C(69)	3932(12)	832(9)	6552(9)	74(5)
C(5)	758(13)	1259(11)	8942(10)	83(5)
C(6)	5043(11)	1163(8)	7493(8)	62(4)
C(7)	4187(15)	2981(9)	9885(8)	84(5)
C(8)	3354(17)	-164(12)	11181(9)	97(6)
C(76)	3090(11)	-138(8)	9766(8)	64(4)
C(10)	4529(15)	-2042(10)	8724(11)	98(6)
C(11)	2508(14)	2674(10)	7306(10)	93(6)
C(12)	3687(14)	420(11)	5963(8)	89(6)
C(13)	6652(10)	1588(9)	7256(9)	73(5)
C(14)	4114(12)	-810(9)	7926(8)	77(5)
C(15)	1655(13)	-1180(10)	8366(9)	86(5)
C(16)	4701(13)	-1355(10)	7719(10)	91(6)
C(17)	6599(12)	2344(10)	8442(9)	83(5)
C(18)	2668(15)	3261(10)	6877(12)	101(6)
C(19)	1127(12)	683(9)	7210(8)	71(5)
C(20)	187(13)	747(10)	7062(10)	93(6)
F(8)	2286(11)	-632(8)	4709(8)	178(6)
C(22)	5133(17)	-212(10)	6043(9)	93(6)
F(7)	3334(9)	-1501(9)	4592(8)	176(6)
C(24)	155(15)	1489(14)	9400(11)	116(7)
C(25)	1622(14)	126(9)	6913(9)	85(5)
C(26)	3900(14)	248(11)	10795(10)	92(6)
C(27)	1882(12)	2109(8)	7151(9)	71(5)
F(9)	2586(14)	-1448(10)	5481(6)	220(9)
C(29)	173(12)	-224(11)	8589(10)	90(6)
C(30)	3801(12)	255(9)	10098(9)	77(5)
C(31)	4891(13)	-1957(10)	8107(12)	92(6)
C(32)	4250(19)	-101(12)	5738(10)	102(7)
C(33)	4817(12)	722(8)	6867(7)	65(4)
C(34)	1188(19)	-343(11)	6447(12)	111(7)
C(75)	1861(11)	-466(11)	8650(8)	73(5)
C(36)	3725(11)	-870(8)	8580(8)	65(4)
C(37)	7409(11)	1979(10)	7449(9)	85(5)
C(38)	2181(17)	3285(12)	6264(12)	104(6)
C(39)	1401(13)	2186(11)	6519(9)	89(5)
C(41)	4728(14)	2680(9)	9406(8)	87(6)

C(42)	-275(19)	277(16)	6603(14)	138(9)
C(43)	6(13)	-935(12)	8286(11)	101(6)
C(44)	3016(13)	2164(9)	9508(9)	84(5)
C(45)	260(20)	-246(15)	6292(13)	127(9)
C(47)	3942(13)	-1484(9)	8963(9)	85(5)
C(48)	1097(12)	-71(10)	8752(8)	73(5)
C(49)	6892(16)	-398(11)	6700(10)	121(7)
C(50)	-144(14)	2573(13)	8763(14)	110(7)
C(51)	7369(13)	2380(10)	8099(10)	92(6)
C(52)	-298(13)	2132(15)	9328(13)	111(7)
C(53)	2523(13)	-551(10)	10157(9)	90(5)
C(54)	463(14)	2359(10)	8296(11)	99(6)
C(55)	759(15)	-1357(12)	8193(10)	100(6)
C(56)	1523(16)	2784(12)	6089(10)	102(6)
C(57)	942(10)	1691(10)	8354(10)	79(5)
C(58)	2623(16)	-554(12)	10867(10)	103(6)

Table S3. Bond lengths [Å] and angles [°] for compound **1.**

Cu(1)-N(1)	2.055(14)
Cu(1)-N(4)	2.102(12)
Cu(1)-P(1)	2.275(4)
Cu(1)-P(2)	2.279(5)
P(1)-C(75)	1.753(17)
P(1)-C(36)	1.810(15)
P(1)-C(76)	1.820(16)
P(2)-C(27)	1.804(16)
P(2)-C(19)	1.845(16)
P(2)-C(57)	1.849(17)
P(3)-F(5)	1.504(14)
P(3)-F(6)	1.507(16)
P(3)-F(7)	1.524(13)
P(3)-F(9)	1.537(13)
P(3)-F(4)	1.541(14)
P(3)-F(8)	1.545(14)
O(2)-C(68)	1.350(18)
O(2)-C(49)	1.42(2)
N(4)-C(44)	1.328(19)
N(4)-C(3)	1.348(17)
O(3)-C(5)	1.384(19)
O(3)-C(48)	1.436(19)
N(2)-C(13)	1.342(17)
N(2)-C(6)	1.377(18)
N(2)-C(1)	1.477(17)
N(1)-C(2)	1.361(17)
N(1)-C(6)	1.364(18)
C(1)-C(2)	1.39(2)
C(1)-C(17)	1.41(2)
C(68)-C(22)	1.37(2)
C(68)-C(33)	1.38(2)
C(2)-C(3)	1.45(2)
C(3)-C(41)	1.38(2)
C(4)-C(44)	1.35(2)
C(4)-C(7)	1.37(2)
C(69)-C(33)	1.40(2)
C(69)-C(12)	1.40(2)
C(5)-C(24)	1.34(2)
C(5)-C(57)	1.42(2)
C(6)-C(33)	1.48(2)
C(7)-C(41)	1.36(2)
C(8)-C(26)	1.34(2)
C(8)-C(58)	1.38(2)
C(76)-C(53)	1.36(2)
C(76)-C(30)	1.38(2)
C(10)-C(31)	1.34(2)
C(10)-C(47)	1.41(2)
C(11)-C(18)	1.38(2)
C(11)-C(27)	1.38(2)
C(12)-C(32)	1.33(2)
C(13)-C(37)	1.34(2)
C(14)-C(16)	1.37(2)
C(14)-C(36)	1.42(2)
C(15)-C(55)	1.35(2)
C(15)-C(75)	1.43(2)
C(16)-C(31)	1.34(2)
C(17)-C(51)	1.32(2)

C(18)-C(38)	1.35(2)
C(19)-C(20)	1.37(2)
C(19)-C(25)	1.38(2)
C(20)-C(42)	1.38(3)
C(22)-C(32)	1.39(3)
C(24)-C(52)	1.34(3)
C(25)-C(34)	1.37(2)
C(26)-C(30)	1.36(2)
C(27)-C(39)	1.39(2)
C(29)-C(48)	1.38(2)
C(29)-C(43)	1.43(2)
C(34)-C(45)	1.37(3)
C(75)-C(48)	1.33(2)
C(36)-C(47)	1.365(19)
C(37)-C(51)	1.46(2)
C(38)-C(56)	1.34(2)
C(39)-C(56)	1.38(2)
C(42)-C(45)	1.38(3)
C(43)-C(55)	1.34(2)
C(50)-C(54)	1.35(3)
C(50)-C(52)	1.39(3)
C(53)-C(58)	1.39(2)
C(54)-C(57)	1.39(2)

N(1)-Cu(1)-N(4)	79.7(5)
N(1)-Cu(1)-P(1)	119.1(4)
N(4)-Cu(1)-P(1)	113.1(3)
N(1)-Cu(1)-P(2)	121.8(4)
N(4)-Cu(1)-P(2)	107.3(4)
P(1)-Cu(1)-P(2)	110.64(17)
C(75)-P(1)-C(36)	102.7(8)
C(75)-P(1)-C(76)	102.9(7)
C(36)-P(1)-C(76)	103.6(7)
C(75)-P(1)-Cu(1)	110.5(6)
C(36)-P(1)-Cu(1)	118.6(5)
C(76)-P(1)-Cu(1)	116.7(5)
C(27)-P(2)-C(19)	100.2(8)
C(27)-P(2)-C(57)	103.3(8)
C(19)-P(2)-C(57)	103.5(8)
C(27)-P(2)-Cu(1)	116.3(6)
C(19)-P(2)-Cu(1)	120.6(6)
C(57)-P(2)-Cu(1)	110.8(6)
F(5)-P(3)-F(6)	93.0(12)
F(5)-P(3)-F(7)	93.3(9)
F(6)-P(3)-F(7)	88.7(10)
F(5)-P(3)-F(9)	176.9(13)
F(6)-P(3)-F(9)	90.0(11)
F(7)-P(3)-F(9)	85.9(10)
F(5)-P(3)-F(4)	90.1(9)
F(6)-P(3)-F(4)	93.0(10)
F(7)-P(3)-F(4)	176.0(9)
F(9)-P(3)-F(4)	90.5(10)
F(5)-P(3)-F(8)	89.3(11)
F(6)-P(3)-F(8)	177.7(11)
F(7)-P(3)-F(8)	91.3(9)
F(9)-P(3)-F(8)	87.7(9)
F(4)-P(3)-F(8)	86.8(9)
C(68)-O(2)-C(49)	119.6(14)
C(44)-N(4)-C(3)	115.5(14)

C(44)-N(4)-Cu(1)	130.1(13)
C(3)-N(4)-Cu(1)	114.4(10)
C(5)-O(3)-C(48)	123.3(13)
C(13)-N(2)-C(6)	133.6(14)
C(13)-N(2)-C(1)	120.6(13)
C(6)-N(2)-C(1)	105.5(12)
C(2)-N(1)-C(6)	105.8(14)
C(2)-N(1)-Cu(1)	111.7(11)
C(6)-N(1)-Cu(1)	142.5(10)
C(2)-C(1)-C(17)	144.5(16)
C(2)-C(1)-N(2)	103.6(12)
C(17)-C(1)-N(2)	111.8(14)
O(2)-C(68)-C(22)	122.4(16)
O(2)-C(68)-C(33)	117.4(15)
C(22)-C(68)-C(33)	120.2(18)
N(1)-C(2)-C(1)	112.8(14)
N(1)-C(2)-C(3)	120.2(15)
C(1)-C(2)-C(3)	127.0(15)
N(4)-C(3)-C(41)	121.6(14)
N(4)-C(3)-C(2)	113.3(14)
C(41)-C(3)-C(2)	124.7(16)
C(44)-C(4)-C(7)	117.7(17)
C(33)-C(69)-C(12)	118.1(16)
C(24)-C(5)-O(3)	120.5(19)
C(24)-C(5)-C(57)	121.3(19)
O(3)-C(5)-C(57)	117.9(16)
N(1)-C(6)-N(2)	112.1(13)
N(1)-C(6)-C(33)	124.6(14)
N(2)-C(6)-C(33)	123.2(14)
C(41)-C(7)-C(4)	118.5(16)
C(26)-C(8)-C(58)	119.2(18)
C(53)-C(76)-C(30)	117.8(15)
C(53)-C(76)-P(1)	123.3(13)
C(30)-C(76)-P(1)	118.8(12)
C(31)-C(10)-C(47)	118.6(18)
C(18)-C(11)-C(27)	124.2(19)
C(32)-C(12)-C(69)	121.0(19)
C(37)-C(13)-N(2)	125.5(17)
C(16)-C(14)-C(36)	119.0(15)
C(55)-C(15)-C(75)	119.1(17)
C(31)-C(16)-C(14)	121.7(18)
C(51)-C(17)-C(1)	126.8(17)
C(38)-C(18)-C(11)	118(2)
C(20)-C(19)-C(25)	119.8(16)
C(20)-C(19)-P(2)	123.1(14)
C(25)-C(19)-P(2)	117.0(14)
C(19)-C(20)-C(42)	121(2)
C(68)-C(22)-C(32)	119.0(18)
C(52)-C(24)-C(5)	122(2)
C(34)-C(25)-C(19)	120.3(19)
C(8)-C(26)-C(30)	122.2(19)
C(11)-C(27)-C(39)	114.1(16)
C(11)-C(27)-P(2)	118.7(14)
C(39)-C(27)-P(2)	127.2(14)
C(48)-C(29)-C(43)	114.6(17)
C(26)-C(30)-C(76)	120.2(17)
C(10)-C(31)-C(16)	121.3(19)
C(12)-C(32)-C(22)	121.3(19)
C(68)-C(33)-C(69)	119.8(15)

C(68)-C(33)-C(6)	123.6(16)
C(69)-C(33)-C(6)	116.3(15)
C(45)-C(34)-C(25)	118(2)
C(48)-C(75)-C(15)	112.7(16)
C(48)-C(75)-P(1)	122.2(16)
C(15)-C(75)-P(1)	125.1(14)
C(47)-C(36)-C(14)	117.6(15)
C(47)-C(36)-P(1)	125.8(14)
C(14)-C(36)-P(1)	116.6(12)
C(13)-C(37)-C(51)	116.1(15)
C(56)-C(38)-C(18)	122(2)
C(56)-C(39)-C(27)	122.9(18)
C(7)-C(41)-C(3)	120.4(18)
C(45)-C(42)-C(20)	117(2)
C(55)-C(43)-C(29)	116.5(18)
N(4)-C(44)-C(4)	126.1(18)
C(34)-C(45)-C(42)	123(2)
C(36)-C(47)-C(10)	121.6(17)
C(75)-C(48)-C(29)	130.5(19)
C(75)-C(48)-O(3)	113.0(15)
C(29)-C(48)-O(3)	116.5(17)
C(54)-C(50)-C(52)	120(2)
C(17)-C(51)-C(37)	118.9(16)
C(24)-C(52)-C(50)	119(2)
C(76)-C(53)-C(58)	121.8(17)
C(50)-C(54)-C(57)	122(2)
C(43)-C(55)-C(15)	127(2)
C(38)-C(56)-C(39)	118.8(19)
C(54)-C(57)-C(5)	115.5(17)
C(54)-C(57)-P(2)	125.3(17)
C(5)-C(57)-P(2)	119.3(13)
C(8)-C(58)-C(53)	118.6(18)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	87(2)	52(1)	62(1)	-2(1)	6(1)	0(1)
P(1)	74(3)	54(3)	60(3)	3(2)	3(2)	1(2)
P(2)	85(3)	61(3)	69(3)	0(2)	4(2)	5(2)
P(3)	123(5)	103(5)	73(4)	8(3)	14(3)	5(4)
F(4)	134(12)	166(13)	213(15)	8(11)	64(11)	4(10)
F(5)	180(15)	420(30)	83(10)	-38(14)	3(9)	31(16)
F(6)	270(20)	106(12)	330(30)	-36(14)	67(18)	15(12)
O(2)	96(9)	72(8)	86(8)	-8(7)	15(7)	14(7)
N(4)	99(11)	60(8)	40(8)	-5(6)	17(7)	-1(8)
O(3)	99(9)	82(9)	73(8)	-1(7)	6(6)	6(7)
N(2)	51(9)	65(8)	67(9)	7(7)	-11(7)	-6(7)
N(1)	92(10)	53(8)	63(9)	-37(7)	-16(8)	8(7)
C(1)	54(11)	79(11)	50(10)	-11(9)	-7(8)	-1(9)
C(68)	88(13)	48(10)	76(12)	-23(10)	25(10)	8(9)
C(2)	69(12)	66(11)	57(11)	7(9)	-6(9)	-2(9)
C(3)	75(12)	55(10)	38(9)	3(8)	8(8)	3(9)
C(4)	124(18)	90(14)	59(11)	-37(11)	22(11)	-3(13)
C(69)	64(12)	85(13)	75(12)	7(10)	25(9)	-4(9)
C(5)	101(15)	77(13)	74(13)	-14(11)	14(11)	13(11)
C(6)	71(11)	66(10)	50(10)	1(9)	11(9)	2(9)

C(7)	133(18)	61(12)	57(12)	-14(10)	-3(11)	-20(12)
C(8)	138(19)	104(16)	47(12)	9(12)	-4(13)	18(14)
C(76)	63(11)	60(10)	69(11)	2(9)	1(9)	-14(8)
C(10)	136(19)	67(14)	92(16)	0(12)	6(13)	13(12)
C(11)	131(17)	65(13)	84(13)	18(11)	8(12)	9(12)
C(12)	128(17)	95(15)	42(11)	-10(11)	-2(11)	-18(13)
C(13)	33(10)	90(12)	97(13)	9(10)	18(9)	0(9)
C(14)	96(13)	64(12)	72(12)	23(10)	14(10)	-4(10)
C(15)	84(15)	64(13)	108(15)	1(11)	-2(11)	8(10)
C(16)	125(17)	60(12)	90(14)	-3(11)	18(12)	11(11)
C(17)	60(12)	106(14)	83(13)	-1(11)	-2(10)	-6(11)
C(18)	118(17)	75(14)	109(17)	20(13)	-2(14)	-8(12)
C(19)	83(13)	54(11)	76(12)	6(9)	-11(10)	-3(9)
C(20)	69(14)	94(14)	114(16)	-5(12)	-22(11)	-7(11)
F(8)	215(16)	119(11)	198(15)	69(11)	-12(12)	-16(10)
C(22)	150(20)	69(12)	63(13)	-34(11)	40(13)	-18(13)
F(7)	95(10)	235(17)	198(14)	-47(13)	18(9)	3(10)
C(24)	120(18)	130(20)	101(16)	-16(15)	36(14)	33(16)
C(25)	124(16)	53(11)	79(13)	-5(10)	1(11)	-3(11)
C(26)	129(17)	81(14)	65(13)	-21(11)	-10(12)	9(12)
C(27)	86(13)	46(10)	80(13)	-2(9)	12(10)	0(9)
F(9)	380(20)	222(17)	58(8)	23(9)	13(11)	114(16)
C(29)	59(13)	79(14)	134(17)	19(12)	19(11)	-1(10)
C(30)	92(14)	69(11)	69(13)	5(10)	4(10)	5(10)
C(31)	96(15)	54(13)	124(18)	-15(13)	0(13)	-5(10)
C(32)	170(20)	84(15)	59(13)	-32(11)	31(15)	-41(16)
C(33)	92(14)	53(10)	52(10)	-5(8)	21(9)	-12(9)
C(34)	140(20)	76(14)	120(19)	-12(14)	9(16)	-3(14)
C(75)	46(11)	107(15)	67(11)	25(10)	15(8)	21(10)
C(36)	78(11)	43(10)	74(12)	6(9)	5(9)	-2(8)
C(37)	43(11)	123(16)	90(14)	14(12)	5(9)	-12(10)
C(38)	120(19)	79(15)	114(19)	19(14)	23(15)	7(14)
C(39)	106(15)	88(14)	73(13)	4(11)	-13(11)	-7(11)
C(41)	155(18)	60(11)	48(10)	-23(9)	18(11)	-11(11)
C(42)	120(20)	140(20)	150(20)	22(19)	-55(19)	-34(19)
C(43)	58(13)	102(16)	143(19)	28(14)	5(11)	-22(12)
C(44)	126(16)	65(12)	64(12)	-9(10)	27(11)	-14(11)
C(45)	150(30)	110(20)	120(20)	-6(16)	-22(19)	-20(18)
C(47)	144(17)	43(10)	68(11)	10(10)	4(11)	-2(11)
C(48)	62(13)	95(14)	61(11)	14(10)	6(9)	-21(11)
C(49)	170(20)	95(15)	103(16)	11(13)	40(15)	25(15)
C(50)	82(16)	114(19)	130(20)	-17(17)	0(14)	29(13)
C(51)	66(13)	111(16)	98(15)	-19(12)	-4(11)	-25(11)
C(52)	67(14)	140(20)	130(20)	-27(18)	21(13)	11(14)
C(53)	101(15)	86(13)	80(14)	8(11)	-5(11)	-28(11)
C(54)	113(17)	75(14)	110(17)	6(12)	7(14)	23(12)
C(55)	68(14)	119(17)	112(16)	18(13)	-11(12)	-2(13)
C(56)	131(19)	97(16)	76(14)	25(13)	3(12)	12(14)
C(57)	46(10)	75(13)	117(16)	-9(12)	4(10)	-3(9)
C(58)	138(19)	113(17)	59(14)	24(12)	15(12)	2(14)

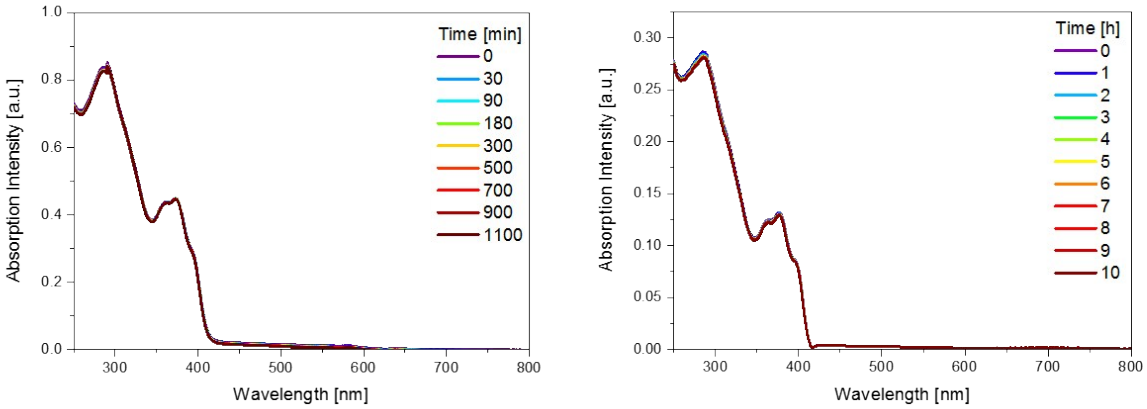


Figure S1. Absorbance of **1** in ACN solution (left) and spin-coated films (right) over time.

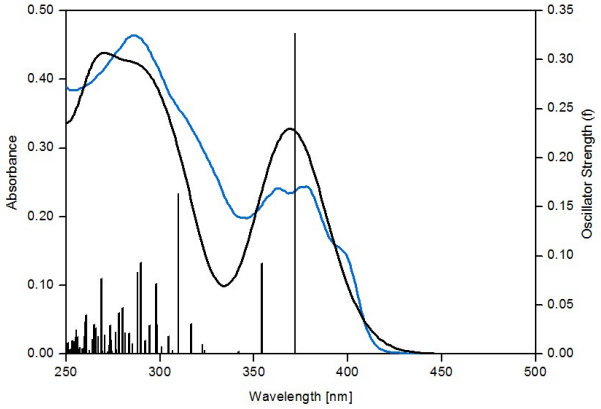
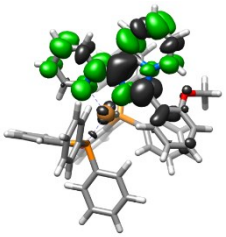
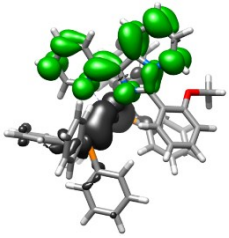
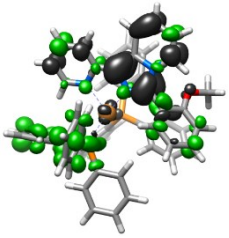
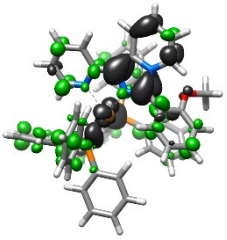
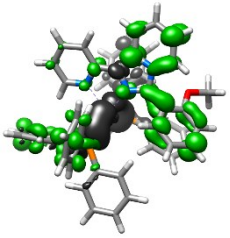
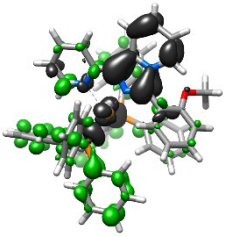
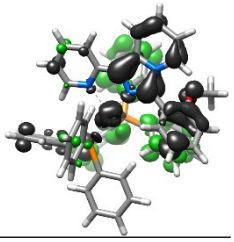


Figure S2. Calculated (black line) and experimental (blue line) electronic absorption spectra of **1** in ACN solution. The excited states are shown as vertical bars with heights equal to the oscillator strength values. The theoretical curve was obtained using the program GaussSum 2.2.5.

Table S5. Selected TD-DFT singlet transitions displaying high values of oscillator strength (f) for **1** in the GS geometry.

Transition	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major contributions	EDDM[a]
1	3.33	372	0.3269	HOMO→LUMO (92%)	
2	3.50	354	0.0920	H-1→LUMO (93%)	
7	4.00	310	0.1638	HOMO→L+3 (51%) HOMO→L+4 (30%)	
12	4.16	298	0.0710	H-1→L+3 (28%) HOMO→L+6 (27%) HOMO→L+7 (15%)	
16	4.28	290	0.0927	H-1→L+3 (16%) H-1→L+4 (75%)	
18	4.30	288	0.0834	H-1→L+5 (21%) HOMO→L+5 (12%) HOMO→L+7 (43%)	
34	4.61	267	0.0764	H-5→L+1 (18%) H-4→L+1 (16%) HOMO→L+11 (30%)	

[a] in the EDDM black indicates a decrease in electron density while green indicates an increase.

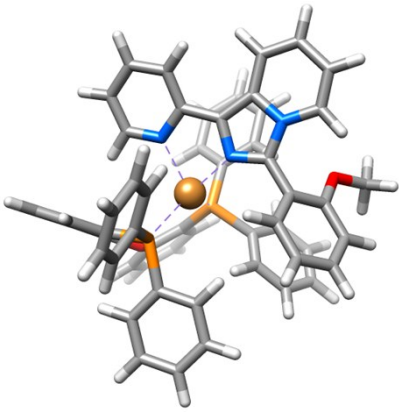


Figure S3. DFT-optimized structure of **1** in the GS.

Table S6. Selected X-ray and DFT-calculated bond distances (Å) and angles (°) for **1**.

	Cu–P1	Cu–P2	Cu–N1	Cu–N4	P1–Cu–P2	N1–Cu–N4	P1–Cu–N1	P1–Cu–N4	P2–Cu–N1	P2–Cu–N4
X-ray	2.272(6)	2.275(6)	2.03(2)	2.157(15)	110.7(2)	79.3(7)	119.1(5)	113.2(4)	121.5(5)	107.9(5)
GS	2.376	2.400	2.150	2.199	119.73	77.78	124.39	108.45	109.50	107.26
S_1	2.370	2.418	2.154	2.160	118.77	77.84	127.07	109.73	107.17	107.22
T_1	2.369	2.409	2.142	2.198	119.50	77.50	125.74	109.03	108.67	106.40

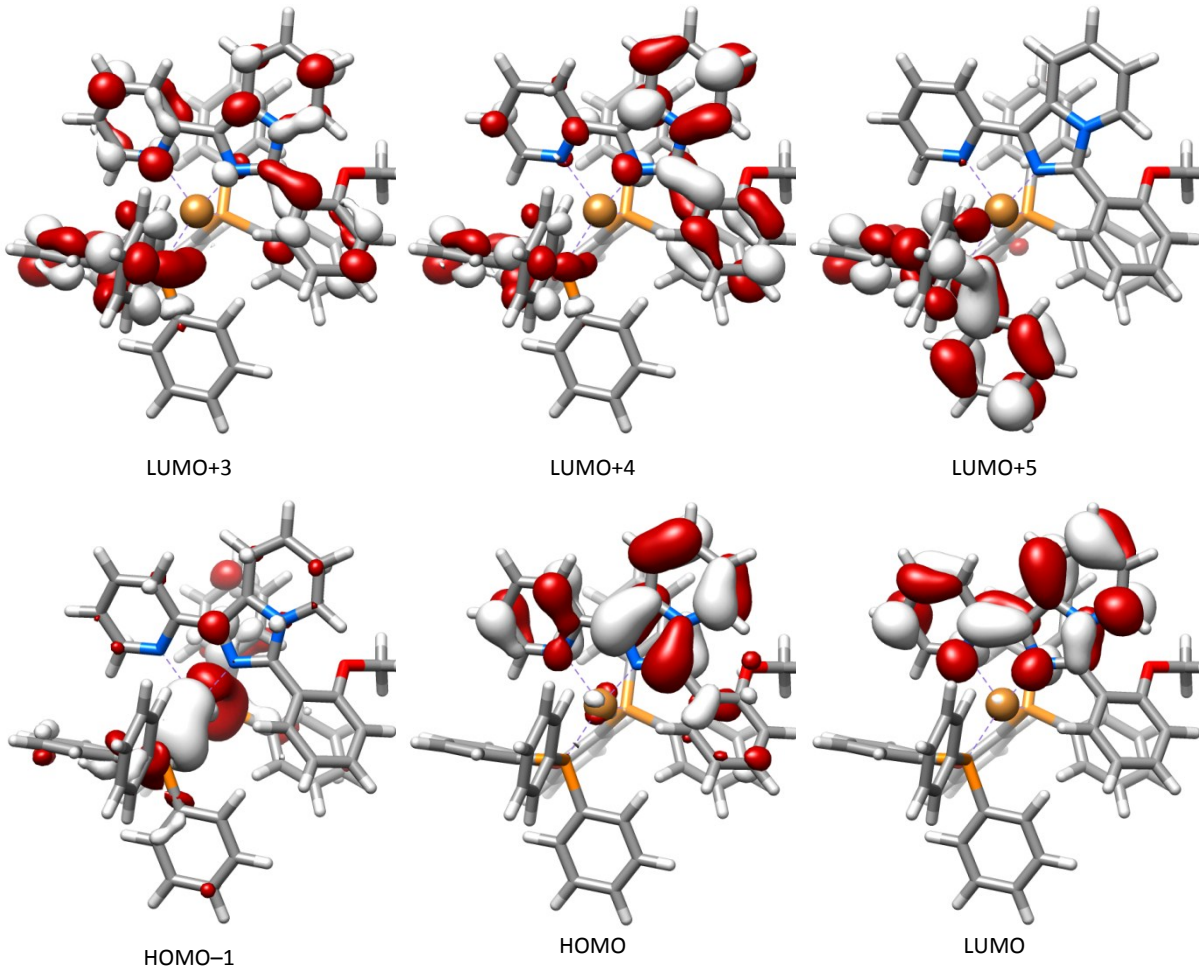


Figure S4. Selected frontier orbitals for **1** in the GS geometry.

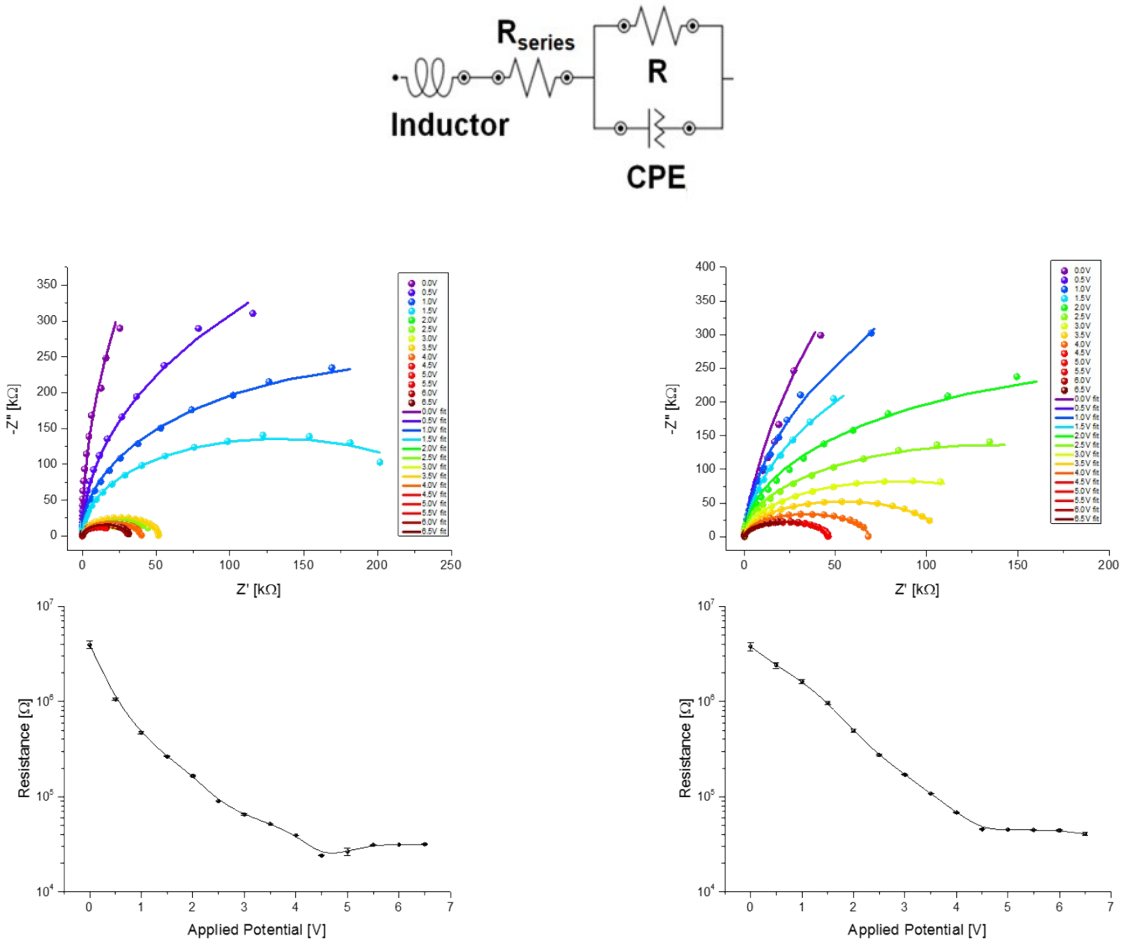


Figure S5. Top. Equivalent circuit used for the fitting. Central. Nyquist plots of fresh (left) and used (right) devices with **1** with the respective fittings (solid lines) upon increasing applied voltage. Bottom. Resistance changes versus applied voltage of fresh (left) and used (right) devices with **1**.

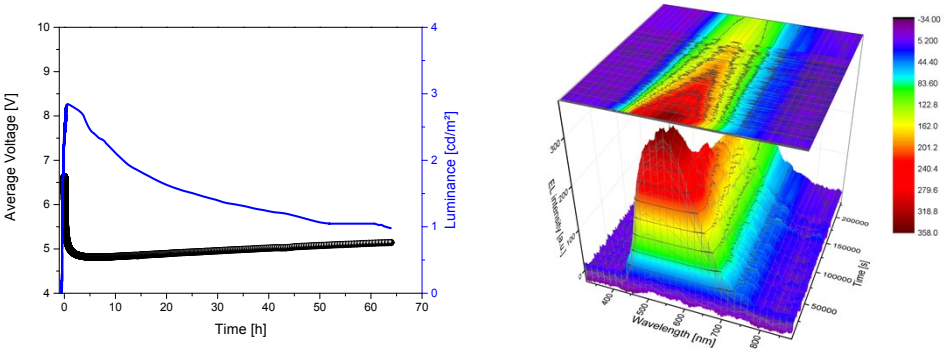


Figure S6. Left. Average voltage and luminance versus time of devices with **1** driven under a pulsed current using a block wave at a frequency of 1 kHz with a duty cycle of 50% and an average current of 1 mA. Right: EL spectra of devices with **1** at selected times.

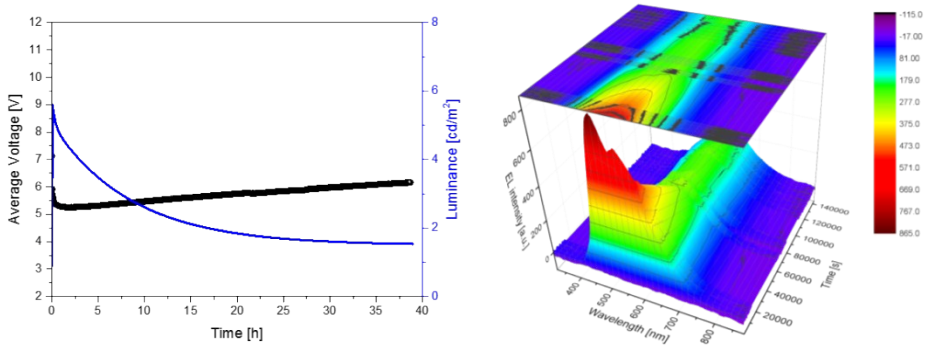


Figure S7. Left. Average voltage and luminance versus time of devices with **1** driven by a pulsed current using a block wave at a frequency of 1 kHz with a duty cycle of 50% and an average current of 2.5 mA. Central. 3D plot of the changes of the EL spectrum over time. Right. EL spectra of devices with **1** at selected times to highlight the rapid change in the shape of the EL band.

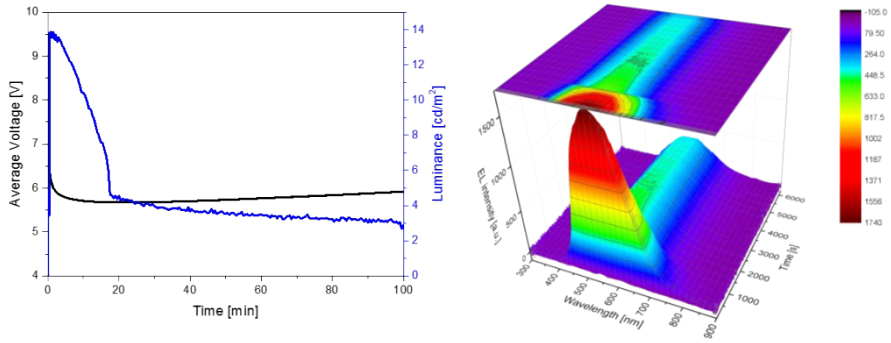


Figure S8. Left. Average voltage and luminance versus time of devices with **1** driven by a pulsed current using a block wave at a frequency of 1 kHz with a duty cycle of 50% and an average current of 7.5 mA. Right. EL spectra of devices with **1** at selected times.

Table S7. Figures-of-merit of devices with **1** featuring different thicknesses and driven at different pulsed currents of 5 and 7.5 mA using a block wave at a frequency of 1 kHz with a duty cycle of 50%.

Applied Average Current [mA]	5		7.5	
Active layer thickness [nm]	45	90	45	90
Luminance[cd/m^2]	2.6	7.5	4.6	13.9
Efficacy [cd/A]	0.008	0.022	0.009	0.028
Lifetime ($t_{1/2}$) [h]	15.9	3.5	0.82	0.28