A new mixed-ligand copper(II) complex of (*E*)-*N*'-(2-hydroxybenzylidene) acetohydrazide: Synthesis, characterization, NLO behavior, DFT calculation and biological activities

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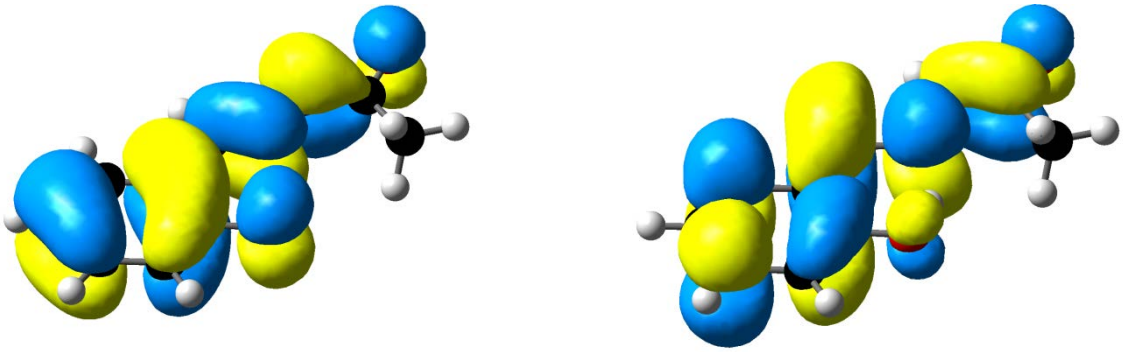

E_{HOMO} = -5.92 eV E_{LUMO} = -1.59 eV

Fig. S1. Molecular orbital surfaces and energy levels of HL

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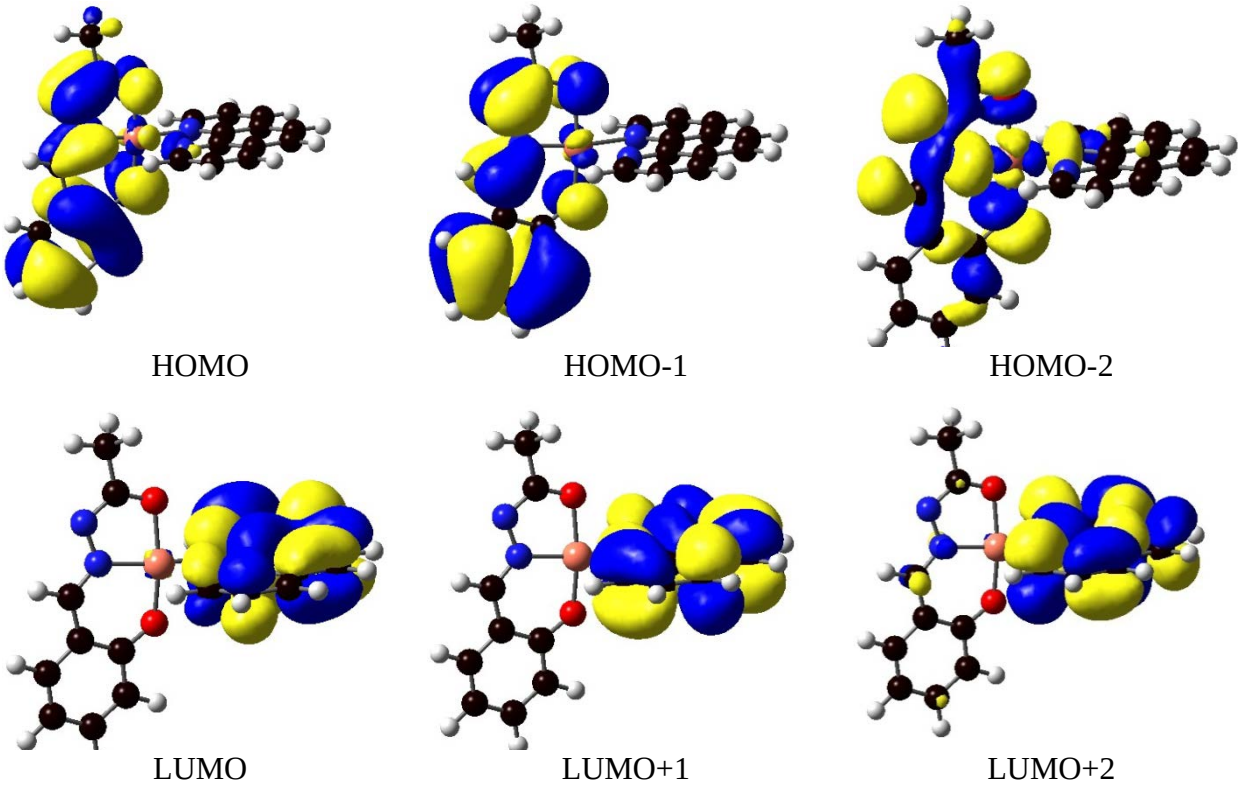

Fig. S2. Contour plots of some selected MOs (α-spin) of [CuL(phen)].

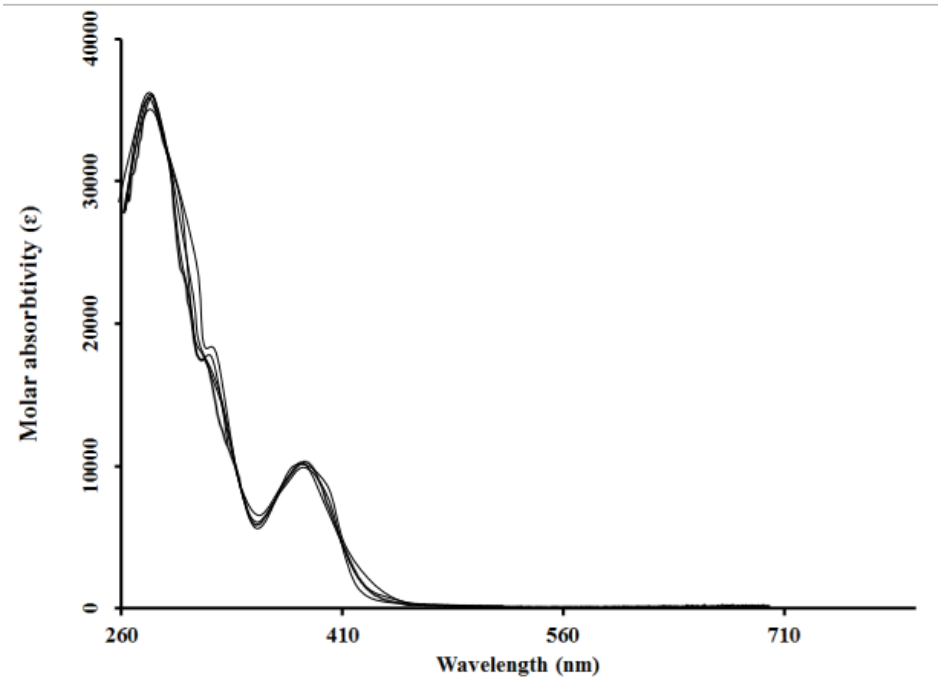

Fig. S3. UV-Vis spectrum of [CuL(phen)] under the effect of irradiation 3 h in DMSO.

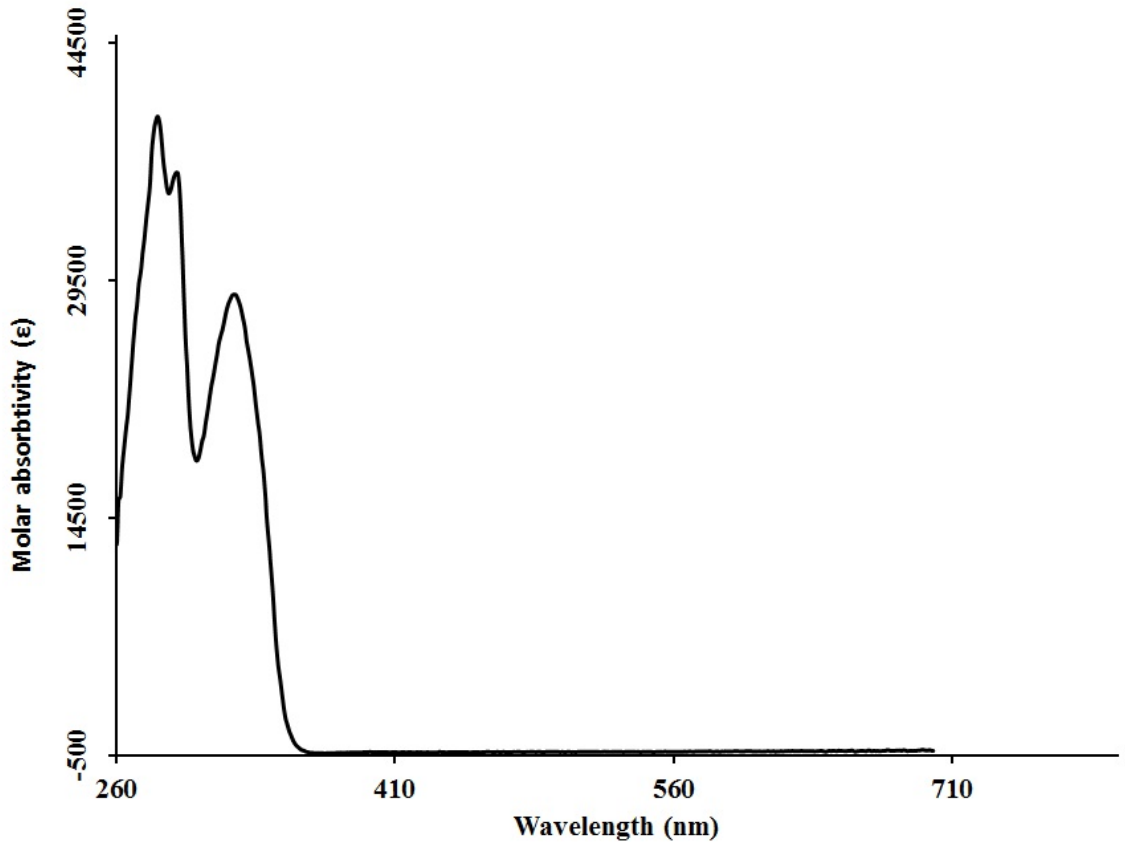

Fig. S4. UV-Vis spectrum of HL.

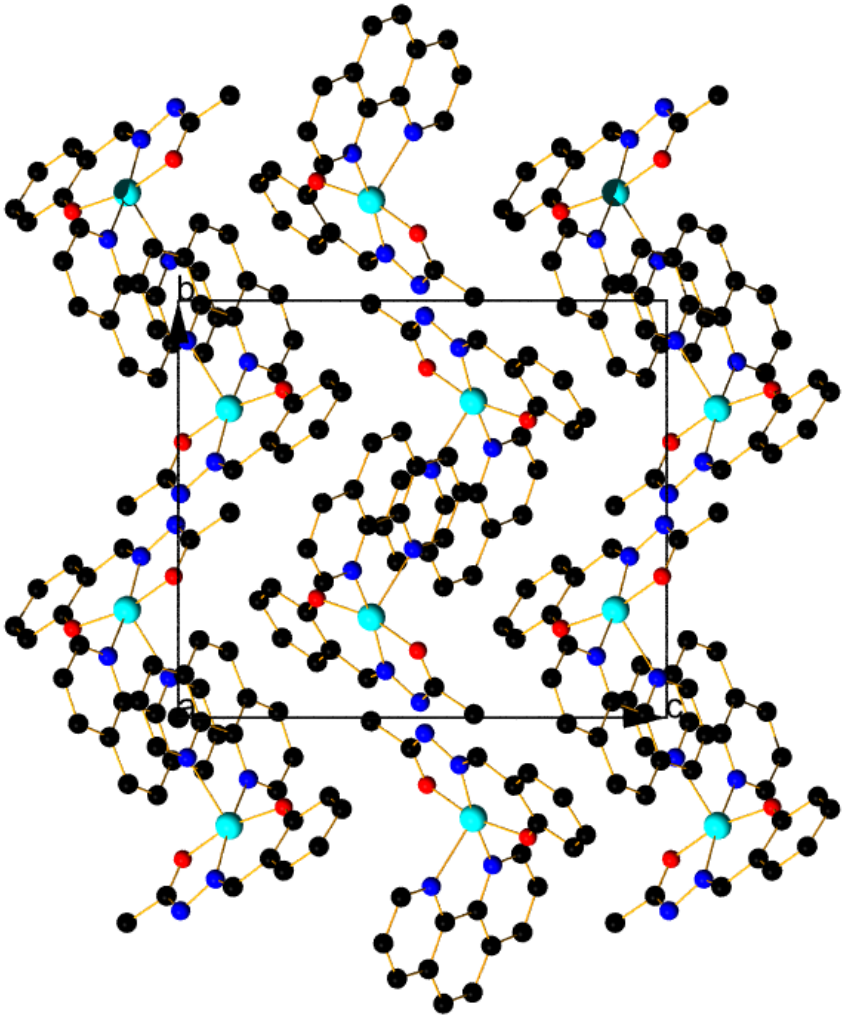

Fig. ~~S3~~S5. Packing diagram of the complex along the a axis.

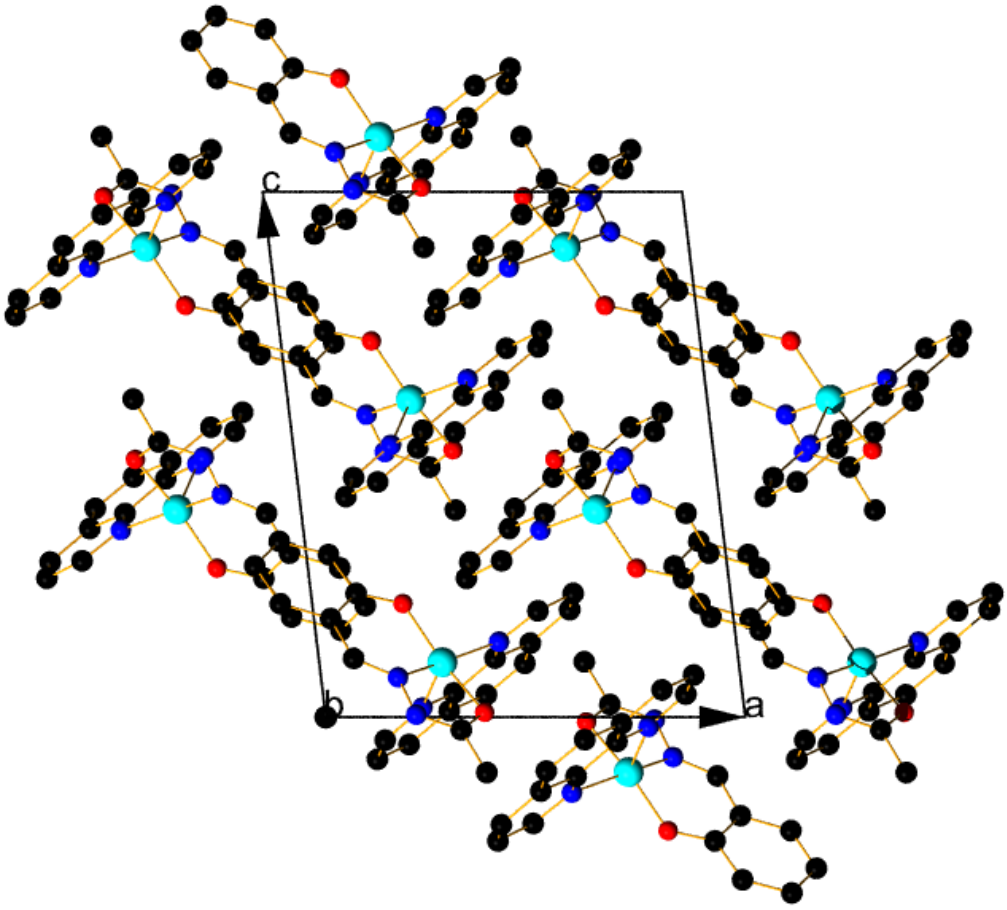

Fig. ~~S4~~S6. Packing diagram of the complex along the b axis.

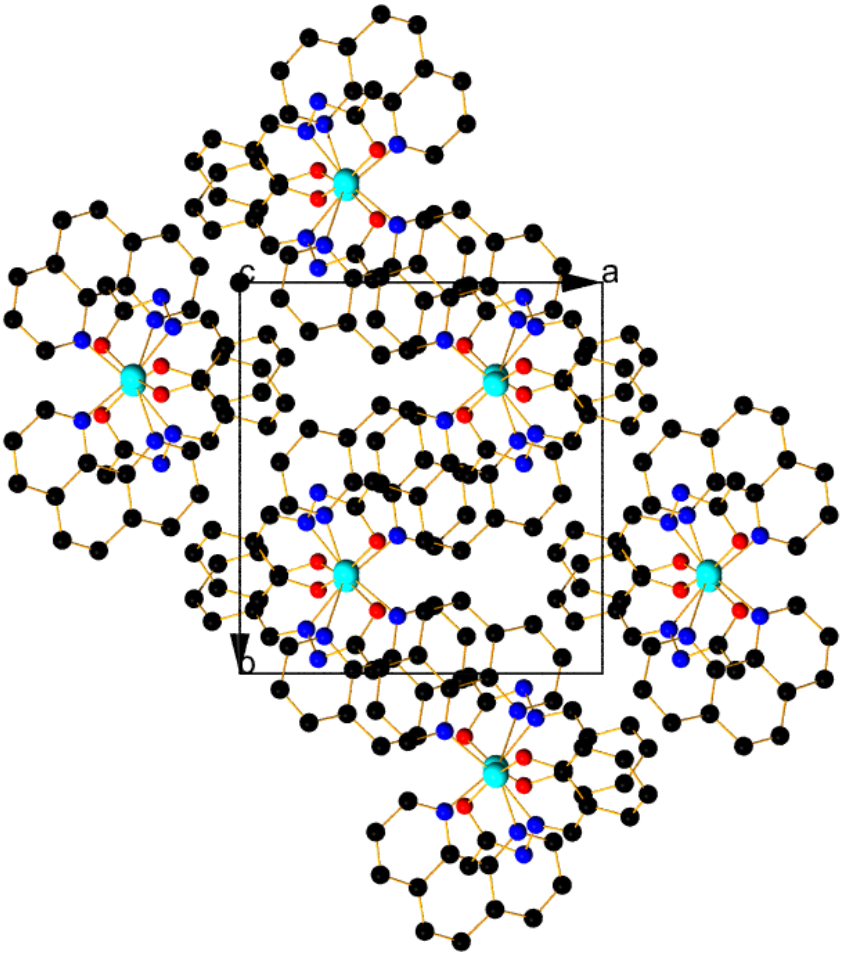

Fig. ~~S5~~S7. Packing diagram of the complex along the c axis.

Table S1. Energy and frontier molecular orbital compositions of [CuL(phen)] (α spin)

MO	Energy (eV)	symmetry	L (%)	Cu (%)	Phen (%)
L+10	1.14	A	89	10	1
L+9	1.1	A	0	94	6
L+8	1.07	A	0	0	100
L+7	0.96	A	5	93	2
L+6	0.84	A	7	92	1
L+5	0.52	A	4	85	11
L+4	-0.15	A	0	0	100
L+3	-0.7	A	96	1	3
L+2	-0.91	A	2	1	97
L+1	-2.13	A	0	0	100
LUMO	-2.23	A	0	0	99
HOMO	-4.63	A	96	3	1
H-1	-5.32	A	98	2	0
H-2	-5.36	A	76	19	5
H-3	-6.41	A	83	12	5
H-4	-6.61	A	97	3	0
H-5	-6.94	A	60	16	24
H-6	-7	A	11	3	86
H-7	-7.29	A	31	28	41
H-8	-7.37	A	0	0	100
H-9	-7.83	A	72	26	2
H-10	-8.33	A	59	22	19

Table S2. Energy and frontier molecular orbital compositions of [CuL(phen)] (β spin)

MO	Energy (eV)	Symmetry	L (%)	Cu(%)	Phen (%)
L+10	1.11	A	0	92	8
L+9	1.07	A	0	0	100
L+8	0.97	A	5	93	2
L+7	0.85	A	7	93	0
L+6	0.52	A	4	85	11
L+5	-0.15	A	0	0	100
L+4	-0.66	A	96	2	2
L+3	-0.91	A	2	1	97
L+2	-1.66	A	34	61	5
L+1	-2.13	A	0	0	100
LUMO	-2.22	A	0	1	99
HOMO	-4.58	A	95	4	1
H-1	-5.28	A	97	3	0
H-2	-6.05	A	85	12	3
H-3	-6.52	A	74	19	7
H-4	-6.62	A	83	12	5
H-5	-6.96	A	14	12	74
H-6	-7.04	A	30	22	48
H-7	-7.36	A	0	2	98
H-8	-7.52	A	67	28	5
H-9	-7.63	A	61	37	2
H-10	-7.96	A	13	84	3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [CuL(phen)]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

x		y	z	U(eq)
Cu(1)	7063(1)	2411(1)	3955(1)	38(1)
N(3)	8164(2)	1132(2)	4241(2)	36(1)
O(1)	7836(2)	2861(2)	2838(1)	47(1)
N(2)	5651(2)	3528(2)	3563(1)	38(1)
O(2)	6201(2)	1610(1)	4908(1)	45(1)
C(13)	8923(2)	2536(2)	2644(2)	38(1)
N(4)	7834(2)	373(2)	4952(2)	39(1)
C(19)	9170(2)	945(2)	3881(2)	39(1)
C(11)	5798(2)	4617(2)	3877(2)	37(1)
N(1)	7667(2)	4045(2)	4817(2)	41(1)
C(20)	6807(2)	729(2)	5240(2)	39(1)
C(12)	6871(2)	4897(2)	4539(2)	38(1)
C(17)	10760(2)	1333(2)	2841(2)	46(1)
C(18)	9602(2)	1626(2)	3123(2)	38(1)
C(14)	9471(2)	3110(2)	1905(2)	44(1)
C(10)	4639(2)	3261(3)	2976(2)	49(1)
C(2)	8890(3)	5408(3)	5802(2)	66(1)
C(15)	10606(3)	2810(2)	1654(2)	48(1)
C(7)	4914(3)	5466(2)	3592(2)	47(1)
C(4)	7037(3)	6029(2)	4877(2)	49(1)
C(3)	8092(3)	6255(3)	5520(2)	62(1)
C(8)	3878(3)	5144(3)	2953(2)	56(1)
C(1)	8649(3)	4303(3)	5439(2)	54(1)
C(21)	6320(2)	83(2)	6055(2)	48(1)
C(6)	5103(3)	6590(3)	3974(2)	59(1)
C(16)	11261(2)	1912(2)	2123(2)	48(1)
C(5)	6108(3)	6856(2)	4572(2)	62(1)
C(9)	3750(3)	4053(3)	2644(2)	60(1)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	36(1)	36(1)	43(1)	0(1)	7(1)	6(1)
N(3)	35(1)	37(1)	37(1)	-1(1)	6(1)	1(1)
O(1)	43(1)	50(1)	50(1)	10(1)	11(1)	14(1)
N(2)	35(1)	45(1)	34(1)	-2(1)	6(1)	4(1)
O(2)	40(1)	43(1)	54(1)	3(1)	13(1)	7(1)
C(13)	37(1)	37(1)	40(1)	-4(1)	5(1)	1(1)
N(4)	41(1)	39(1)	38(1)	3(1)	7(1)	2(1)
C(19)	40(1)	35(1)	42(1)	0(1)	2(1)	7(1)
C(11)	39(1)	44(1)	30(1)	5(1)	12(1)	8(1)
N(1)	39(1)	44(1)	38(1)	4(1)	0(1)	-1(1)
C(20)	36(1)	40(1)	42(1)	-4(1)	4(1)	-3(1)
C(12)	44(1)	40(1)	32(1)	2(1)	15(1)	1(1)
C(17)	42(1)	46(1)	52(2)	2(1)	9(1)	8(1)
C(18)	35(1)	41(1)	39(1)	-2(1)	6(1)	1(1)
C(14)	47(2)	42(1)	42(2)	5(1)	6(1)	3(1)
C(10)	40(1)	66(2)	41(2)	-6(1)	5(1)	-2(1)
C(2)	60(2)	92(3)	44(2)	-8(2)	3(2)	-32(2)
C(15)	50(2)	51(2)	45(2)	0(1)	11(1)	-6(1)
C(7)	54(2)	51(2)	39(1)	13(1)	24(1)	20(1)
C(4)	66(2)	45(1)	39(2)	-5(1)	23(1)	-7(1)
C(3)	79(2)	59(2)	51(2)	-14(2)	24(2)	-23(2)
C(8)	40(2)	84(2)	47(2)	22(2)	10(1)	21(2)
C(1)	45(2)	69(2)	48(2)	9(1)	-1(1)	-7(1)
C(21)	41(1)	53(2)	50(2)	4(1)	10(1)	-3(1)
C(6)	76(2)	50(2)	56(2)	13(1)	32(2)	24(2)
C(16)	39(1)	53(2)	55(2)	3(1)	15(1)	4(1)
C(5)	95(3)	38(1)	61(2)	-1(1)	43(2)	8(2)
C(9)	39(2)	96(2)	45(2)	8(2)	3(1)	7(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [CuL(phen)].

x	y	z	U(eq)
H(19)	9652	332	4125	47
H(17)	11195	729	3153	55
H(14)	9050	3712	1577	52
H(10)	4524	2505	2779	59
H(2)	9592	5556	6232	79
H(15)	10938	3212	1166	58
H(3)	8246	6992	5755	74
H(8)	3280	5681	2743	68
H(1)	9202	3724	5644	65
H(21A)	6495	502	6653	71
H(21B)	6708	-652	6124	71
H(21C)	5447	-13	5907	71
H(6)	4512	7148	3802	71
H(16)	12027	1707	1951	58
H(5)	6209	7602	4798	74
H(9)	3072	3837	2213	72