Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Synthesis of Cu(II) Schiff base complex using a bidentate N_2O_2 donor ligand: Crystal structure, photophysical properties and antibacterial activities

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Figure Captions

Fig. S1 ^{1}H NMR spectrum of HL in DMSO-d_6

Fig. S2 ^{13}C NMR spectrum of HL in DMSO-d_6

Fig. S3 (a) The two-dimensional structure of HL viewed along the [100] direction; (b) The three-dimensional structure of HL formed by C-H---Cl, C-H--- π and C-H---O hydrogen bonds. Dotted lines represent the weak interactions.

Fig. S4 The FTIR spectra of HL and Cu(II) complex

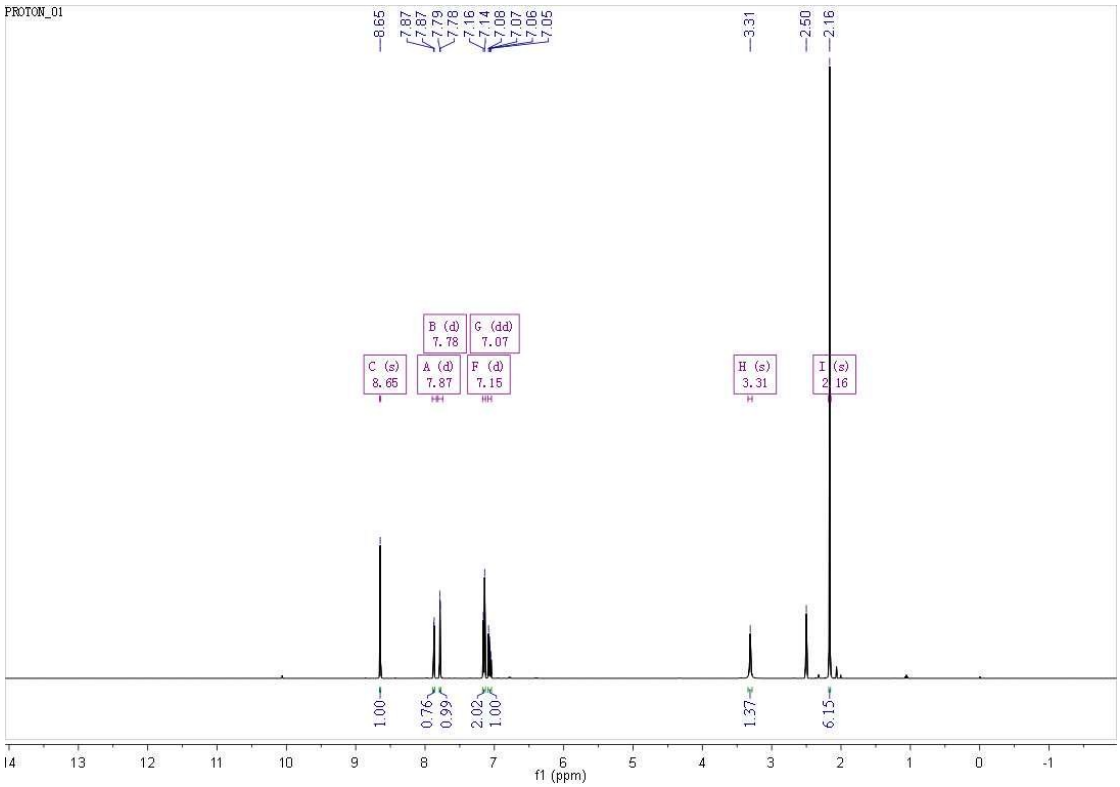


Fig. S1 ^{1}H NMR spectrum of HL in DMSO-d_6

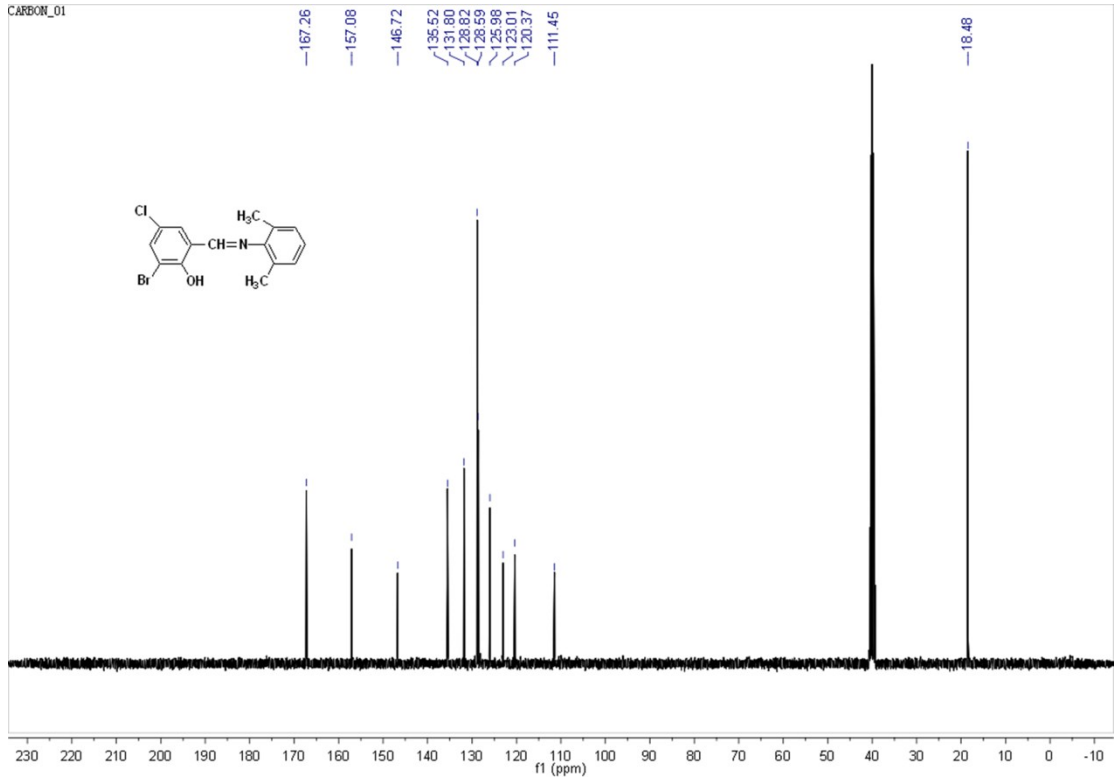
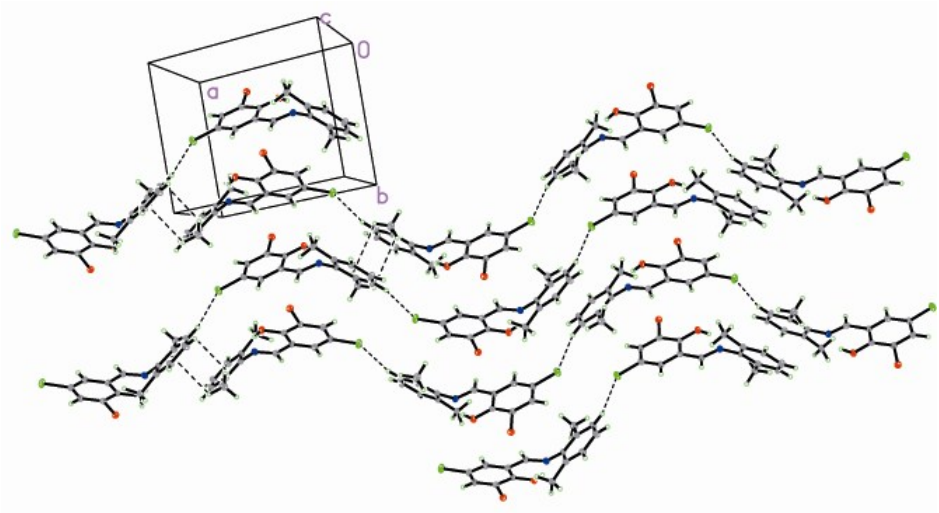
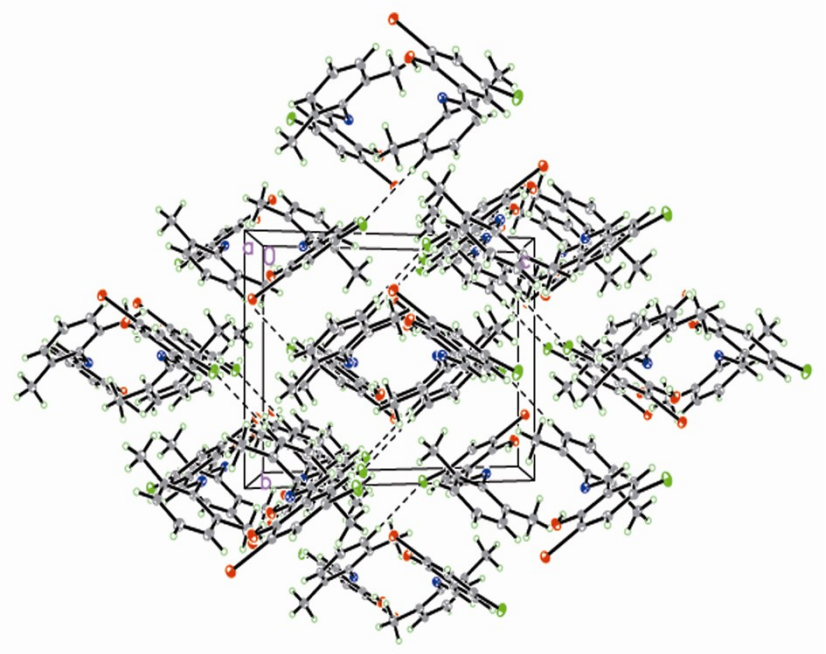


Fig. S2 ^{13}C NMR spectrum of HL in DMSO-d_6



(a)



(b)

Fig. S3 (a) The two-dimensional structure of HL viewed along the [100] direction;
(b) The three-dimensional structure of HL formed by C-H---Cl, C-H--- π and C-H---O hydrogen bonds. Dotted lines represent the weak interactions.

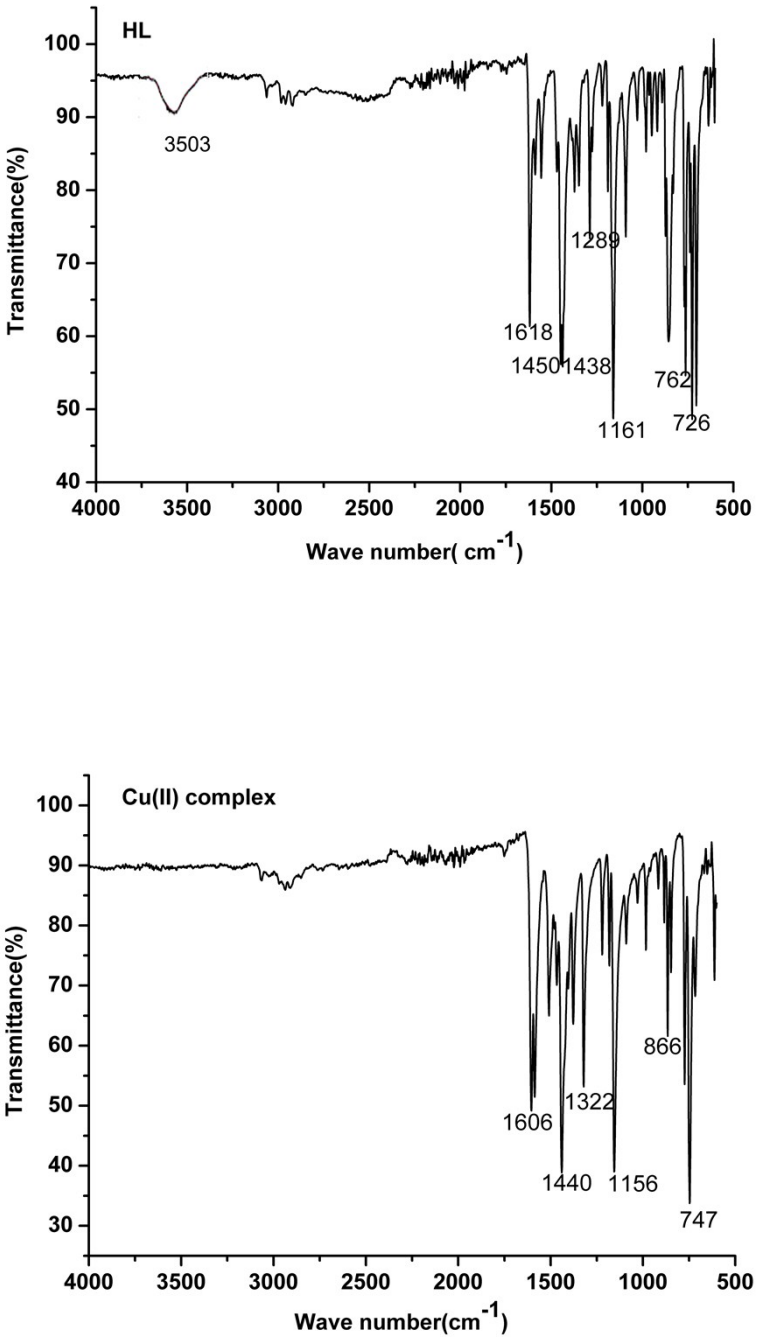


Fig. S4 The FTIR spectra of HL and Cu(II) complex

Table captions:

Table S1 Selected bond lengths (nm) and bond angles (º) for HL and Cu(II) complex

Table S2 Parameters of hydrogen bonds and halogen-halogen interaction for HL and Cu(II) complex

Table S1 Selected bond lengths (nm) and bond angles (°) for HL and Cu(II) complex

Bonds	*d*	Bonds	*d*	Bonds	*d*
HL					
Br(1)-C(2)	0.1890(2)	Cl(1)-C(4)	0.1729(2)	O(1)-C(1)	0.1343(3)
N(1)-C(7)	0.1276(3)	N(1)-C(8)	0.1437(3)	C(6)-C(7)	0.1457(3)
O(1)-H(1O)	0.093(3)	C(8)-C(9)	0.1407(3)	C(7)-H(7)	0.09500
Cu(II) complex					
Cu(1)-O(1)$^{\#1}$	0.18841(12)	Cu(1)-O(1)	0.18841(12)	Cu(1)-N(1)	0.19772(15)
Cu(1)-N(1)$^{\#1}$	0.19772(15)	Br(1)-C(3)	0.18899(18)	Cl(1)-C(5)	0.17495(18)
O(1)-C(2)	0.1295(2)	N(1)-C(7)	0.1292(2)	N(1)-C(8)	0.1446(2)
C(7)-H(7)	0.09500	C(1)-C(7)	0.1441(2)	C(5)-C(6)	0.1368(3)
Angle	ω	Angle	ω	Angle	ω
HL					
C(1)O(1)H(1O)	103.1(19)	C(7)N(1)C(8)	118.7(2)	O(1)-C(1)-C(2)	119.9(2)
O(1)-C(1)-C(6)	121.9(2)	C(3)-C(2)-Br(1)	119.69(17)	C(1)-C(2)-Br(1)	118.62(16)
C(1)C(6)C(7)	120.3(2)	N(1)C(7)C(6)	122.3(2)	C(5)C(4)Cl(1)	119.58(18)
C(3)C(4)Cl(1)	119.20(18)	C(6)C(1)C(2)	118.2(2)	C(2)C(3)C(4)	118.8(2)
Cu(II) complex					
O(1)$^{\#1}$Cu(1)O(1)	156.81(8)	O(1)$^{\#1}$Cu(1)N(1)	92.75(6)	O(1)Cu(1)N(1)	93.13(6)
O(1)$^{\#1}$Cu(1)N(1)$^{\#1}$	93.13(6)	O(1)Cu(1)N(1)$^{\#1}$	92.75(6)	N(1)Cu(1)N(1)$^{\#1}$	150.41(9)
C(2)O(1)Cu(1)	127.53(12)	C(7)N(1)C(8)	116.08(15)	C(7)-N(1)-Cu(1)	123.05(12)
C(8)-N(1)-Cu(1)	120.41(11)	C(6)-C(1)-C(7)	116.40(16)	O(1)-C(2)-C(1)	124.45(15)
C(4)-C(3)-Br(1)	119.32(13)	C(2)-C(3)-Br(1)	117.66(13)	C(6)-C(5)-Cl(1)	119.55(15)
C(4)-C(5)-Cl(1)	119.21(14)	N(1)-C(7)-C(1)	126.26(16)	C(9)-C(8)-N(1)	118.05(16)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1,y,-z+1/2

Table S2 Parameters of hydrogen bonds and halogen-halogen interaction for HL and Cu(II) complex

Compound	D—H…A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
HL	C(12)-H(12)…Cl(1)^{i}	0.0950	0.2890	0.3803	161.4
	C(14)-H(14c)…O(1)^{ii}	0.0980	0.2706	0.3145	107.7
	C(15)-H(15)…Cg	0.0980	0.3201	0.3615	107.3
Cu(II) complex	C(14)-H(14C)---Cl(1)$^{\#2}$	0.1749	0.2911	0.3776	168.5
	C(10)-H(10)…Cg$^{\#3}$	0.0950	0.2826	0.3470	125.4