

Supporting information

Halogen-bonding contacts determining the crystal structure and fluorescence properties of organic salts

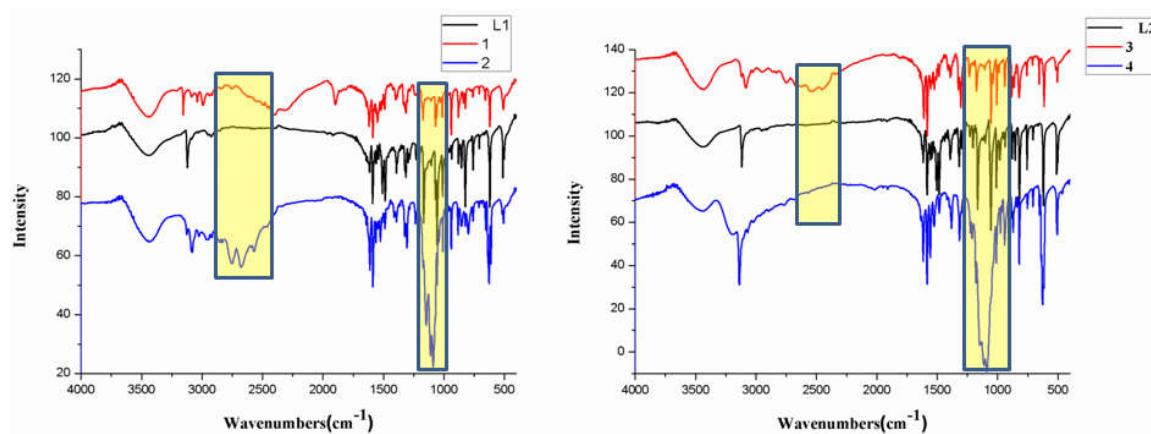


Fig. S1 IR spectra of compounds *L*₁, *L*₂ and salts **1-4**. The differences are highlighted.

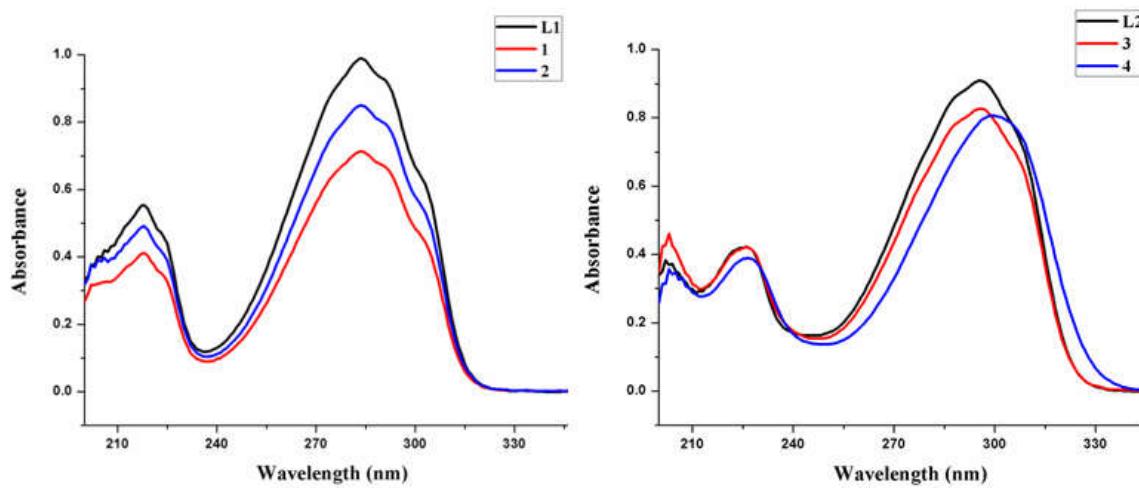
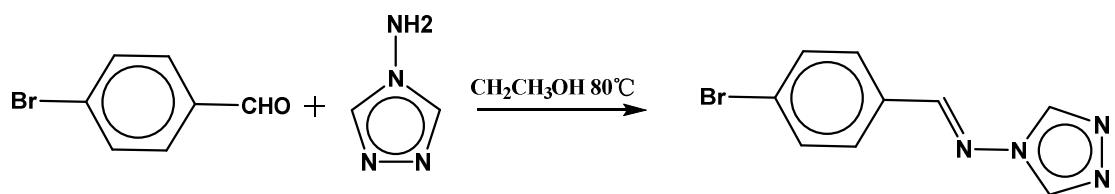


Fig. S2 UV-visible absorption spectra for ligand *L*₁, *L*₂ and salts **1-4** in methanol solution (2.5×10^{-6} mol L⁻¹).

Table S1 Geometrical parameters for halogen bonds in compounds L_1 , L_2 and crystals **2**, **3**.

Y-X···D	X···D (Å)	Symmetry operation
Compound L_1		
Br···N1	3.296	-1.5+x, 1.5-y, 1/2+z
Compound L_2		
I···N1	3.210	-1.5+x, 1/2-y, 1/2+z
crystal 2		
O4···Br1	3.240	2-x, 2-y, 2-z
C4···Br1	3.524	1-x, 2-y, 2-z
crystal 3		
Cl···I	3.344	1+x, -2+y, z
Cl···C1	3.376	-x, 2-y, 1-z



Scheme S1 The synthetic route for compound L_1 .



Scheme S2 The synthetic route for compound L_2 .

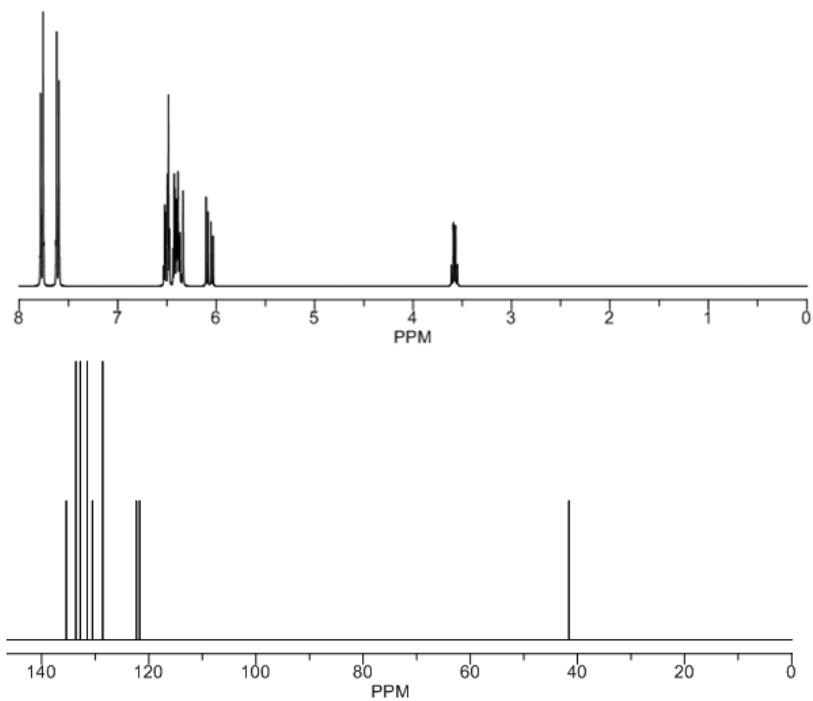


Fig. S3 ^1H NMR and ^{13}C NMR of compound L_1 .

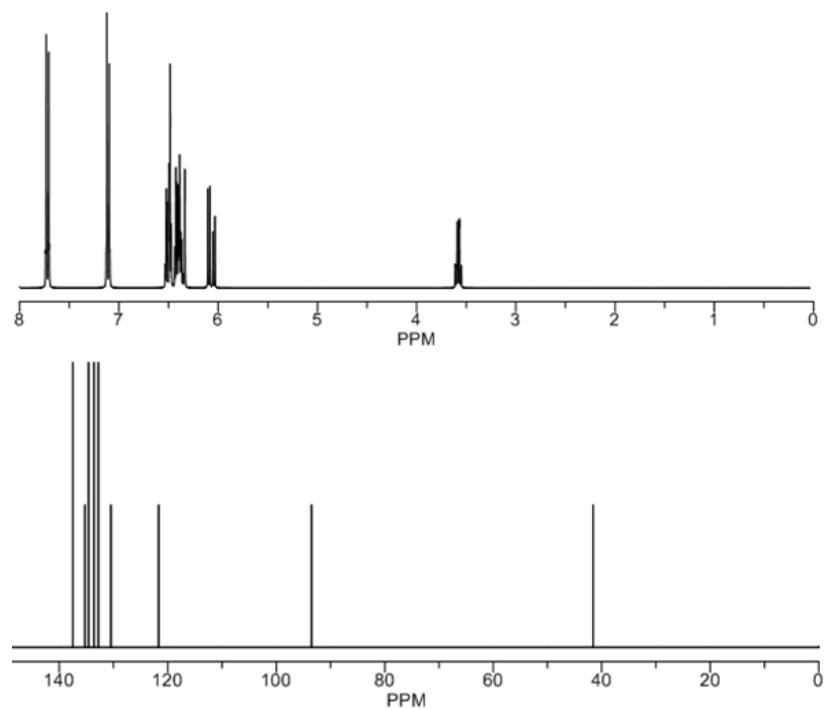


Fig. S4 ^1H NMR and ^{13}C NMR of compound L_2 .