

Electronic Supporting Information

Silver(I) Coordination Polymers Based on Halogenated Cyanoforamidine: Roles of Oxyanions and Halogen Atoms in the Structural Diversity

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Fig. S1. The PXRD patterns for **1**.

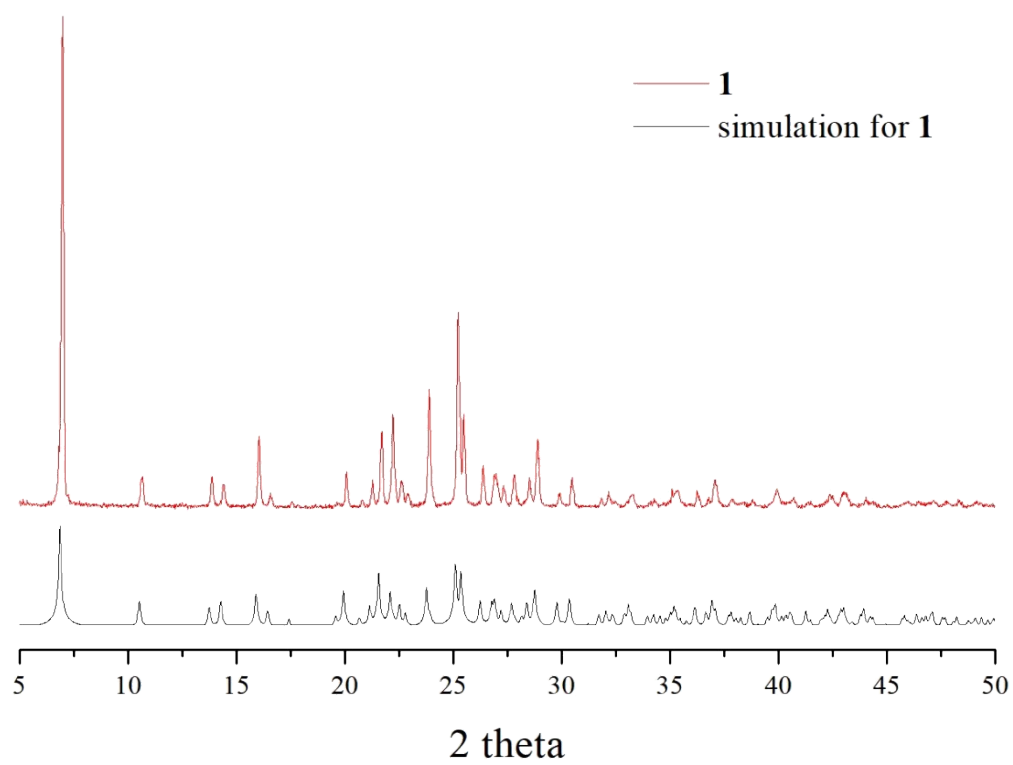


Fig. S2. The PXRD patterns for **2**.

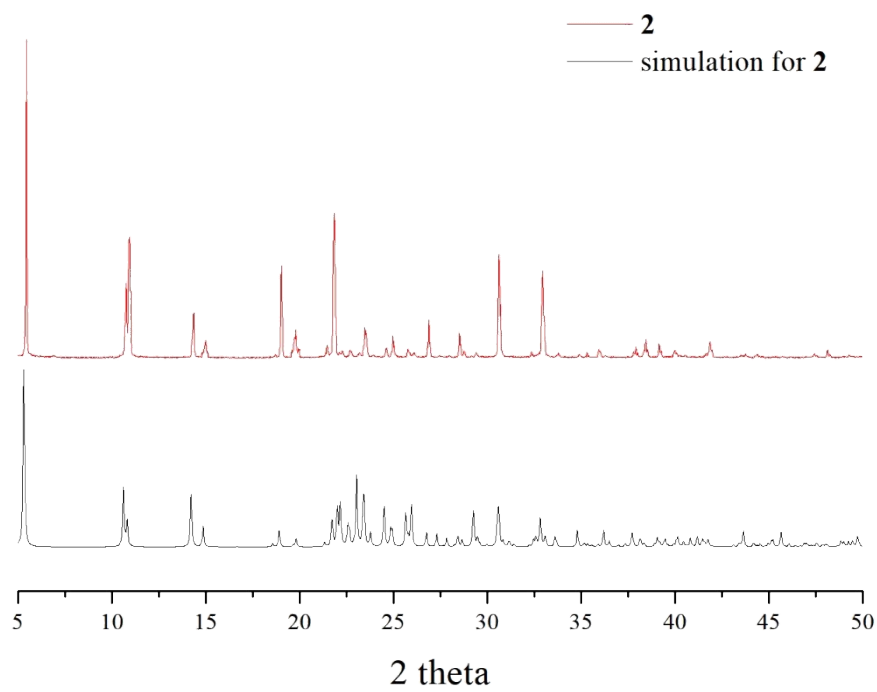


Fig. S3. The PXRD patterns for **3**.

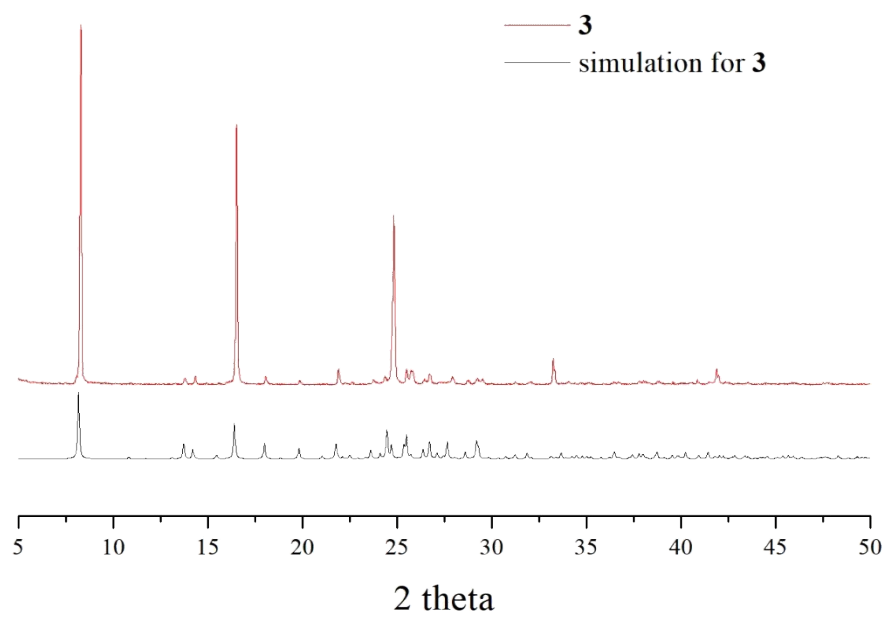


Fig. S4. The PXRD patterns for **4**.

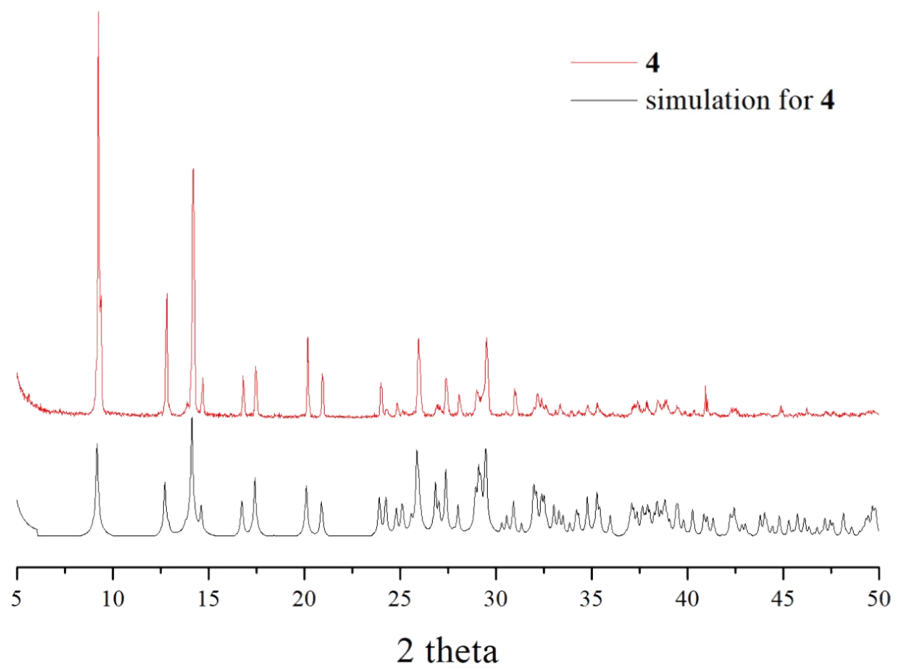


Fig. S5. The PXRD patterns for **5**.

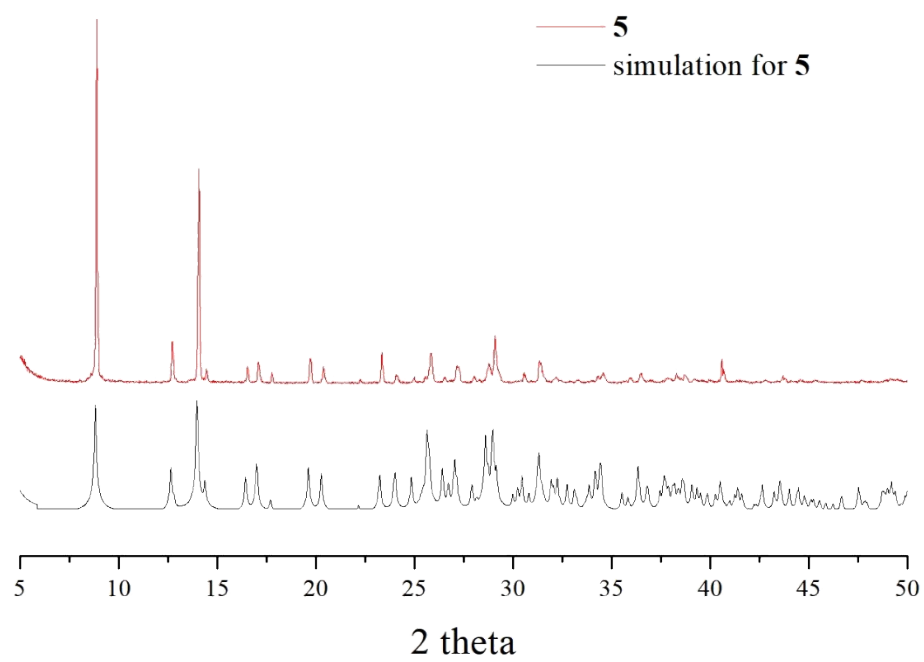


Fig. S6. The PXRD patterns for **6**.

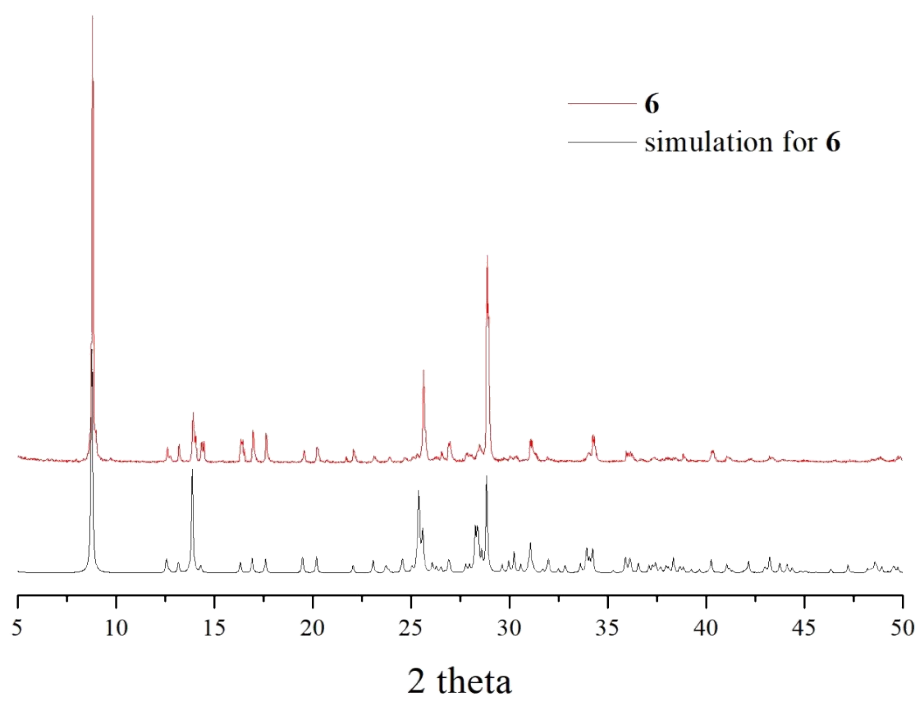


Fig. S7. Hirshfeld surfaces and fingerprint plots for O-H interaction (a) **4**, (b) **5** and (c) **6**.

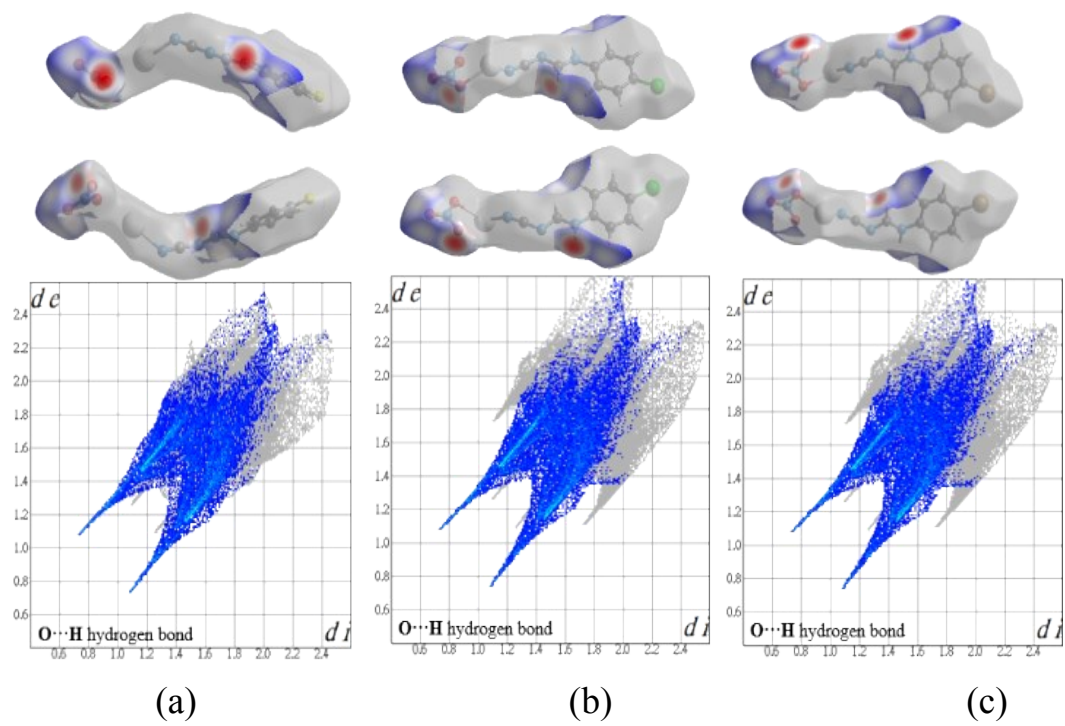


Fig. S8. Fingerprint plots for Ag-Ag interaction (above) and X-H interaction (below) (a) **4**, (b) **5** and (c) **6**.

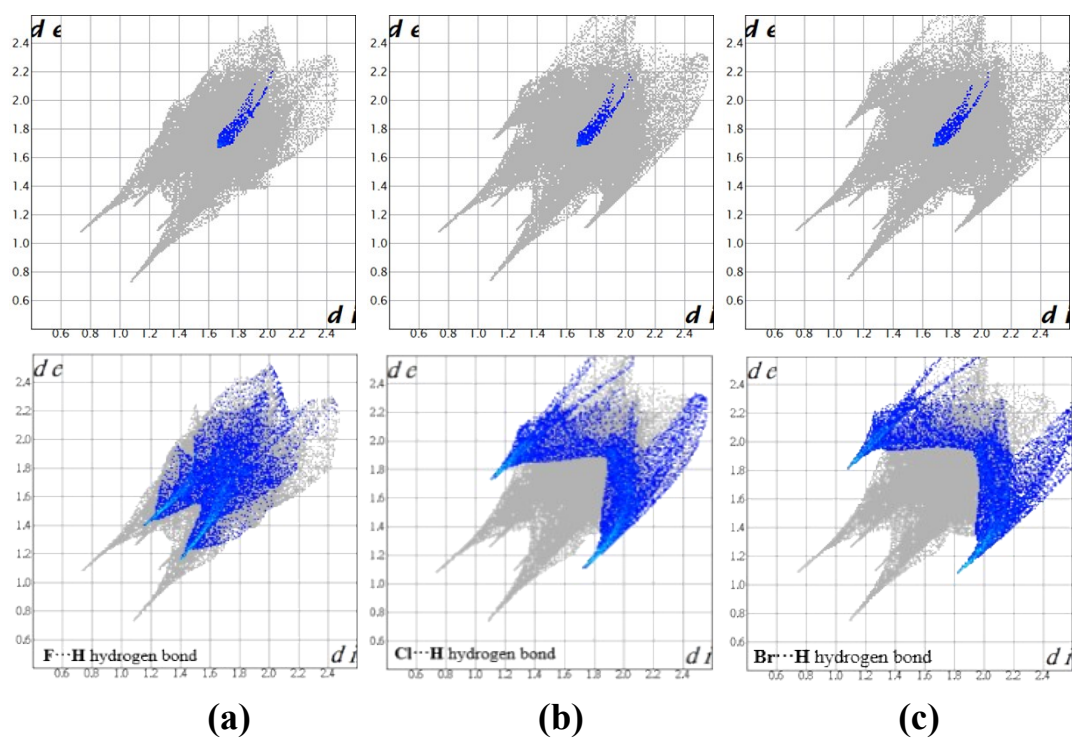


Fig. S9. Hirshfeld surfaces and fingerprint plots for Ag-O interaction (a) 4, (b) 5 and (c) 6.

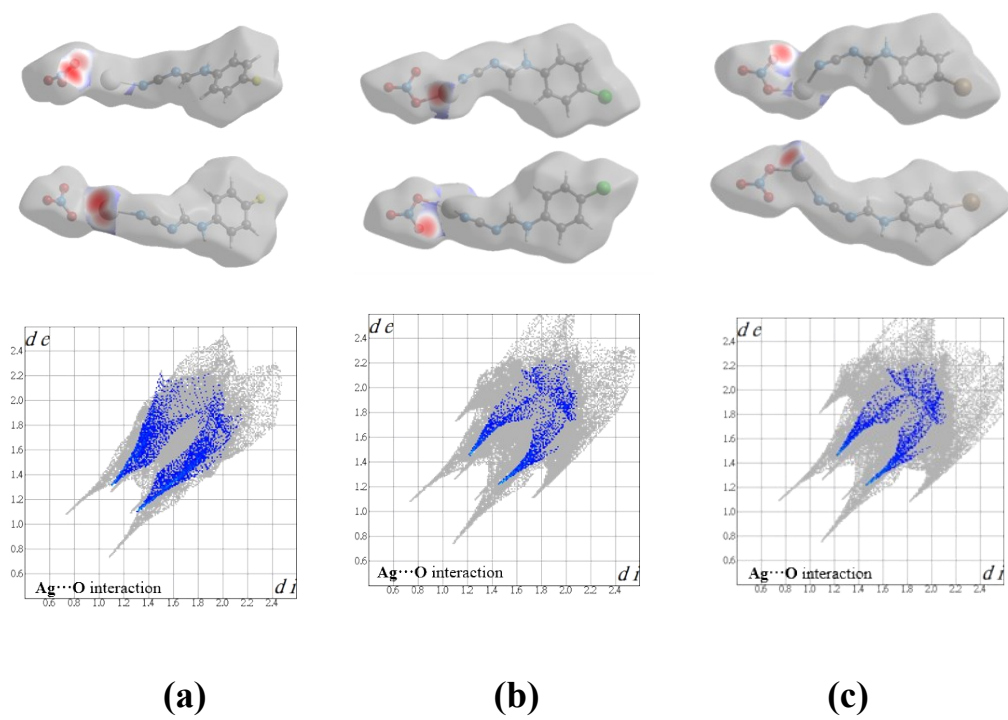


Fig. S10. Hirshfeld surfaces and fingerprint plots for π -- π interaction (a) 4, (b) 5 and (c) 6.

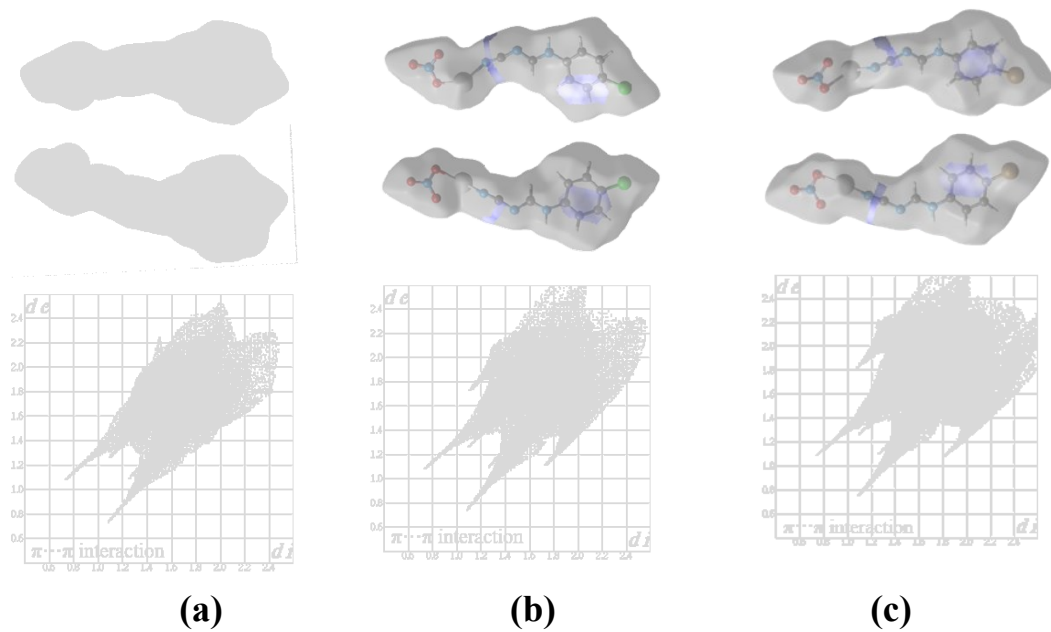


Fig. S11. Hirshfeld surfaces for X-H interaction (a) **4**, F-H (b) **5** Cl-H and (c) **6**. Br-H interaction.

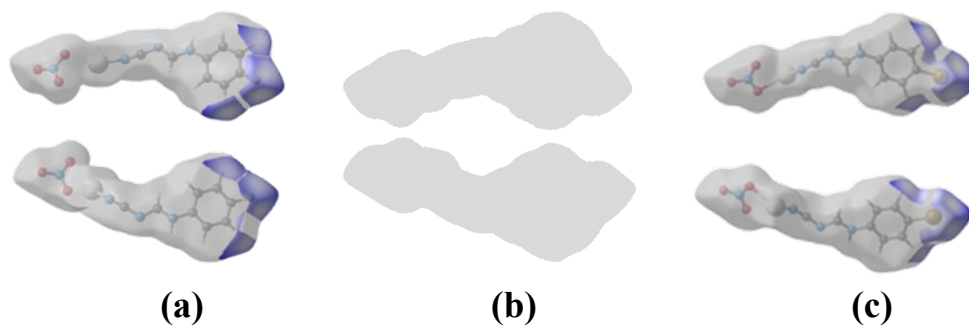


Fig. S12. Crystal void (isovalue 0.002 e au⁻³) along a-axis for (a) **4**, (b) **5** and (c) **6**.

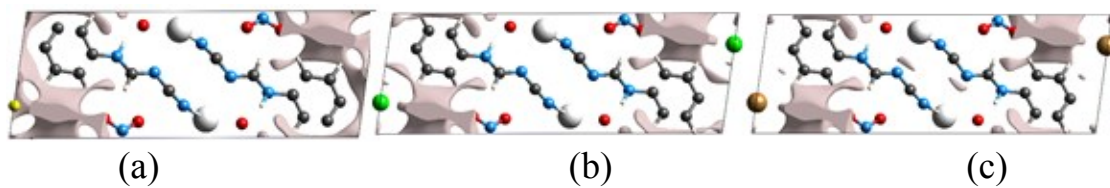


Fig. S13. Hirshfeld surfaces for Ag-Ag interaction (a) **4**, (b) **5** and (c) **6**.

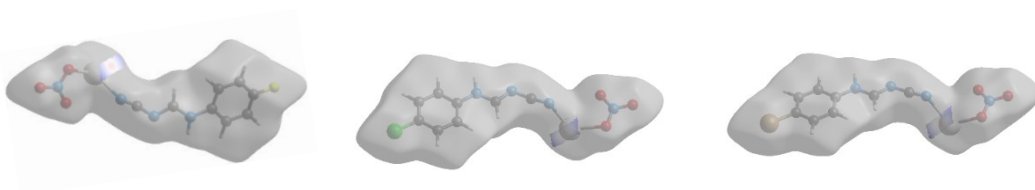


Fig. S14. Uv-Vis spectra of the free ligands in ethanol.

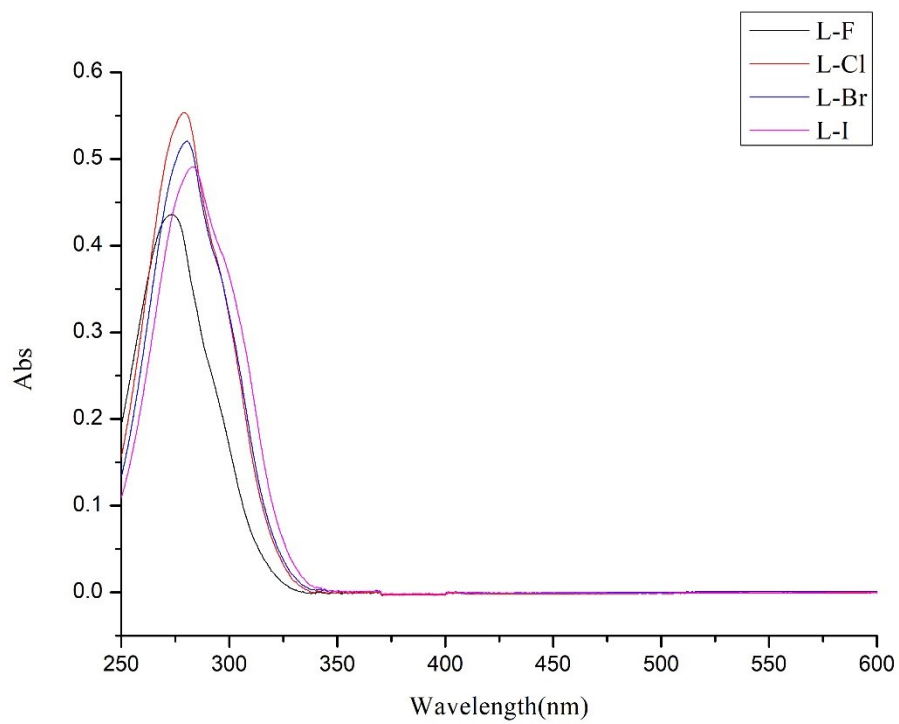


Fig. S15. Solid state UV-vis absorption spectra for ligands and complexes

1 – 3.

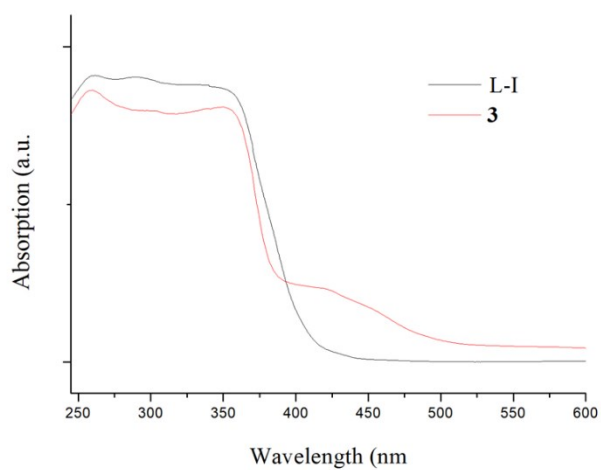
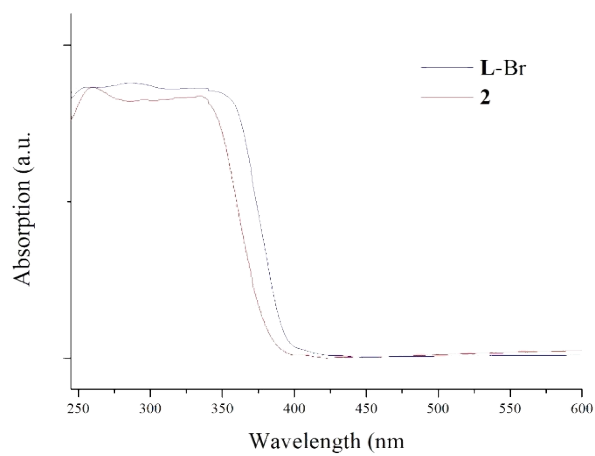
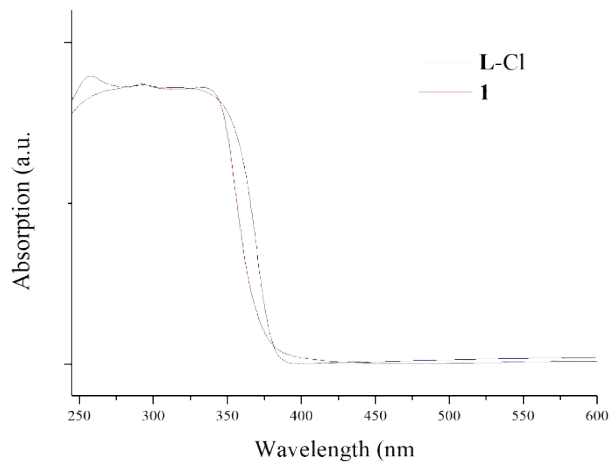


Fig. S16. Solid state UV-vis absorption spectra for ligands and complexes **4** – **6**.

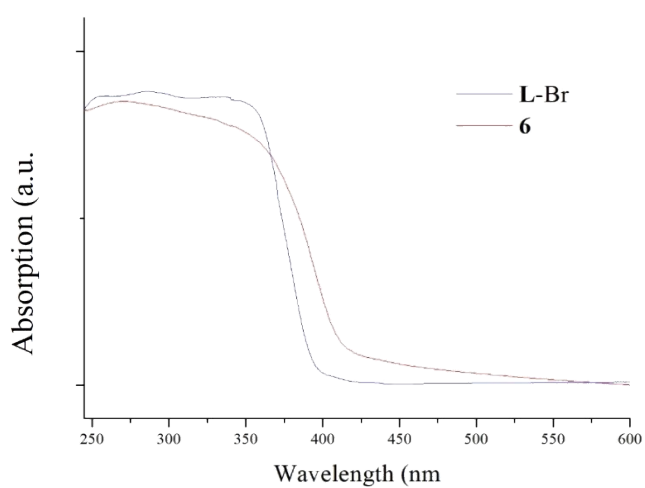
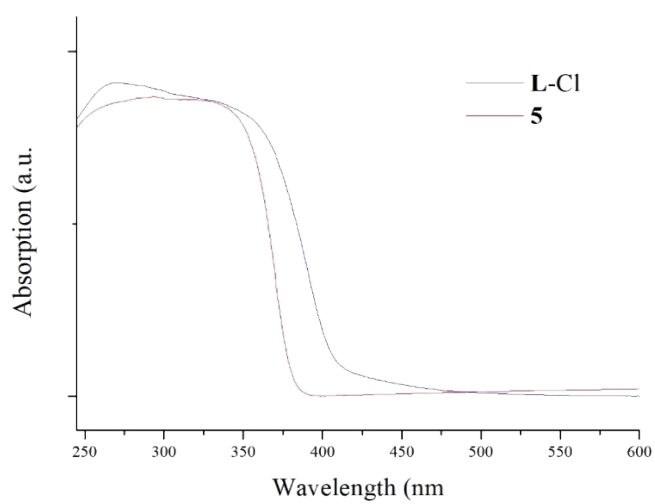
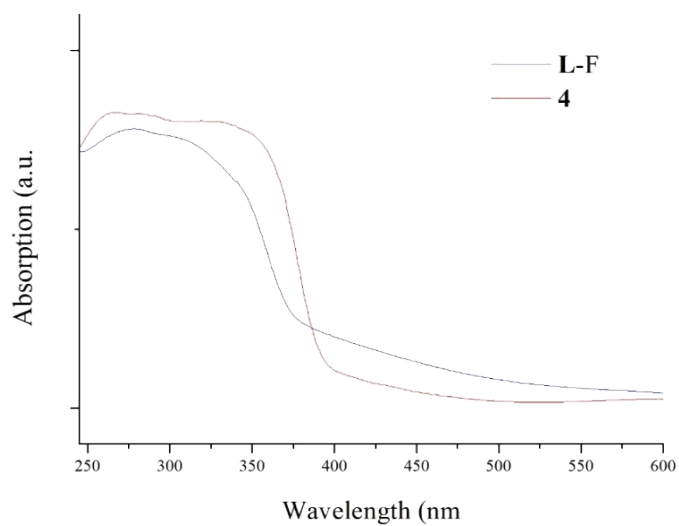


Table S1. Selected distances (Å) and angles (°) of the weak C-H---X hydrogen bonds in **4** – **6**.

		4		
C-H---F	H---F	∠C-H---F	C---F	
C(7) ⁱ -H(7A) ⁱ ---F	2.725	160.18	3.615(6)	
C(5) ⁱⁱ -H(5A) ⁱⁱ ---F	2.788	131.18	3.472(5)	Sy
C(5) ⁱⁱⁱ -H(5A) ⁱⁱⁱ ---F	2.873	146.42	3.684(5)	mm
		5		etry
C-H---Cl	H---Cl	∠C-H---Cl	C---Cl	cod
C(5) ⁱ -H(5A) ⁱ ---Cl	3.063	155.62	3.929(5)	e: (i)
C(7) ⁱⁱ -H(7A) ⁱⁱ ---Cl	3.174	129.51	3.834(5)	1 –
C(7) ⁱⁱⁱ -H(7A) ⁱⁱⁱ ---Cl	3.000	154.06	3.859(5)	x, 1
		6		– y,
C-H---Br	H---Br	∠C-H---Br	C---Br	– z;
C(5) ⁱ -H(5A) ⁱ ---Br	3.142	155.33	4.008(7)	(ii)
C(7) ⁱⁱ -H(7A) ⁱⁱ ---Br	3.293	129.36	3.949(6)	1 –
C(7) ⁱⁱⁱ -H(7A) ⁱⁱⁱ ---Br	3.068	154.94	3.930(7)	x, –
				y, –
				z;
				(iii)
				2-x,
				– y, –
				z, for 4 and 5 . (i) 1 – x, 2 – y, 2 – z; (ii) 1 – x, 3 – y, 2 – z; (iii) –x, 3 – y, 2 –
				z, for 6 .

Table S2. Selected bond lengths (Å) and angles (°) for **1 - 3**.

	1	2	3
N(1)-C(1)	1.143(5)	1.141(6)	1.157(8)
N(2)-C(1)	1.332(5)	1.328(6)	1.308(8)
N(2)-C(2)	1.328(4)	1.325(5)	1.296(7)
N(3)-C(2)	1.295(4)	1.291(5)	1.305(7)
N(3)-C(3)	1.418(4)	1.416(5)	1.409(7)
N(4)-C(9)			1.137(8)
N(5)-C(9)			1.304(8)
N(5)-C(10)			1.288(8)
N(6)-C(10)			1.303(7)
N(6)-C(11)			1.422(8)

Table S3. Selected bond lengths (Å) and angles (°) for **4 - 6**.

	4	5	6
N(1)-C(1)	1.155(4)	1.154(6)	1.143(7)
N(2)-C(1)	1.313(4)	1.315(6)	1.307(8)
N(2)-C(2)	1.321(4)	1.320(6)	1.312(9)
N(3)-C(2)	1.306(4)	1.308(6)	1.297(7)
N(3)-C(3)	1.418(4)	1.427(5)	1.420(8)
