Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Materials

Diverse Ag(I) complexes constructed from asymmetric pyridyl- and pyrimidyl amide ligands: roles of Ag---Ag and π-π interactions

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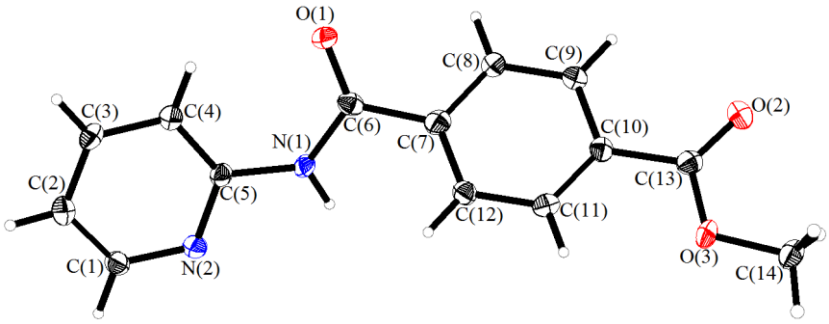
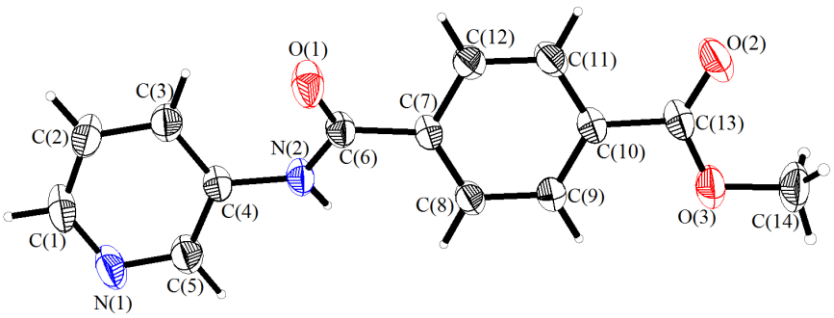
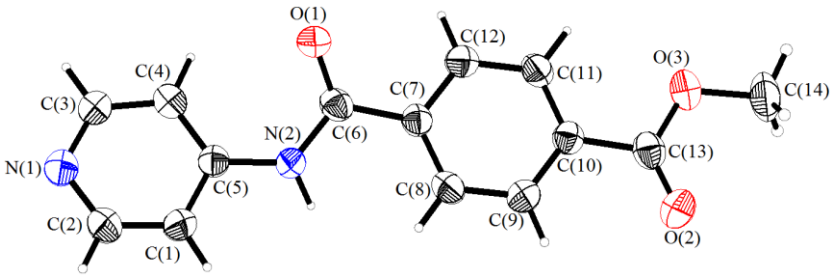
Fig. S1. The molecular structures of (a) $\mathbf{L}^{1}$, (b) $\mathbf{L}^{2}$ and (c) $\mathbf{L}^{3}$.



(a)



(b)



(c)

Fig. S2. A packing diagram of **4** showing that the cations are linked by the ClO_4^- anions to form a 2D net.

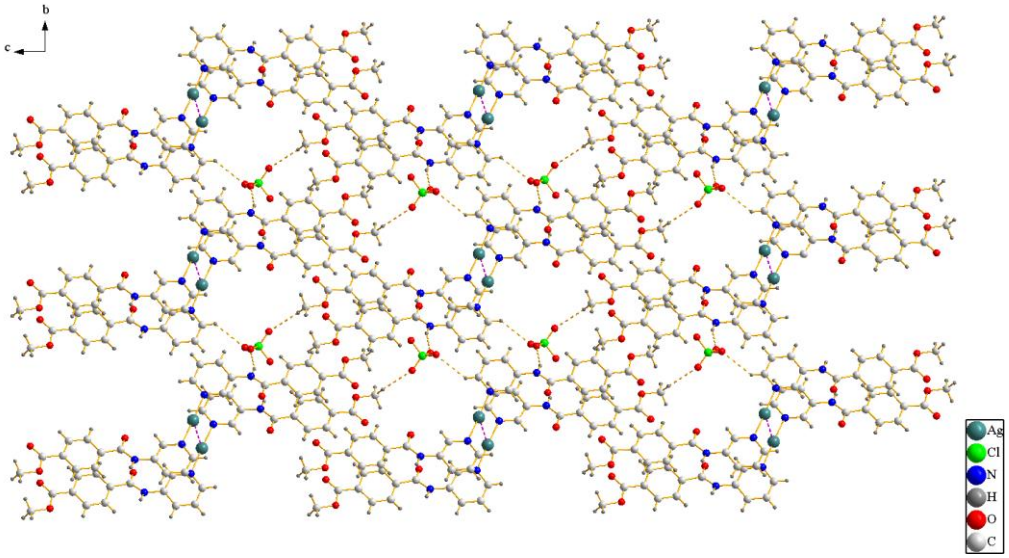


Fig. S3. The molecules of **5** are interlinked through C-H---O hydrogen bonds to form a 2D net.

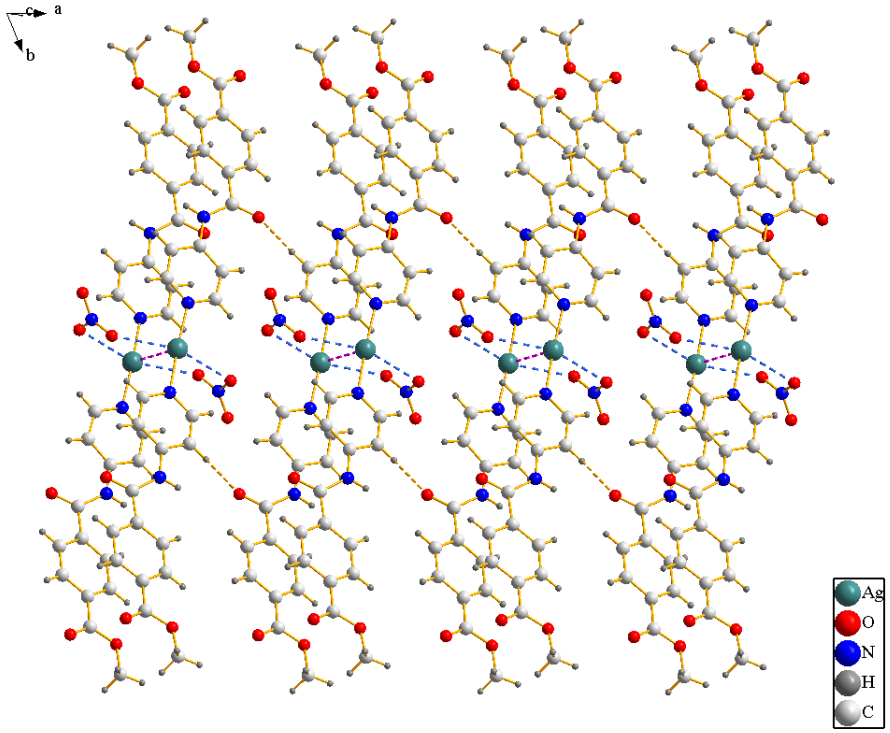


Fig. S4. The cations of **6** are interlinked by the ClO_4^- anions to form a 2D net.

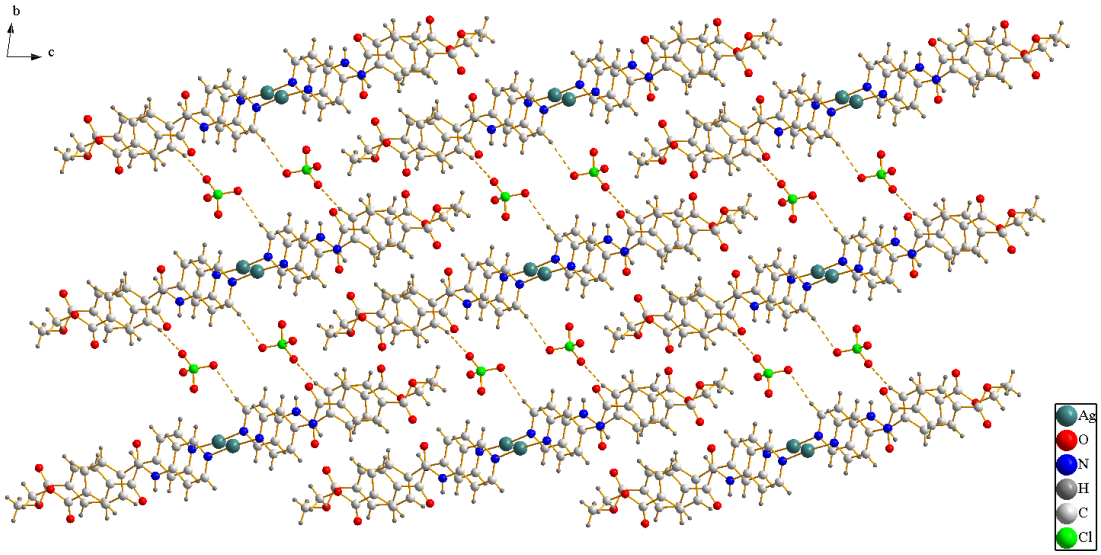
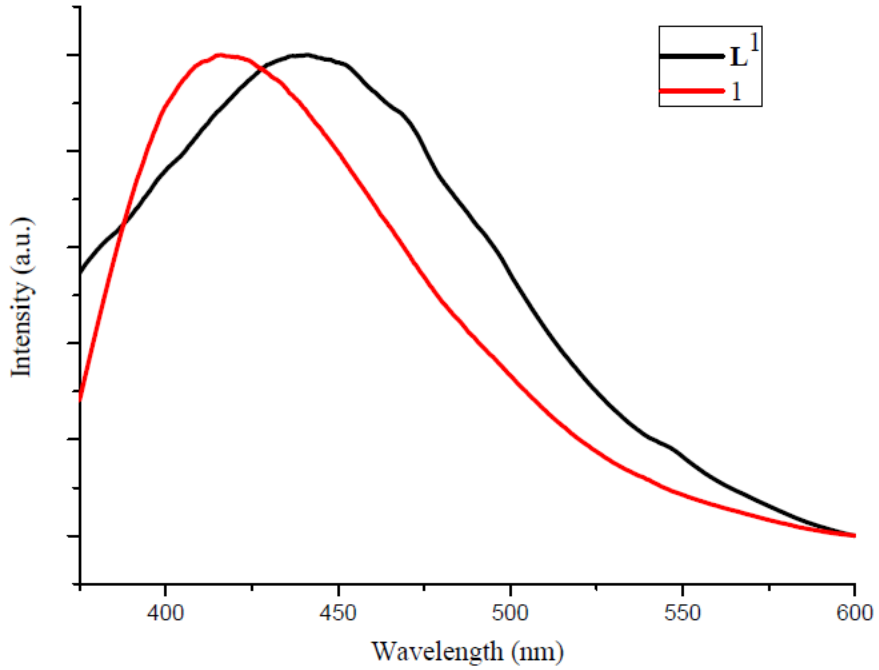
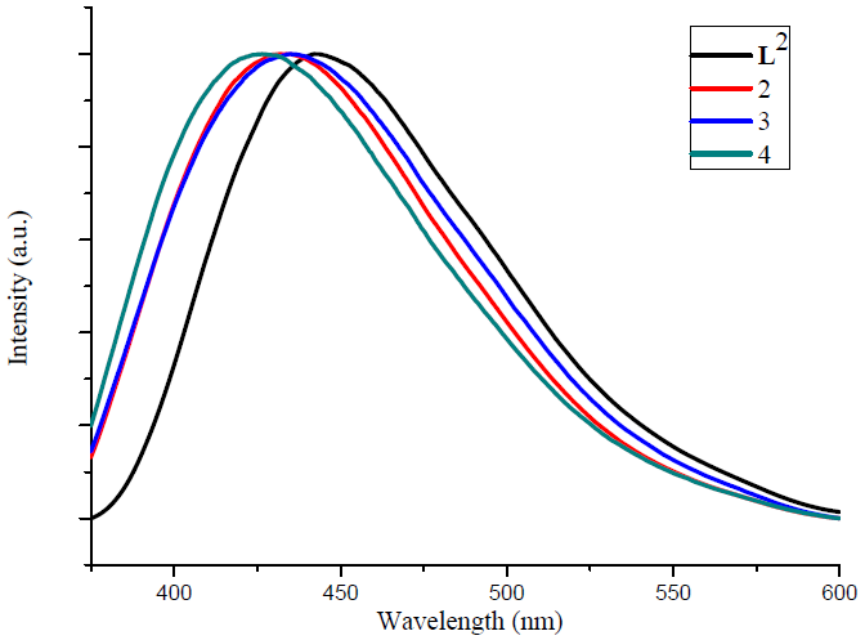


Fig. S5. Fluorescent emission spectra of (a) **1**, (b) **2** – **4**, (c) **5** - **6** and (d) **7** – **9** and their corresponding ligands.

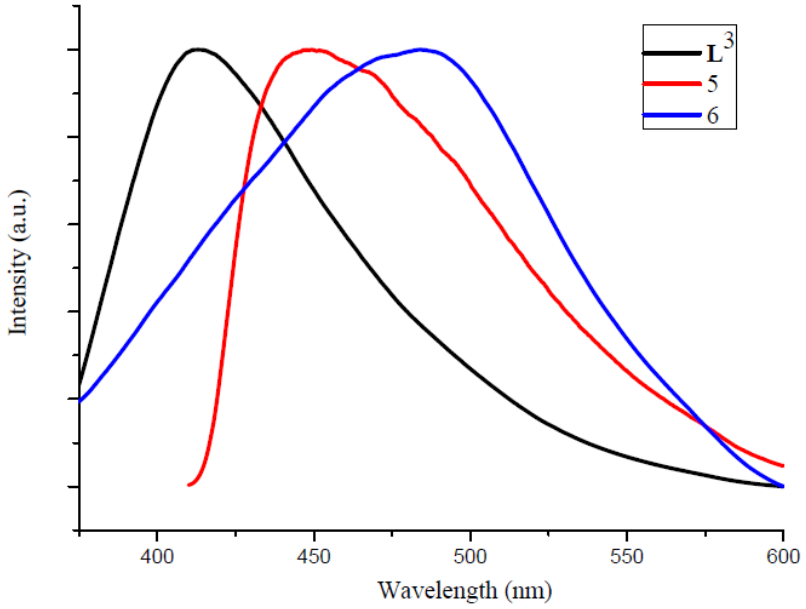


(a)

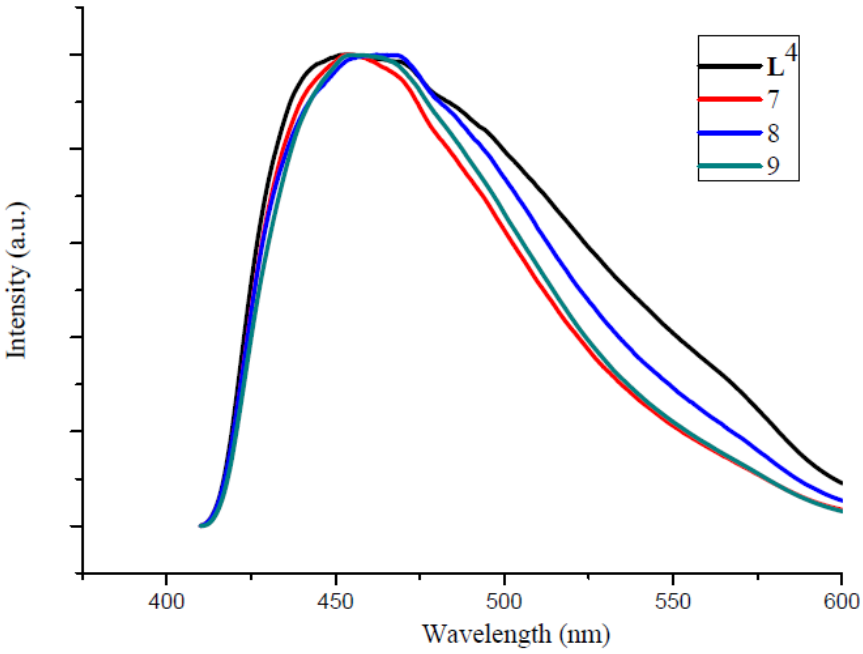


(b)

Fig. S5. Fluorescent emission spectra of (a) **1**, (b) **2** – **4**, (c) **5** - **6** and (d) **7** – **9** and their corresponding ligands. (cont.)

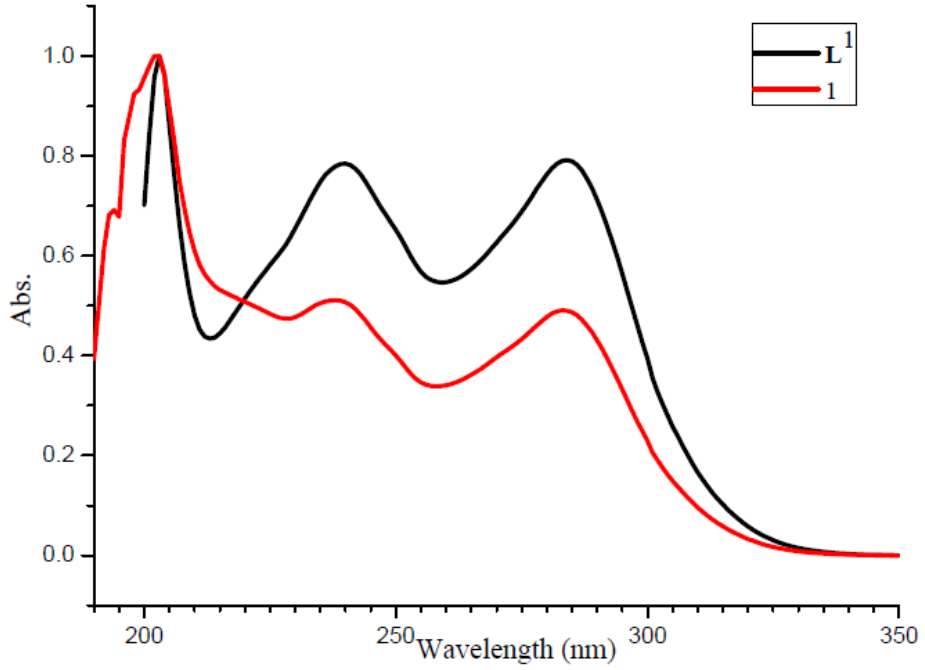


(c)

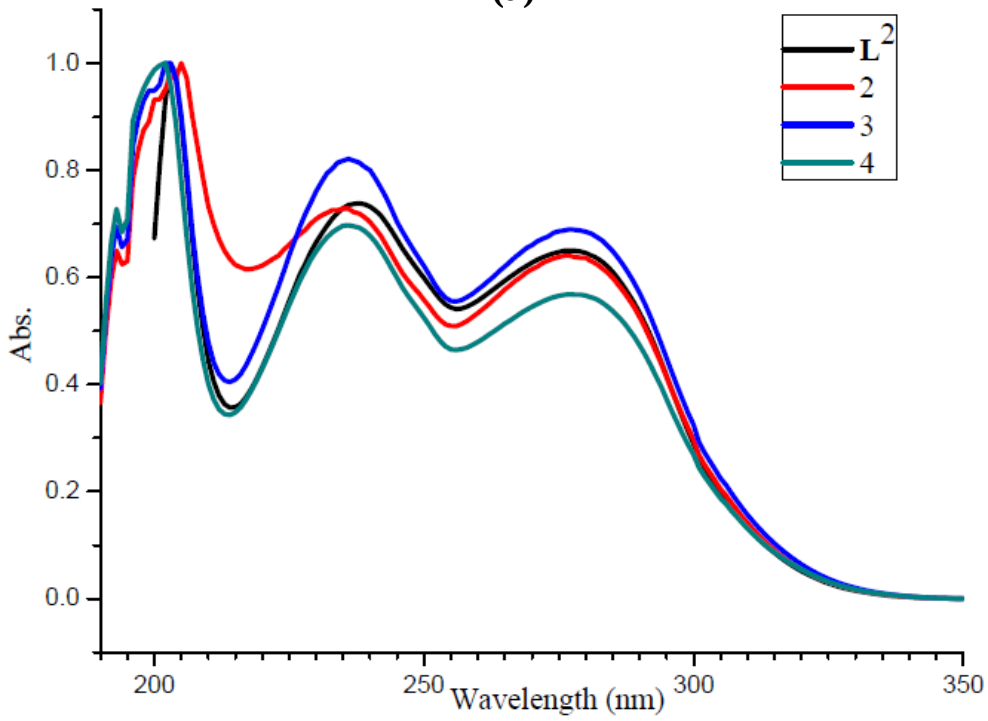


(d)

Fig. S6. Uv spectra of (a) **1**, (b) **2** – **4**, (c) **5** - **6** and (d) **7** – **9** and their corresponding ligands.

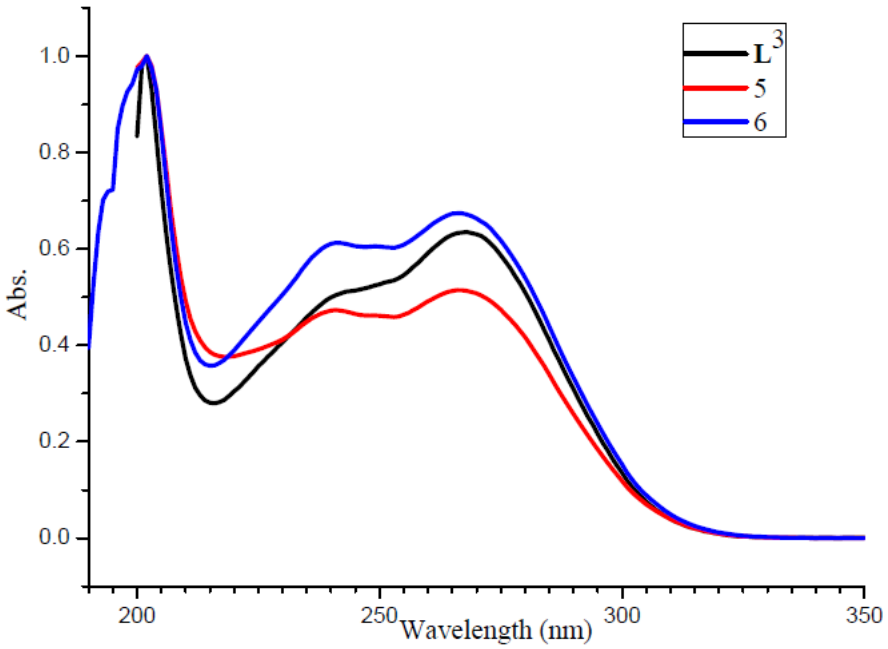


(a)

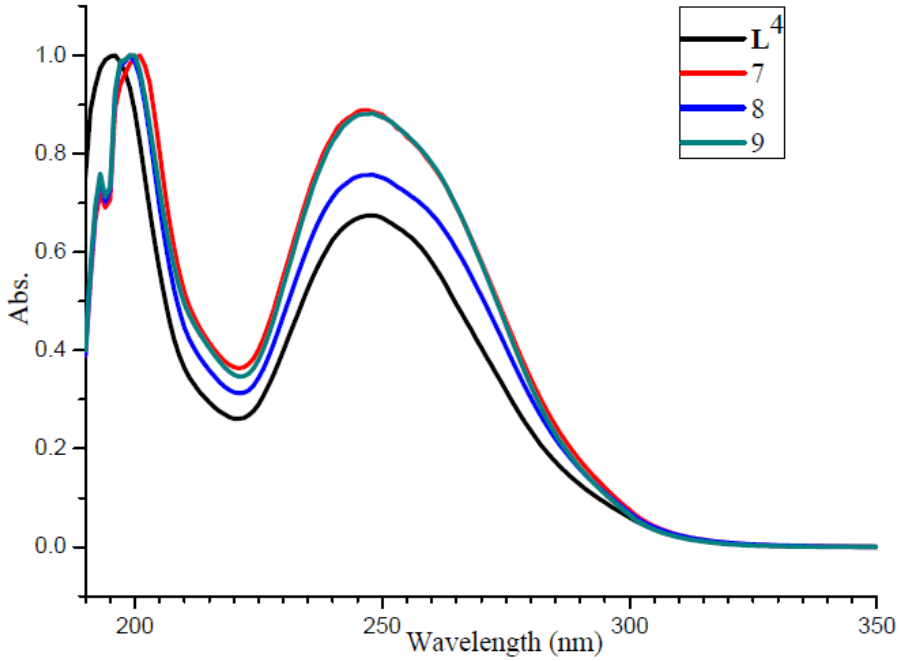


(b)

Fig. S6. Uv spectra of (a) **1**, (b) **2** – **4**, (c) **5** - **6** and (d) **7** – **9** and their corresponding ligands. (cont.)



(c)



(d)

Table S1. Selected bond distances (Å) and angles (°) for **1** – **6**.

1			
Ag(1)-N(1)	2.196 (2)	N(1)-Ag(1)-O(7)	129.1 (1)
Ag(1)-O(7)	2.372 (2)	N(1)-Ag(1)-O(10)	139.6 (1)
Ag(1)-O(10)	2.365 (2)	O(10)-Ag(1)-O(7)	84.2 (1)
Ag(2)-N(3)	2.242 (2)	N(3)-Ag(2)-O(10)	173.0 (1)
Ag(2)-O(8A)	2.590 (2)	N(3)-Ag(2)-O(8A)	92.8 (1)
Ag(2)-O(10)	2.246 (2)	O(10)-Ag(2)-O(8A)	90.2 (1)
2			
Ag(1)-N(1)	2.191 (1)	N(1)-Ag(1)-N(1A)	180.0
Ag(2)-O(4)	2.291 (2)	O(4)-Ag(2)-O(5)	52.3 (1)
Ag(2)-O(5)	2.552 (1)	O(4)-Ag(2)-O(4B)	180.0
		O(5)-Ag(2)-O(5B)	180.0
3			
Ag-N(1)	2.159 (2)	N(1)-Ag-N(1A)	180.0
4			
Ag-N(1)	2.172(2)	N(1)-Ag-N(3)	173.6(1)
Ag-N(3)	2.178(2)		
5			
Ag-N(1)	2.138(2)	N(1)-Ag-N(3)	174.1(1)
Ag-N(3)	2.139(2)		
6			
Ag-N(1)	2.141(2)	N(4)-Ag-N(1)	174.6(1)
Ag-N(3)	2.141(2)		

Symmetry code A: -x + 2, -y - 2, -z for **1**; A: -x + 1, -y + 2, -z; B: -x + 2, -y + 1, -z for **2**; A: -x + 1, -y, -z for **3**; A: -x + 1, -y + 1, -z + 1 for **4**; A: -x + 1, -y , -z for **5**.

Table S2. Selected bond distances (Å) and angles (°) for **7 - 9**.

	7	**8**	**9**
Ag-N(4)	2.277(3)	2.275(5)	2.280(3)
Ag-N(1)	2.334(2)	2.337(4)	2.314(3)
Ag-O(4)	2.394(2)	2.391(4)	2.404(3)
Ag-O(1)	2.423(2)	2.411(4)	2.443(3)
N(4)-Ag-N(1)	166.5(1)	165.4(2)	169.0(1)
N(4)-Ag-O(4)	77.4(1)	77.7(2)	76.9(1)
N(1)-Ag-O(4)	93.1(1)	91.8(2)	94.8(1)
N(4)-Ag-O(1)	115.0(1)	115.7(2)	114.4(1)
N(1)-Ag-O(1)	73.6(1)	73.5(1)	73.8(1)
O(4)-Ag-O(1)	166.1(1)	164.3(1)	168.6(1)

Table S3. The Uv absorption wavelengths of $\mathbf{L^1}$ – $\mathbf{L^4}$ and **1** – **9** in CH_3CN (nm).

$\mathbf{L^1}$	203, 241, 285	**4**	202, 236, 277
$\mathbf{L^2}$	203, 240, 280	**5**	202, 241, 266
$\mathbf{L^3}$	202, 246,271	**6**	202, 241, 267
$\mathbf{L^4}$	196, 249	**7**	199, 248
1	199, 238, 283	**8**	198, 248
2	205, 235, 276	**9**	196, 247
3	202, 236, 277		

Table S4. The ^{1}H NMR chemical shifts of **1** – **9** in DMSO-d_6.

Complex	Chemical shifts (ppm)
1	11.00 (1H, s, NH), 8.40 (1H, d, H-py), 8.18 (1H, d, H-py), 8.11 (4H, dd, H-bz), 7.87 (1H, t, H-py), 7.20 (1H, t, H-py), 3.89 (3H, s, OCH_3)
2	10.70 (1H, s, NH), 8.97 (1H, d, H-py), 8.34 (1H, d, H-py), 8.22 (1H, d, H-py), 8.11 (4H, dd, H-bz), 7.47 (1H, q, H-py), 3.90 (3H, s, OCH_3)
3	10.69 (1H, s, NH), 8.97 (1H, d, H-py), 8.34 (1H, d, H-py), 8.22 (1H, d, H-py), 8.11 (4H, dd, H-bz), 7.46 (1H, q, H-py), 3.90 (3H, s, OCH_3)
4	10.70 (1H, s, NH), 8.93 (1H, d, H-py), 8.34 (1H, d, H-py), 8.20 (1H, d, H-py), 8.10 (4H, dd, H-bz), 7.47 (1H, q, H-py), 3.90 (3H, s, OCH_3)
5	10.90 (1H, s, NH), 8.52 (1H, d, H-py), 8.10 (4H, dd, H-bz), 7.86 (2H, d, H-py), 3.90 (3H, s, OCH_3)
6	10.83 (1H, s, NH), 8.50 (1H, d, H-py), 8.09 (4H, dd, H-bz), 7.82 (2H, d, H-py), 3.90 (3H, s, OCH_3)
7	11.23 (1H, s, NH), 8.76 (2H, d, H-pm), 8.06 (4H, dd, H-bz), 7.29 (1H, d, H-pm), 3.89 (3H, s, OCH_3)
8	11.24 (1H, s, NH), 8.79 (2H, d, H-pm), 8.06 (4H, dd, H-bz), 7.30 (1H, d, H-pm), 3.89 (3H, s, OCH_3)
9	11.24 (1H, s, NH), 8.77 (2H, d, H-pm), 8.06 (4H, dd, H-bz), 7.30 (1H, d, H-pm), 3.89 (3H, s, OCH_3)