Silver-pyrazole complexes as hybrid multifunctional materials with metallomesogenic and photoluminescent behaviour

Paloma Ovejero,[a] Eduardo Asensio,[a] José Vicente Heras,[a] José Antonio Campo,[a] Mercedes Cano,*[,a] M. Rosario Torres,[b] Cristina Núñez[c,d] and Carlos Lodeiro*[,c,d]

Table S1 Selected bond distances (Å) and angles (º) for [$Hpz^{R(12)py}$] (**1**)

N1–N2	1.361(2)	N1–N2–C3	104.4(2)
N1–C5	1.346(3)	N2–N1–C5	113.0(2)
N2–C3	1.334(3)	N2–C3–C4	110.8(2)
C3–C4	1.395(3)	N1–C5–C4	105.5(3)
C4–C5	1.377(3)	C3–C4–C5	106.3(2)
C5–C6	1.460(3)	N2 C3–C11	119.5(3)
C3–C11	1.482(3)	N1–C5–C6	122.1(2)

Table S2 Hydrogen bond geometries (lenghts in Å and angles in degrees) for [$Hpz^{R(12)py}$] (**1**) and [$Ag(Hpz^{R(14)py})_2$][NO_3]·CH_2Cl_2 (**6·CH_2Cl_2**)

Compound	D – H ⋯ A	d(D – H)	d(H ⋯ A)	d(D ⋯ A)	<(D – H⋯A)
1	N1 – H1 ⋯ N3 [a]	1.16	2.09	3.065(3)	139.8
	C15 – H15⋯O2 [b]	0.93	2.74	3.65(1)	167.0
6·CH_2Cl_2	N2 – H2 ⋯ O2	1.11	1.72	2.825(8)	176.4
	N5 – H5 ⋯ O2	1.17	1.59	2.758(8)	171.8
	C59 – H59B – O3 [c]	0.97	2.37	3.21(2)	145.1
	C59 – H59A – O4 [d]	0.97	2.56	3.37(2)	141.2
	C59 – H59A – O3 [d]	0.97	2.44	3.40(2)	168.6
	C22 – H22 – O4 [e]	0.93	2.64	3.54(2)	164.6

[a] $-x+1, -y+2, -z$; [b] $-x+1, -y+1, -z+1$; [c] $-x+1, -y+1, -z+1$; [d] $x+1, y, z+1$; [e] $x+1, y, z$

Table S3 Selected bond distances (Å) and angles (º) for [$Ag(Hpz^{R(14)py})_2$][NO_3]·CH_2Cl_2 (**6**·CH_2Cl_2)

Ag–N1	2.182(7)	N1–Ag–N3	66.3(3)
Ag–N3	2.720(8)	N1–Ag–N4	114.5(3)
Ag–N4	2.423(7)	N1–Ag–N6	164.6(2)
Ag–N6	2.246(7)	N3–Ag–N4	168.0(2)
Ag–Ag [a]	3.152(2)	N3–Ag–N6	105.2(3)
N7–O2	1.260(8)	N4–Ag–N6	71.0(3)
N7–O3	1.213(8)	O2–N7–O3	119.3(9)
N7–O4	1.223(8)	O2–N7–O4	119.0(9)
		O3–N7–O4	121.6(9)

[a] $-x+1, -y+2, -z$

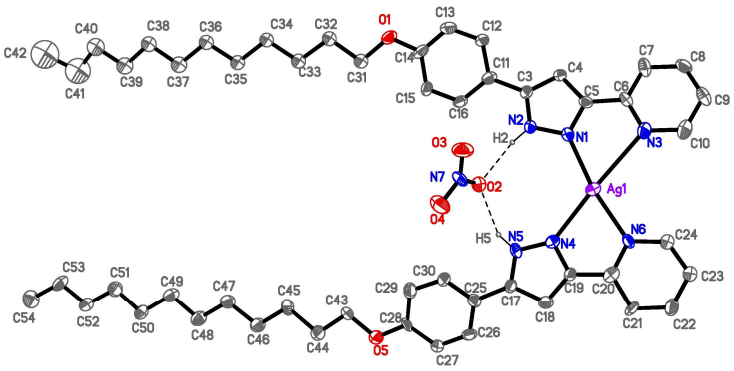

Figure S1 Ortep plot for $[Ag(Hpz^{R(12)py})_2][NO_3]$ **5**