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Silver pyrazole complexes with tunable liquid crystals and luminescent properties

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SUPPLEMENTARY INFORMATION

Table S1. Selected lengths (Å) and angles (°) for **5**

Ag1-N3	2.117(5)	N3-Ag1-N1	173.8(2)
Ag1-N1	2.127(5)	N2-N1-Ag1	119.6(4)
N1-N2	1.346(7)	C5-N1-Ag1	134.7(5)
N3-N4	1.358(8)	N4-N3-Ag1	121.7(4)
		C8-N3-Ag1	133.0(4)
		N1-N2-H2	123.3
		N3-N4-H4	121.3

Table S2. Hydrogen-bond geometries of **5**

D – H ... A	d(D – H) [Å]	d(H ... A) [Å]	d(D ... A) [Å]	<(D – H ... A) [°]
N2 – H2 ... O6	0.88	1.91	2.72(1)	151.6
N4 – H4 ... O7	0.88	1.87	2.72(2)	161.8
C31 – H31 ... O1 ^a	0.93	2.62	3.50(1)	157.1
C15 – H15A ... O2 ^b	0.96	2.75	3.45(1)	130.4
C15 – H15B ... O3 ^c	0.96	2.63	3.45(1)	143.8
C22 – H22C ... O5 ^d	0.96	2.47	3.42(2)	172.7
C25 – H25 ... O1 ^e	0.93	2.49	3.33(1)	150.5

^a -x+2, -y+1, -z+1; ^b x+1, y-1, z; ^c x+1, y, z-1; ^d x, y+1, z; ^e x-1, y, z+1

Table S3. Selected lengths (Å) and angles (°) for **10**

Ag1-N1	2.095(5)	C5-N1-Ag1	129.1(4)
Ag2-N3	2.119(5)	N2-N1-Ag1	125.3(4)
Ag1-N1 ^a	2.095(5)	C15-N3-Ag2	129.4(4)
Ag2-N3 ^b	2.119(5)	N4-N3-Ag2	125.4(4)
N1-N2	1.364(6)	N3-N4-H4	118.1
N4-N3	1.371(6)	N1-N2-H2	116.8

^a -x+1, -y+1, -z+1; ^b -x, -y+1, -z+2

Table S4. Hydrogen-bond geometries of **10**

D – H ... A	d(D – H) [Å]	d(H ... A) [Å]	d(D ... A) [Å]	<(D – H ... A) [°]
N2 – H2 ... O3	0.94	1.94	2.865(6)	169.8
N4 – H4 ... O5 ^a	1.06	1.75	2.805(6)	171.5
C22 – H22A ... O1 ^b	0.96	2.57	3.40(1)	144.3

^a x-1, y, z; ^b -x+1, y+1/2, -x+3/2

Table S5. Yields and analytical data of the compounds

complex n		MOLECULAR FORMULA	Yield (%)	Molecular weight (gmol ⁻¹)	Elemental analysis					
					calculated (%)			experimental (%)		
					C	H	N	C	H	N
12	1	C ₇₈ H ₁₂₀ N ₄ O ₄ AgCH ₃ C ₆ H ₄ SO ₃	55	1456.9	70.1	8.8	3.9	70.2	9.2	3.6
14	2	C ₈₆ H ₁₃₆ N ₄ O ₄ AgCH ₃ C ₆ H ₄ SO ₃	51	1569.1	71.2	9.2	3.6	71.7	9.4	3.8
16	3	C ₉₄ H ₁₅₂ N ₄ O ₄ AgCH ₃ C ₆ H ₄ SO ₃	50	1681.4	72.2	9.5	3.3	72.0	10.0	3.2
18	4	C ₁₀₂ H ₁₆₈ N ₄ O ₄ AgCH ₃ C ₆ H ₄ SO ₃	52	1793.6	73.0	9.8	3.1	73.5	9.8	3.1
1	5	C ₃₄ H ₃₂ N ₄ O ₄ AgCF ₃ SO ₃	75	817.6	51.4	4.0	6.9	51.4	4.1	7.0
12	6	C ₇₈ H ₁₂₀ N ₄ O ₄ AgCF ₃ SO ₃	56	1434.8	66.1	8.4	3.9	66.5	8.9	3.6
14	7	C ₈₆ H ₁₃₆ N ₄ O ₄ AgCF ₃ SO ₃	52	1547.0	67.6	8.9	3.6	67.6	8.5	3.5
16	8	C ₉₄ H ₁₅₂ N ₄ O ₄ AgCF ₃ SO ₃	55	1659.2	68.8	9.2	3.4	68.7	9.1	3.3
18	9	C ₁₀₂ H ₁₆₈ N ₄ O ₄ AgCF ₃ SO ₃	55	1771.4	69.8	9.6	3.2	70.0	9.6	3.0
1	10	C ₂₀ H ₂₀ N ₄ O ₂ AgCH ₃ C ₆ H ₄ SO ₃	70	627.5	51.7	4.3	8.9	51.5	4.3	8.9
12	11	C ₄₂ H ₆₄ N ₄ O ₂ AgCH ₃ C ₆ H ₄ SO ₃	62	936.1	62.9	7.7	6.0	62.5	7.8	6.3
14	12	C ₄₆ H ₇₂ N ₄ O ₂ AgCH ₃ C ₆ H ₄ SO ₃	58	992.2	64.2	8.0	5.7	64.6	8.3	6.0
16	13	C ₅₀ H ₈₀ N ₄ O ₂ AgCH ₃ C ₆ H ₄ SO ₃	55	1048.3	65.3	8.4	5.3	65.8	8.4	5.3
18	14	C ₅₄ H ₈₈ N ₄ O ₂ AgCH ₃ C ₆ H ₄ SO ₃	53	1104.4	66.3	8.7	5.1	66.0	9.0	5.1
12	15	C ₄₂ H ₆₄ N ₄ O ₂ AgCF ₃ SO ₃	50	913.9	56.5	7.1	6.1	56.0	7.0	5.7
14	16	C ₄₆ H ₇₂ N ₄ O ₂ AgCF ₃ SO ₃	49	970.1	58.2	7.5	5.8	57.8	7.5	6.0
16	17	C ₅₀ H ₈₀ N ₄ O ₂ AgCF ₃ SO ₃	48	1026.2	59.7	7.9	5.5	59.5	8.0	5.6
18	18	C ₅₄ H ₈₈ N ₄ O ₂ AgCF ₃ SO ₃	52	1082.3	61.0	8.2	5.2	61.0	8.4	5.0

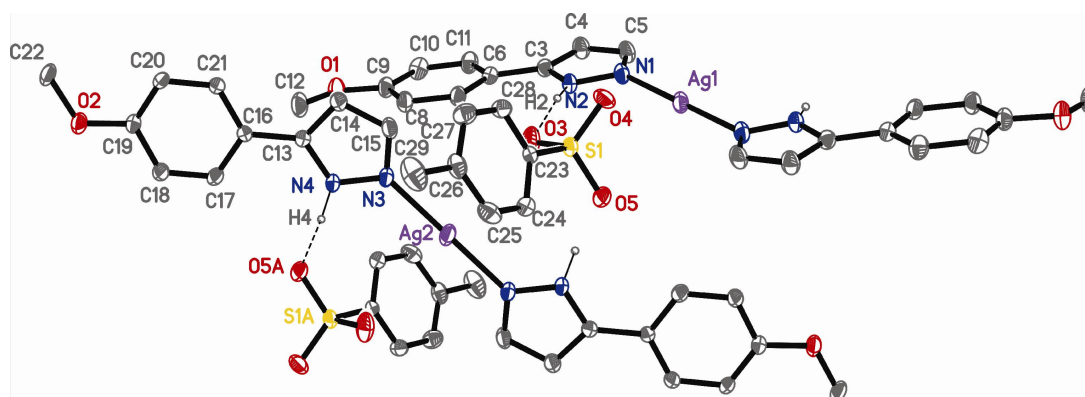


Figure S1. ORTEP plot of $[\text{Ag}(\text{Hpz}^{\text{R}(1)})_2][\text{PTS}]$ (**10**) with 35 % probability. Hydrogen atoms, except H2 and H4, have been omitted for clarity (*symmetry operation for atoms labelled A: $x-1, y, z$*)