

Supporting Information for

Modulation of the Ligand-Based Fluorescence of 3d Metal Complexes upon Spin State Change

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Table S1: Crystallographic data.

Compound	[NiL1]	[CuL1(EtOH)]·2 CHCl ₃
formula	C ₂₆ H ₂₄ N ₄ NiO ₆	C ₃₀ H ₃₂ N ₄ Cl ₆ CuO ₆
CCDC number	1055605	1055606
<i>M_r</i> / g mol ⁻¹	547.20	836.83
crystal system	Triclinic	Triclinic
space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> / Å	4.084(1)	8.651(1)
<i>b</i> / Å	12.918(3)	11.798(2)
<i>c</i> / Å	22.854(6)	18.199(3)
α / °	101.906(19)	71.833(11)
β / °	91.82(2)	86.734(12)
γ / °	94.00(2)	88.122(12)
<i>V</i> / Å ³	1175.6(5)	1761.8(4)
<i>Z</i>	2	2
ρ / g cm ⁻³	1.546	1.577
μ / mm ⁻¹	0.877	1.126
crystal size	0.06 × 0.14 × 0.29	0.084 × 0.103 × 0.115
<i>T</i> / K	133(2)	133(2)
λ (MoK α) / Å	0.71073	0.71073
θ -range / °	1.7–27.8	1.179–28.0
reflns. collected	8045	7594
indep. reflns. (<i>R_{int}</i>)	4136 (0.084)	3682 (0.173)
parameters	334	434
<i>R</i> (<i>F</i>) (all data)	0.0497 (0.1498)	0.1176 (0.1779)
<i>wR</i> ²	0.0720	0.2963
<i>Goof</i>	0.680	0.988

Figure S1: Powder diffraction patterns of all synthesised complexes.

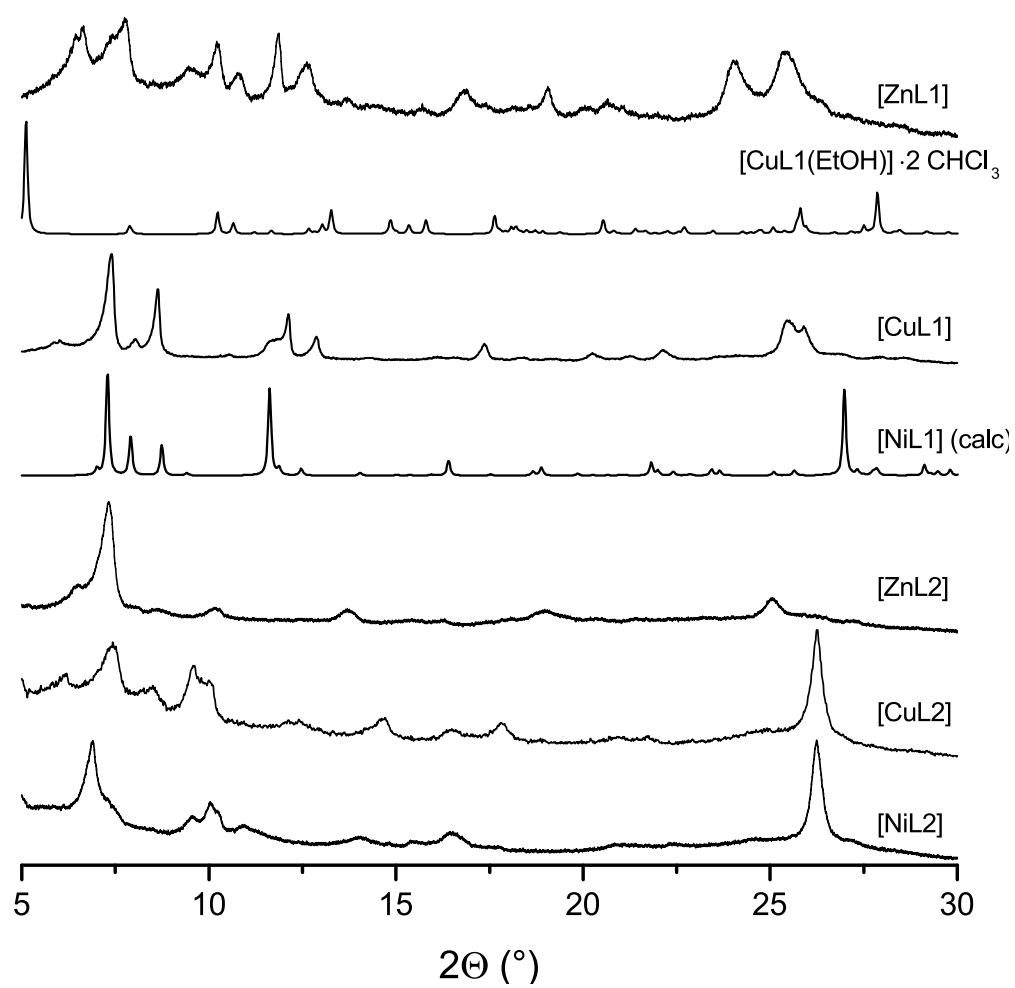


Figure S2: Intensity of characteristic absorption bands for the complex [NiL1] in trichloromethane and pyridine solutions, upon complexation and de-complexation of the pyridine molecules.

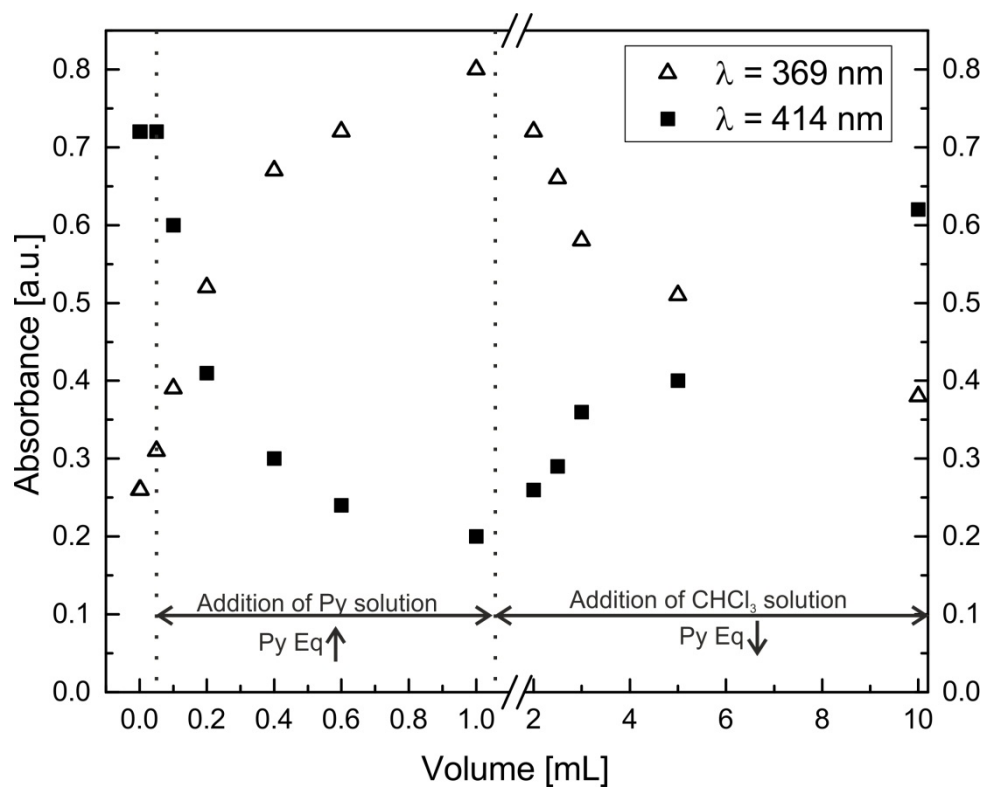


Figure S3: UV-Vis spectra of [NiL1], [NiL2], [ZnL1], and [ZnL2] in CHCl₃/Et₃N and CHCl₃/HCOOH mixtures.

