

Structural and Magnetic Variability of Cobalt(II) Complexes with Bridging Pyrazolate Ligands Bearing Appended Imine Groups

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HL³	
Empirical formula	C ₄₇ H ₅₀ N ₄
Formula weight	670.51
crystal size [mm]	0.78 x 0.75 x 0.11
crystal system	Monoclinic
space group	P2 ₁ /c (No. 14)
<i>a</i> [Å]	25.819(5)
<i>b</i> [Å]	8.1503(16)
<i>c</i> [Å]	24.549(5)
α [°]	90
β [°]	116.88(3)
γ [°]	90
<i>V</i> [Å ³]	4607.8(16)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	0.967
F(000)	1440
μ [mm ⁻¹]	0.056
<i>hkl</i> range	31±, -8 to 10±, ±30
θ range [°]	1.66 to 25.92
measured refl.	38404
unique refl. [<i>R</i> _{int}]	8898[0.2351]
observed refl. (<i>I</i> > 2 σ (<i>I</i>))	3093
ref. param. / restraints	213/0
goodness-of-fit	1.353
<i>R</i> 1, <i>wR</i> 2 (<i>I</i> > 2 σ (<i>I</i>))	0.2291, 0.4933
<i>R</i> 1, <i>wR</i> 2 (all data)	0.3524, 0.5584
resid. el. dens. [e Å ⁻³]	2.682/-0.635

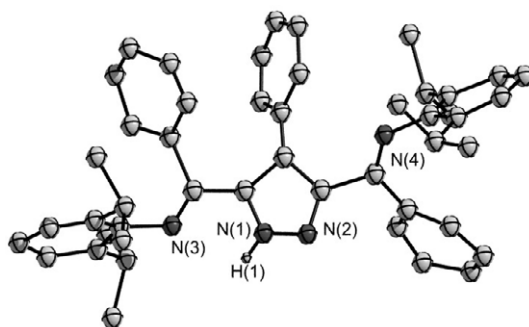


Fig. S1. Molecular structure of HL³. In the interest of clarity most hydrogen atoms have been omitted.

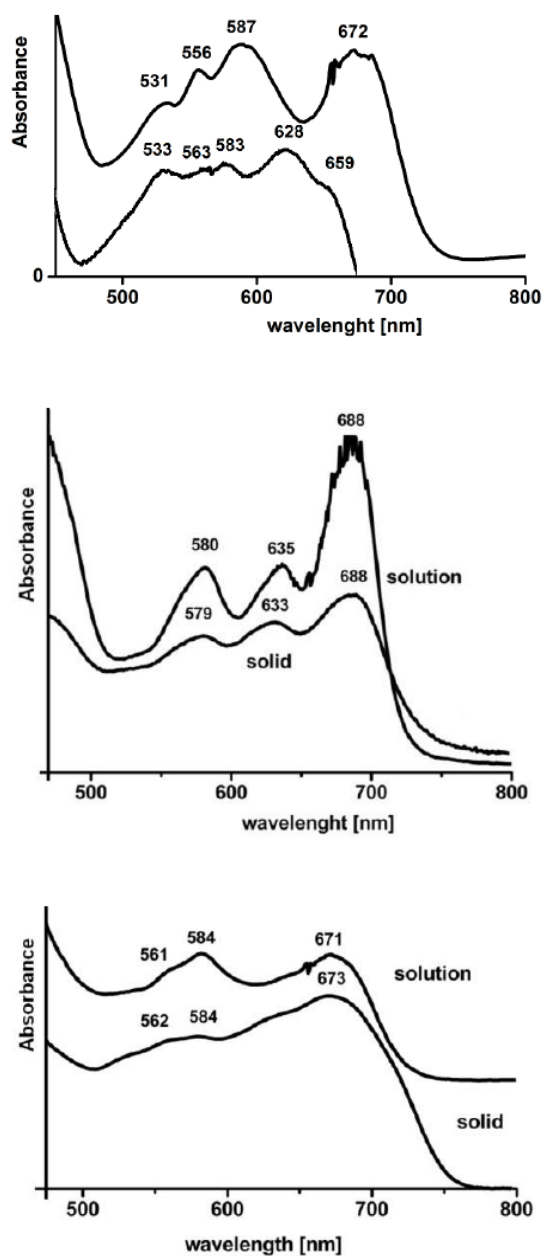


Fig. S2. Part of the UV-Vis spectra of **1** (top), **2** (middle) and **3** (bottom) in the solid state (diffuse reflectance) and in CH_2Cl_2 solutions.

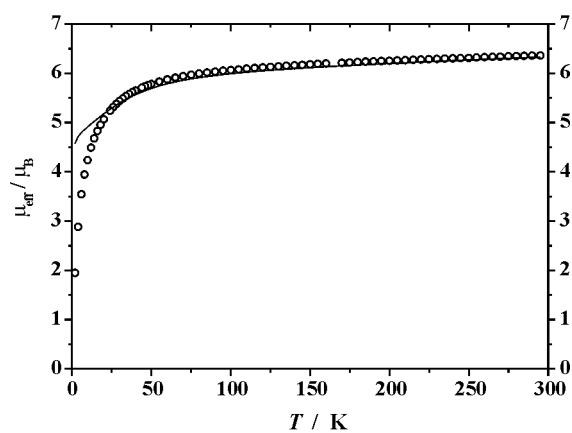


Fig. S3. μ_{eff} vs. T plot for **1**. The solid line represents the calculated curve fit when coupling constant J is excluded. Best fit parameters for **1** are $g = 2.20$, $|D| = 40 \text{ cm}^{-1}$, $PI = 2.5 \%$ (fixed) and $TIP = 19.0 \times 10^{-4} \text{ cm}^3 \text{ mol}^{-1}$ (fixed).

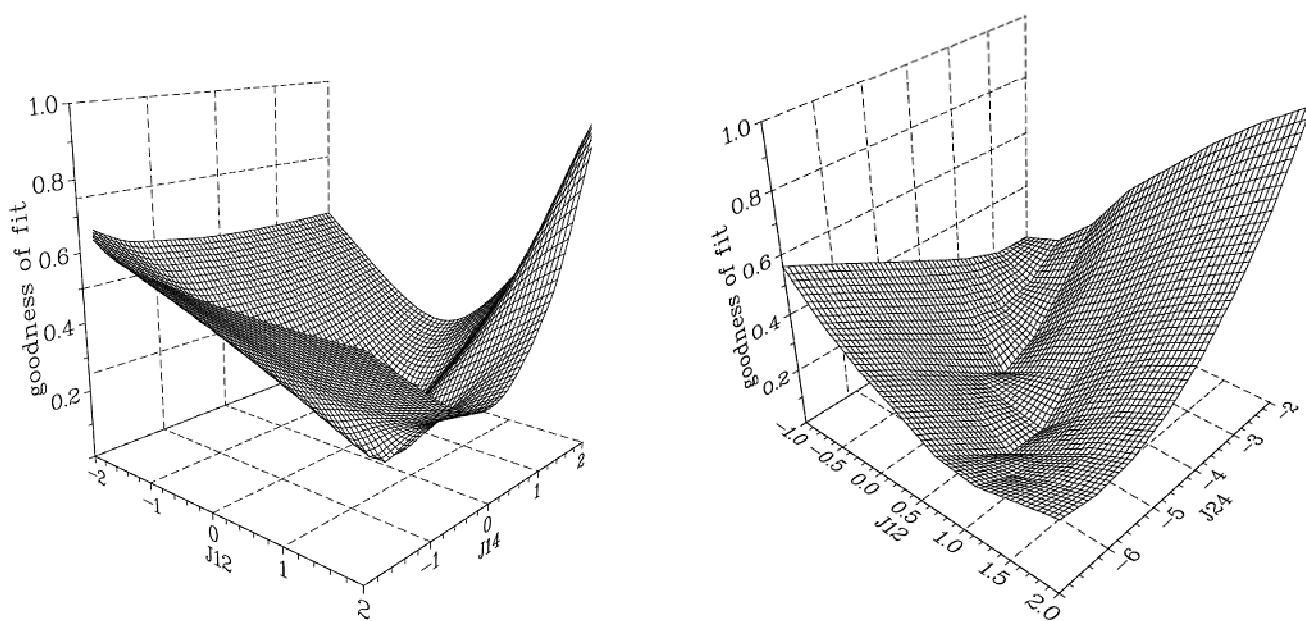


Fig. S4. The 3D error surfaces for the pairs J_2 - J_3 (left) and J_1 - J_2 (right).