

Supplementary Materials

The structural and magnetic properties of Fe^{II} and Co^{II} complexes with 2-(furan-2-yl)-5-pyridin-2-yl-1,3,4-oxadiazole

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Table S1. Parameters of one-component Debye model for 2 derived according Eq.4 in main text.

T/K	$\chi_s/(10^{-6} \text{ m}^3\text{mol}^{-1})$	$\chi_T/(10^{-6} \text{ m}^3\text{mol}^{-1})$	α	τ/s
1.9	0.5414	11.0301	0.21247	5.41E-03
2.1	0.4562	9.8960	0.21788	4.26E-03
2.3	0.4794	9.1067	0.20218	3.59E-03
2.5	0.4587	8.4973	0.20646	3.09E-03
2.7	0.4763	7.8337	0.20290	2.60E-03
2.9	0.4874	7.2190	0.18749	2.18E-03
3.1	0.5046	6.7876	0.17255	1.90E-03
3.3	0.5507	6.3644	0.14523	1.61E-03
3.5	0.4536	6.0045	0.15623	1.27E-03
3.7	0.4878	5.6856	0.12545	1.02E-03
3.9	0.5564	5.4039	0.08493	7.89E-04
4.1	0.4721	5.1482	0.07469	5.26E-04
4.3	0.4780	4.9185	0.05209	3.33E-04
4.5	0.4524	4.7052	0.03086	2.06E-04
4.7	0.4647	4.5190	0.01977	1.27E-04
4.9	0.3985	4.3466	0.01064	7.43E-05
5.1	0.4092	4.1932	0.00967	4.52E-05
5.3	0.5860	4.0464	0.00928	2.82E-05

Table S2. The g-values for the ground state Kramers doublet calculated for the effective spin $S_{\text{eff}} = 1/2$ for **2** derived from CASSCF/NEVPT2 calculations

	g^1	g^2	g^3
	[Co(fpo) ₂ (H ₂ O) ₂] ²⁺		
CAS(7,5)	2.076654	4.160317	5.232077
CAS(7,10)	2.070967	4.103990	5.307797
	{[Co(fpo) ₂ (H ₂ O) ₂](ClO ₄) ₂ }		
CAS(7,5)	1.589525	2.364502	6.468165
CAS(7,10)	1.620814	2.437684	6.450145
	{[Co(fpo) ₂ (H ₂ O) ₂](ClO ₄) ₄] ²⁻ }		
CAS(7,5)	1.141082	1.469279	6.876476
CAS(7,10)	1.182593	1.537428	6.869937

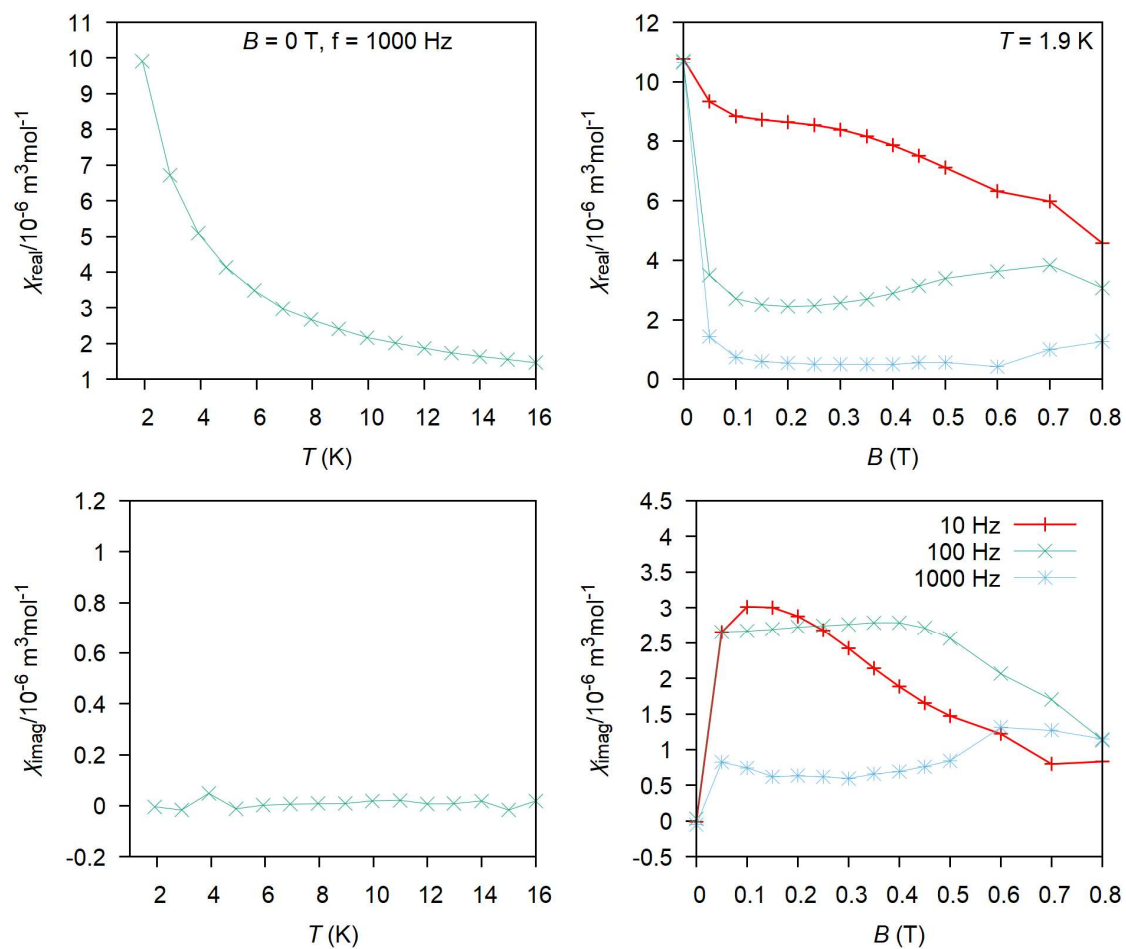


Figure S1. In-phase χ_{real} and out-of-phase χ_{imag} molar susceptibilities for **2** at zero static magnetic field (*left*) and in non-zero static field (*right*). Lines serve as guides for the eyes.