

Electronic Supplementary Information

Magnetic, Electrochemical and Spectroscopic Properties of a Sulfate-bridged Co(II) Imidazole Dimer

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Table S1. Single crystal X-ray diffraction collection summary for **2**.

Compound	2
Formula of the Refinement Model	C ₂₄ H ₃₈ Co ₂ N ₁₀ O ₈ S ₂
Molecular Weight	776.62
Crystal System	monoclinic
Space Group	<i>P</i> 2 ₁ / <i>c</i> (#14)
<i>a</i> / Å	10.9888(11)
<i>b</i> / Å	8.6363(9)
<i>c</i> / Å	17.4813(15)
β / °	94.688(4)°
<i>V</i> / Å ³	1653.5(3)
<i>D</i> _c / g cm ⁻³	1.560
<i>Z</i>	2
Crystal size / mm	0.120 x 0.075 x 0.054
Crystal colour	purple
Crystal habit	prismatic
Temperature / K	150(2)
λ (Mo-K α) / Å	0.71073
μ (Mo-K α) / mm ⁻¹	1.190
<i>T</i> (SADABS) _{min,max}	0.925, 1.0
$2\theta_{\text{max}}$ / °	52.84
<i>hkl</i> range	-13 to 13, -10 to 10, -21 to 21
<i>N</i>	49379
<i>N</i> _{ind}	3393 (<i>R</i> _{merge} 0.0342)
<i>N</i> _{obs}	3155 (<i>I</i> > 2σ(<i>I</i>))
<i>N</i> _{var}	213
Residuals * <i>R</i> 1(<i>F</i>), <i>wR</i> 2(<i>F</i> ²)	0.0242, 0.1010
GoF(all)	1.179
Residual Extrema / e Å ⁻³	-1.046, 0.651

* $R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$ for $F_o > 2\Sigma(F_o)$; $wR2 = \frac{(\sum w(F_o^2 - F_c^2)^2 / \sum (wF_c^2)^2)^{1/2}}{\text{all reflections. } w=1/[\sigma^2(F_o^2)+(0.0630P)^2+0.8196P]}$ where $P=(F_o^2+2F_c^2)/3$

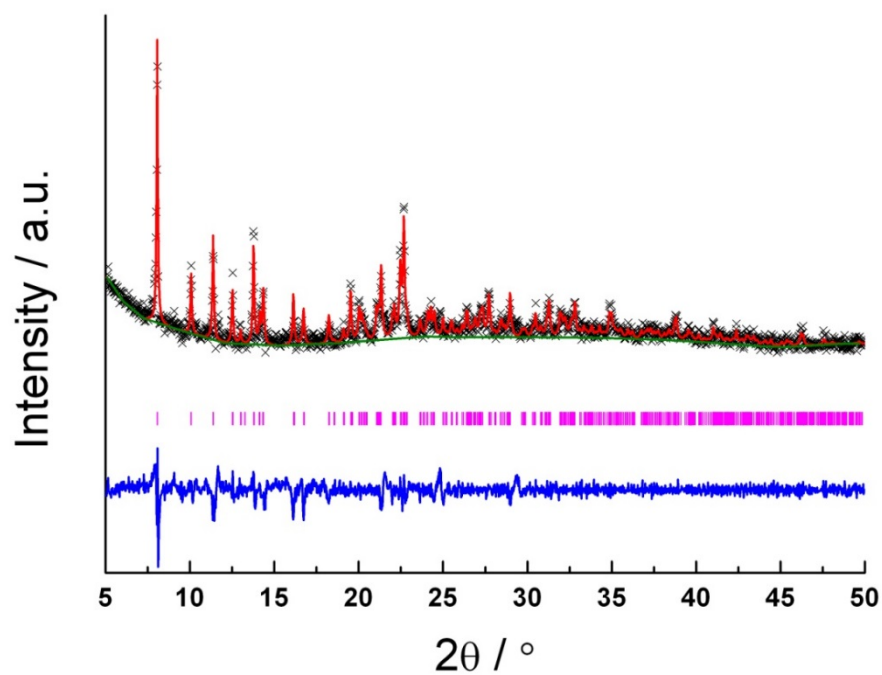


Figure S1. Le Bail fit of **2**: $a = 11.025(4)$, $b = 8.698(2)$, $c = 17.677(5)$ Å, $\beta = 93.29(3)^\circ$ and $V = 1692.4(8)$ Å³.

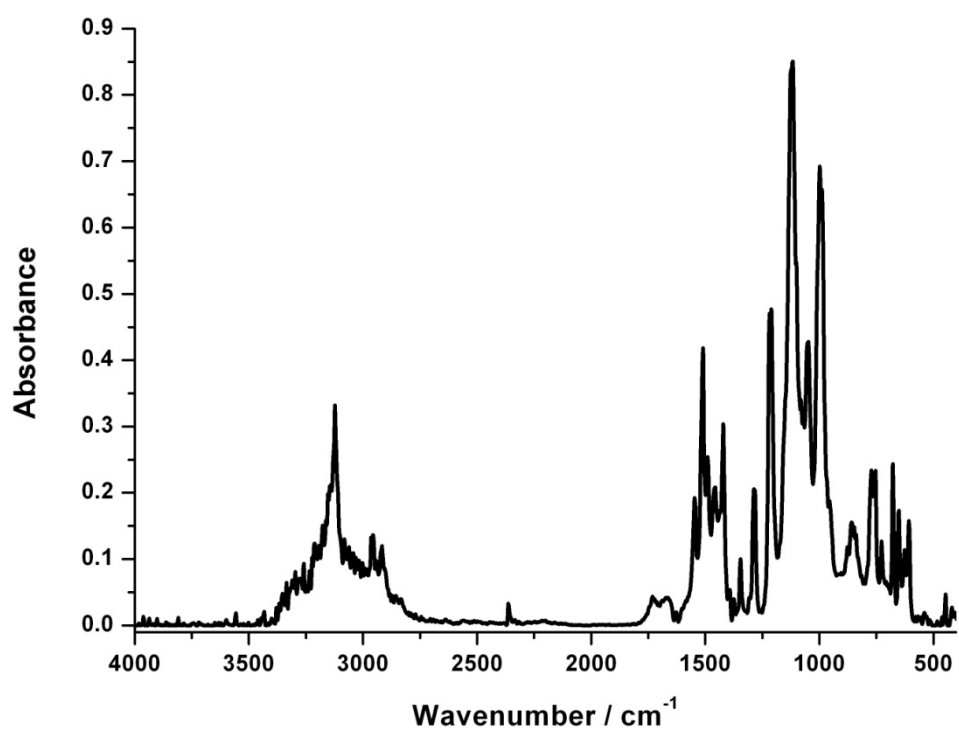


Figure S2. FT-IR spectrum of **2**.

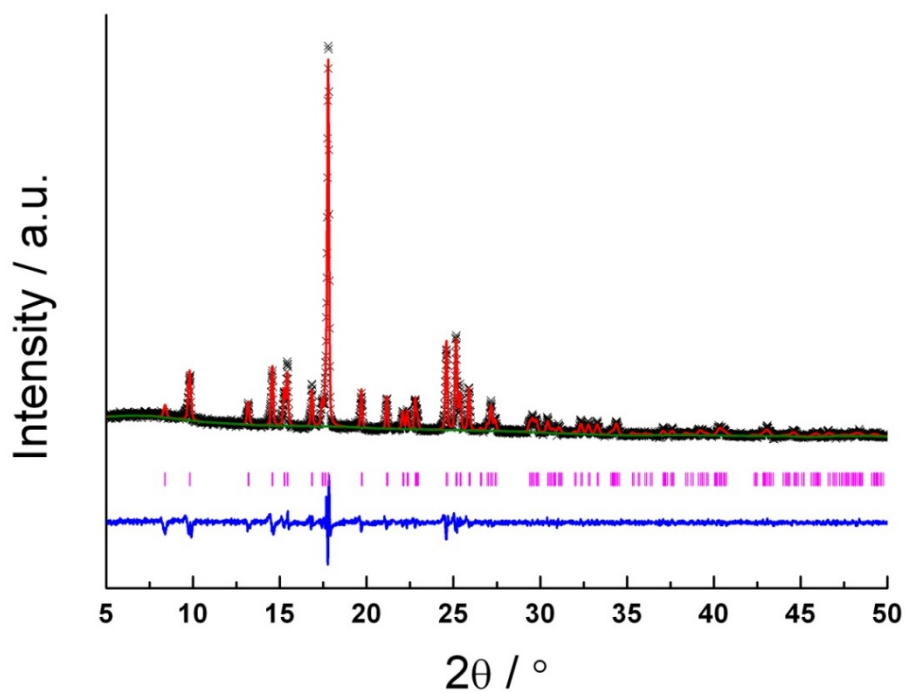


Figure S3. Le Bail fit of **1**: Space group $P3_221$ (#154), $a = b = 12.1377(9)$, $c = 17.393(2)$ Å and $V = 2219.1(3)$ Å³.

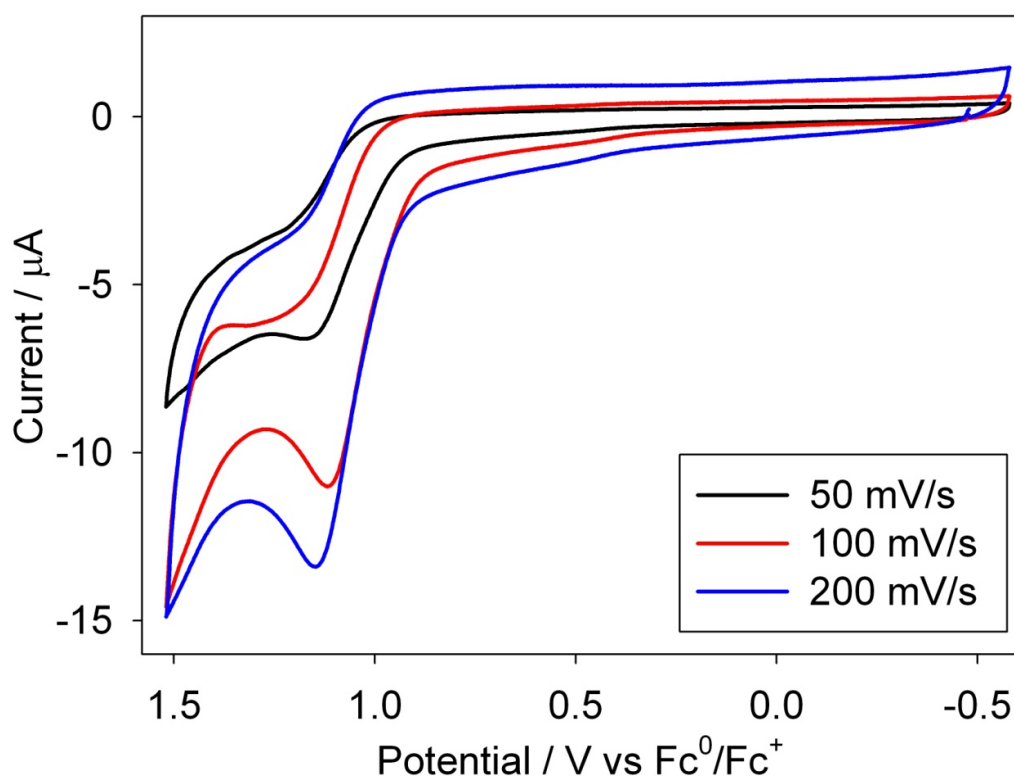


Figure S4. Solution-state cyclic voltammograms of **1** measured at different scan rates.

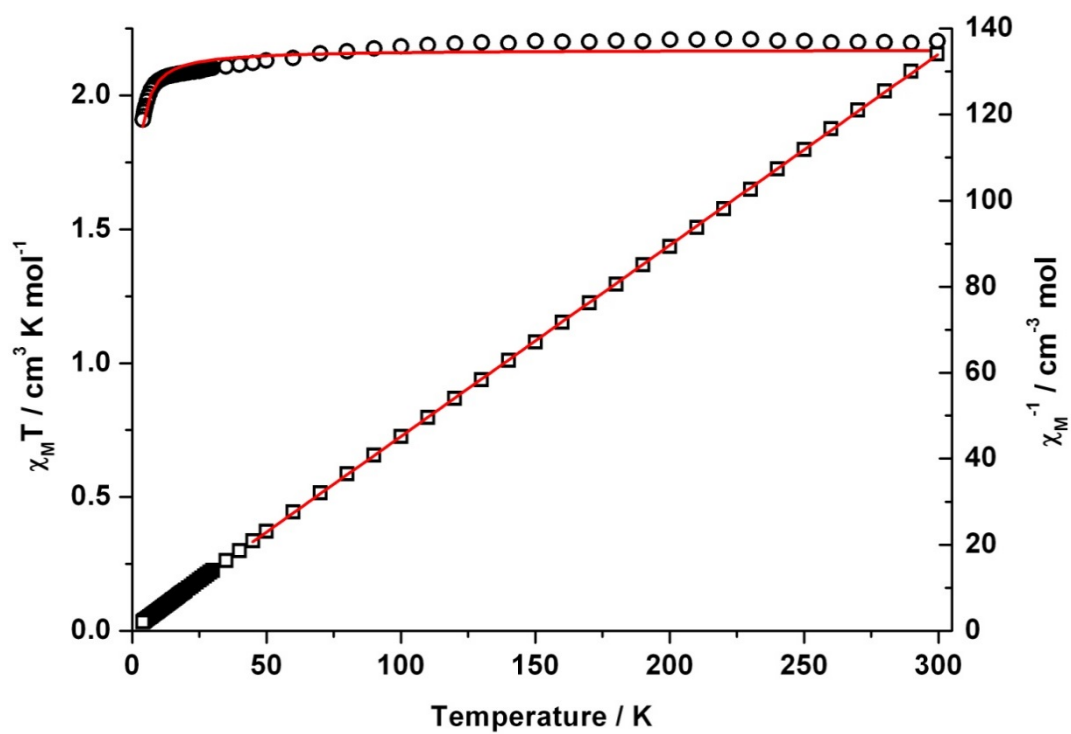


Figure S5. $\chi_M T$ (open circles) and χ_M^{-1} (open squares) vs. temperature plots of **1**. Best fits to the Heisenberg Hamiltonian and Curie-Weiss Law are shown as red lines.

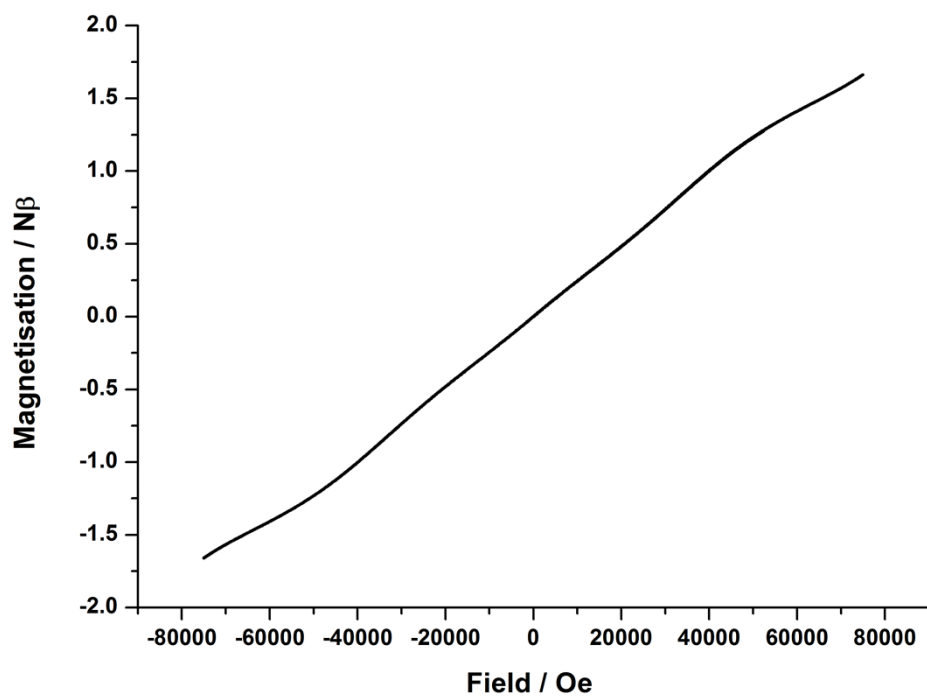


Figure S6. Magnetisation vs. field curve of **2** at 2.25 K.

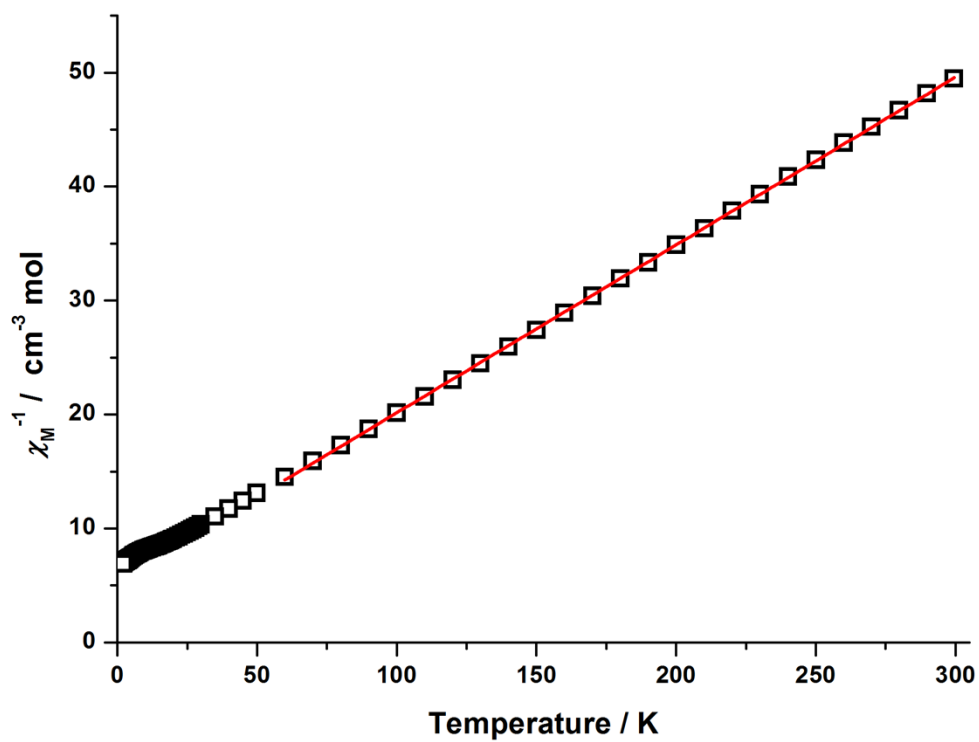


Figure S7. Plot of χ^{-1} vs. temperature for **2**. Red line is the best fit to the Curie Weiss Law.

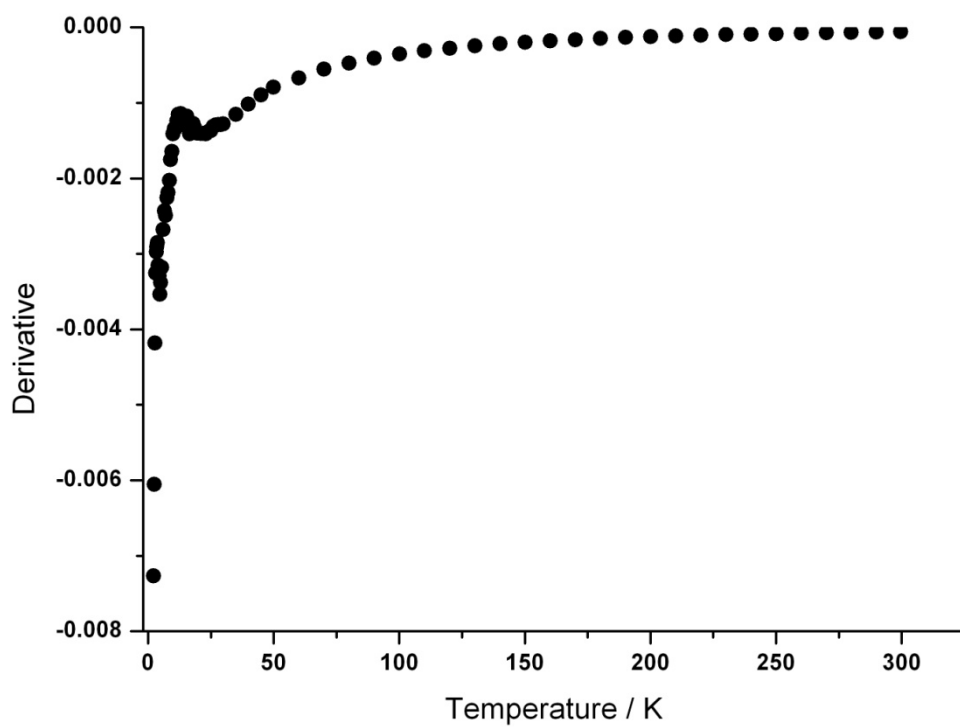


Figure S8. 1st derivative ($d\chi/dT$) of magnetic susceptibility of **2**, indicating the $T_N = 14.5$ K.