



SUPPLEMENTARY MATERIAL TO
Synthesis, crystal structure and properties of [Co(L)₂](ClO₄)₂
(L = 1,3-bis(1*H*-benzimidazol-2-yl)-2-oxapropane)

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IR DATA FOR THE LIGAND

*1,3-Bis(1*H*-benzimidazol-2-yl)-2-oxapropane (L)*. IR (KBr, cm⁻¹): 3049*m,br*, 2947*m*, 2846*m*, 2744*m*, 1625*m*, 1590*m*, 1457*s*, 1432*s*, 1336*s*, 1272*s*, 1232*s*, 1103*s*, 1038*m*, 923*m*, 748*s*, 433*m*.

ANALYTICAL, PHYSICAL AND SPECTRAL DATA OF THE TITLE COMPOUND

*Bis[1,3-bis(1*H*-benzimidazol-2-yl-κN³)-2-oxapropane]cobalt(2+)-diperchlorate (I)*. M.p.: 234 °C; Anal. Calcd. for C₃₂H₂₈Cl₂CoN₈O₁₀: C, 47.19; H, 3.47; N, 13.76 %. Found: C 46.78, H 3.62, N 13.54 %; IR (KBr, cm⁻¹) 3273 (NH stretching), 3080*m* (CH stretching of aromatic ring), 2933 (–CH₂– stretching), 1630*m* (C=N stretching), 1604*m* (C=C stretching), 1484*m*, 1462*s*, 1399*m*, 1283*m*, 1115*s* (Cl=O stretching of perchlorate anion), 1088*s*, 1046*s* (C–O stretching of ethereal bridge), 1009*m*, 745*s* (out of plane bending CH of aromatic ring), 698*m* (Co–N stretching), 627*m* (Cl=O ν₄ stretching mode of perchlorate), 584*w*; MS (*m/z*, (relative abundance, %)): 835.90 (19.2, [(M+23)–2]⁺, {814.45+23 = 837.45}); 279.7 (11.8, [ML+1]⁺ for the ligand); 614.7 (100, [Co(L)₂–1]⁺); 714.1 (26.5, [2L+Co+ClO₄]⁺); 484.6 (16.7, [L+Co+ClO₄]⁺); UV–Vis (MeOH, λ_{max} / nm): 558*w*, 526*sh*, 476*sh*, 280*m*, 274*s*, 268*sh*, 246*s,br*, 218*s*, 212*s*; Molar conductivity (DMF, 25 °C): 126 S m² mol⁻¹. Magnetic moment, μ_{eff} / μ_B: 4.12.

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TABLE S-I. Selected bond lengths and angles

Bond lengths, Å			
Co(1)–N(5)	2.034(2)	Co(1)–N(7)	2.032(4)
Co(2)–N(2)	2.028(2)	Co(2)–N(3)	2.053(4)
Co(1)–O(2)	2.805(3)	Co(2)–O(1)	2.752(2)
O(2)–C(24)	1.431(5)	O(2)–C(25)	1.435(5)
N(2)–C(2)	1.408(5)	N(2)–C(7)	1.333(4)
C(1)–C(2)	1.396(5)	C(7)–C(8)	1.474(5)
Bond angles, °			
N(5)–Co(1)–N(7)	114.3(2)	N(2)–Co(2)–N(3)	112.9(1)
O(1)–Co(2)–N(2)	162.3(6)	O(2)–Co(1)–N(5)	155.7(2)
C(8)–O(1)–C(9)	113.1(3)	C(24)–O(2)–C(25)	112.1(3)
C(2)–N(2)–Co(2)	131.0(2)	C(7)–N(2)–Co(2)	123.6(3)
C(10)–N(3)–Co(2)	125.1(4)	C(16)–N(3)–Co(2)	129.6(2)
C(23)–N(5)–Co(1)	123.8(3)	C(8)–C(7)–N(1)	125.2(3)
C(8)–C(7)–N(2)	122.5(3)	O(1)–C(8)–C(7)	104.0(3)
C(10)–C(9)–O(1)	108.6(3)	N(4)–C(10)–C(9)	122.5(3)
O(2)–C(24)–C(23)	104.7(3)	C(26)–C(25)–O(2)	109.2(3)

TABLE S-II. Selected torsion angles (°)

N(7)–Co(1)–N(5)–C(20)	149.9(3)	N(7)–Co(1)–N(5)–C(23)	–21.8(3)
N(5)–Co(1)–N(7)–C(26)	59.9(4)	N(5)–Co(1)–N(7)–C(27)	–116.7(4)
N(2)–Co(2)–N(3)–C(10)	–66.7(3)	N(3)–Co(2)–N(2)–C(7)	34.0(4)
C(9)–O(1)–C(8)–C(7)	–154.7(3)	C(8)–O(1)–C(9)–C(10)	73.9(3)
Co(1)–N(7)–C(26)–N(8)	–177.1(3)	O(2)–C(25)–C(26)–N(8)	150.5(4)
Co(1)–N(7)–C(27)–C(28)	–4.6(7)	Co(1)–N(7)–C(26)–C(25)	3.3(6)
N(1)–C(7)–C(8)–O(1)	–134.3(4)	Co(1)–N(7)–C(27)–C(32)	177.6(3)
N(5)–C(23)–C(24)–O(2)	–37.8(4)	N(2)–C(7)–C(8)–O(1)	44.2(6)
O(2)–C(25)–C(26)–N(7)	–29.9(6)		

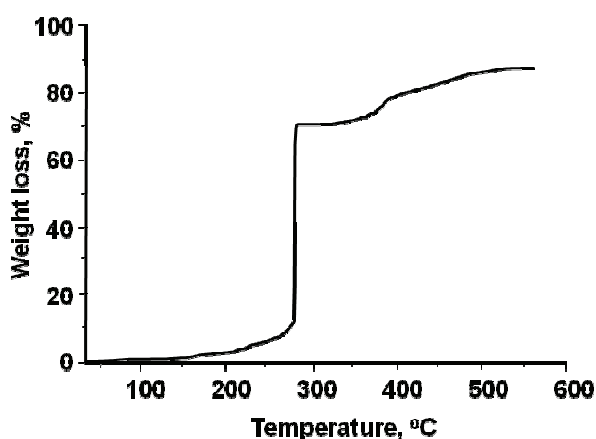


Fig. S-1. TGA curve of the title compound.

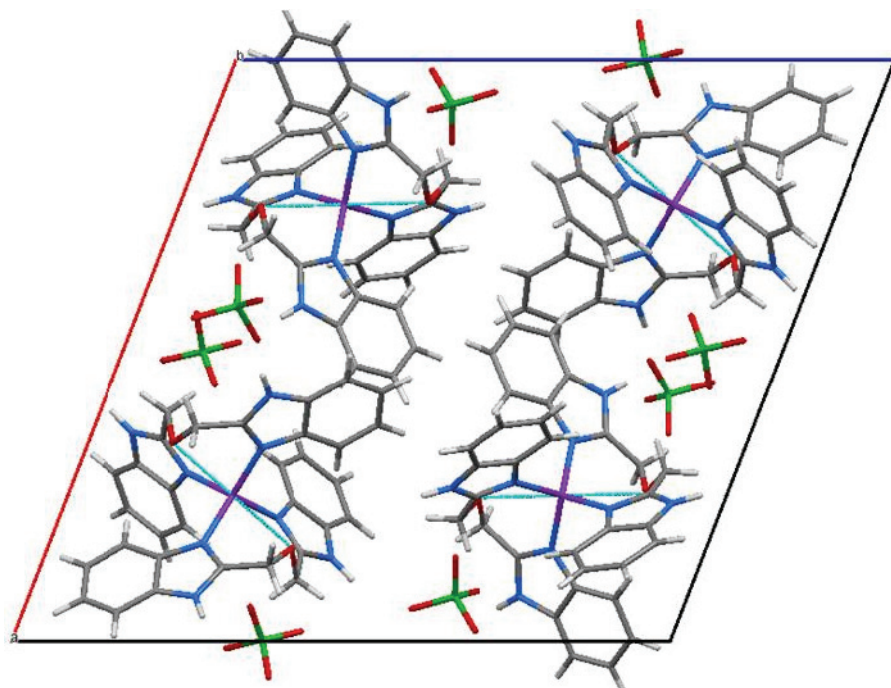


Fig. S-2. A packing diagram of the title compound (view *b*).