

Supporting Information

Effects of electron donating/withdrawing groups in the 5-substituted-2-hydroxybenzaldehyde on the synthesis of neutral cubanes with a Ni^{II}₄O₄ core: Synthesis, crystal structures and magnetic properties

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Table S1 Selected bond lengths (Å) and angles (°) for **1** and **2**

	1	2
Ni(1)-O(1)	2.074(2)	2.0637(18)
Ni(1)-O(2)	2.063(2)	2.062(2)
Ni(1)-O(3)	2.051(2)	2.0417(19)
Ni(2)-O(1)	2.055(2)	2.0474(19)
Ni(2)-O(2)	2.052(2)	2.0594(19)
Ni(2)-O(4)	2.062(2)	2.054(2)
Ni(3)-O(1)	2.056(2)	2.053(2)
Ni(3)-O(3)	2.054(2)	2.0532(18)
Ni(3)-O(4)	2.069(2)	2.0521(18)
Ni(4)-O(2)	2.0474(19)	2.051(2)
Ni(4)-O(3)	2.056(2)	2.0574(19)
Ni(4)-O(4)	2.084(2)	2.0619(18)
Ni(2)-O(1)-Ni(1)	95.32(8)	95.96(8)
Ni(1)-O(3)-Ni(3)	95.84(8)	96.30(7)
Ni(2)-O(2)-Ni(1)	95.78(8)	95.65(8)
Ni(2)-O(1)-Ni(3)	100.18(9)	99.60(8)
Ni(2)-O(4)-Ni(3)	99.52(9)	99.41(8)
Ni(2)-O(4)-Ni(4)	95.04(8)	96.44(7)
Ni(3)-O(1)-Ni(1)	95.06(8)	95.61(7)
Ni(3)-O(3)-Ni(4)	96.67(9)	95.99(8)
Ni(3)-O(4)-Ni(4)	95.32(9)	95.89(8)
Ni(4)-O(2)-Ni(2)	96.47(9)	96.64(8)
Ni(4)-O(2)-Ni(1)	98.91(8)	98.79(8)
Ni(1)-O(3)-Ni(4)	99.02(8)	99.22(8)
Ni(1)-Ni(2)	3.0526	3.0542
Ni(1)-Ni(3)	3.0466	3.0503
Ni(1)-Ni(4)	3.1233	3.1222
Ni(2)-Ni(3)	3.1534	3.1323
Ni(2)-Ni(4)	3.0574	3.0697
Ni(3)-Ni(4)	3.0698	3.0547

Table S2 Crystal data and structure refinement for **1** and **2**.

	1	2
Empirical formula	C ₃₆ H ₄₈ O ₁₆ Ni ₄	C ₄₀ H ₅₆ O ₁₆ Ni ₄
Formula weight	971.58	1027.69
Temperature (K)	298(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/n	P2(1)/c
Unit cell dimensions (Å, °)	a = 14.645(3) b = 14.608(3) c = 20.215(4) β = 104.39(3)	a = 18.262(4) b = 17.467(4) c = 14.722(3) β = 90.39(3)
Volume (Å ³)	4189.0(16)	4695.8(18)
Z	4	4
Calculated density (Mg/m ³)	1.541	1.454
Absorption coefficient (mm ⁻¹)	1.838	1.644
F(000)	2016	2144
Theta range for data collection (°)	2.62 to 25.00	2.52 to 26.00
Index ranges	-17 ≤ h ≤ 17 -17 ≤ k ≤ 17 -23 ≤ l ≤ 24	-21 ≤ h ≤ 22 -21 ≤ k ≤ 21 -18 ≤ l ≤ 18
Reflections collected	20745	44189
Independent reflections	7077 [R _(int) = 0.0348]	9210 [R _(int) = 0.0452]
Data Completeness (%)	96.1	99.9
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	7077 / 9 / 519	9210 / 12 / 557
Goodness-of-fit on <i>F</i> ²	0.858	0.920
Final R indices [I > 2σ (I)]	R ₁ = 0.0311 wR ₂ = 0.0624	R ₁ = 0.0358 wR ₂ = 0.0844
R indices (all data)	R ₁ = 0.0536 wR ₂ = 0.0669	R ₁ = 0.0571 wR ₂ = 0.0906
Largest diff. peak and hole (e.Å ⁻³)	0.395 and -0.249	0.251 and -0.269