Electronic Supporting Information

Tetracobalt(II) cluster with two vertex truncated dicubane topology endogenously supported by carboxylate-based (2-pyridyl)methylamine ligands: magneto-structural and DFT study

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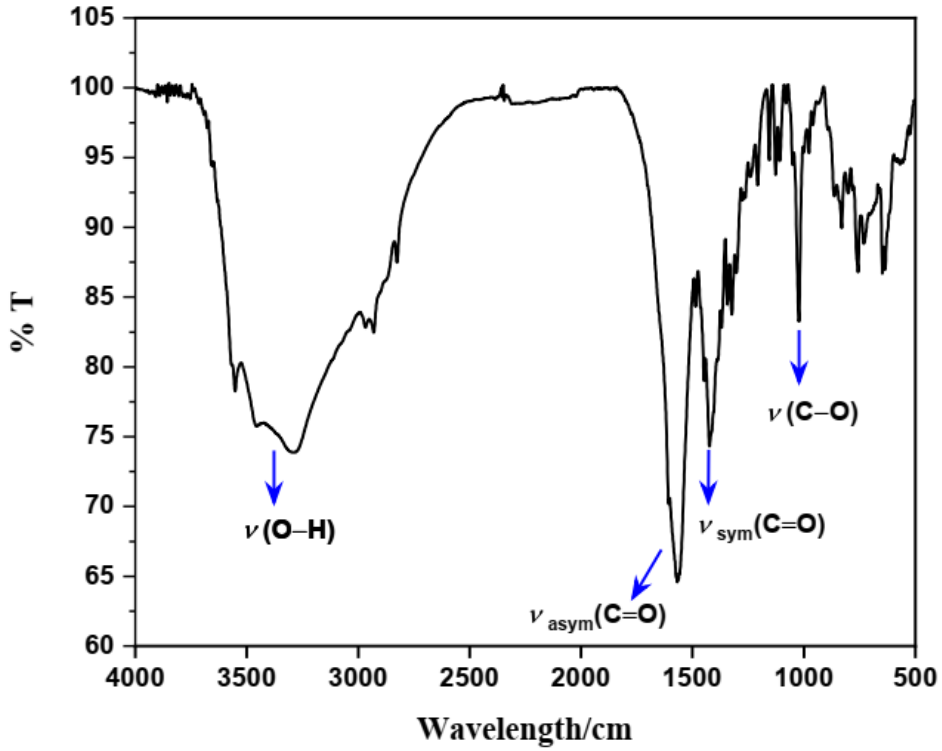


Fig. S1 FT-IR spectrum of $[Co^{II}_4\{L^3\text{-}(CO_2^-)_2\}_2(\mu_3\text{-}OCH_3)_2(CH_3OH)_2(H_2O)_2Cl_2]$ (**1**).

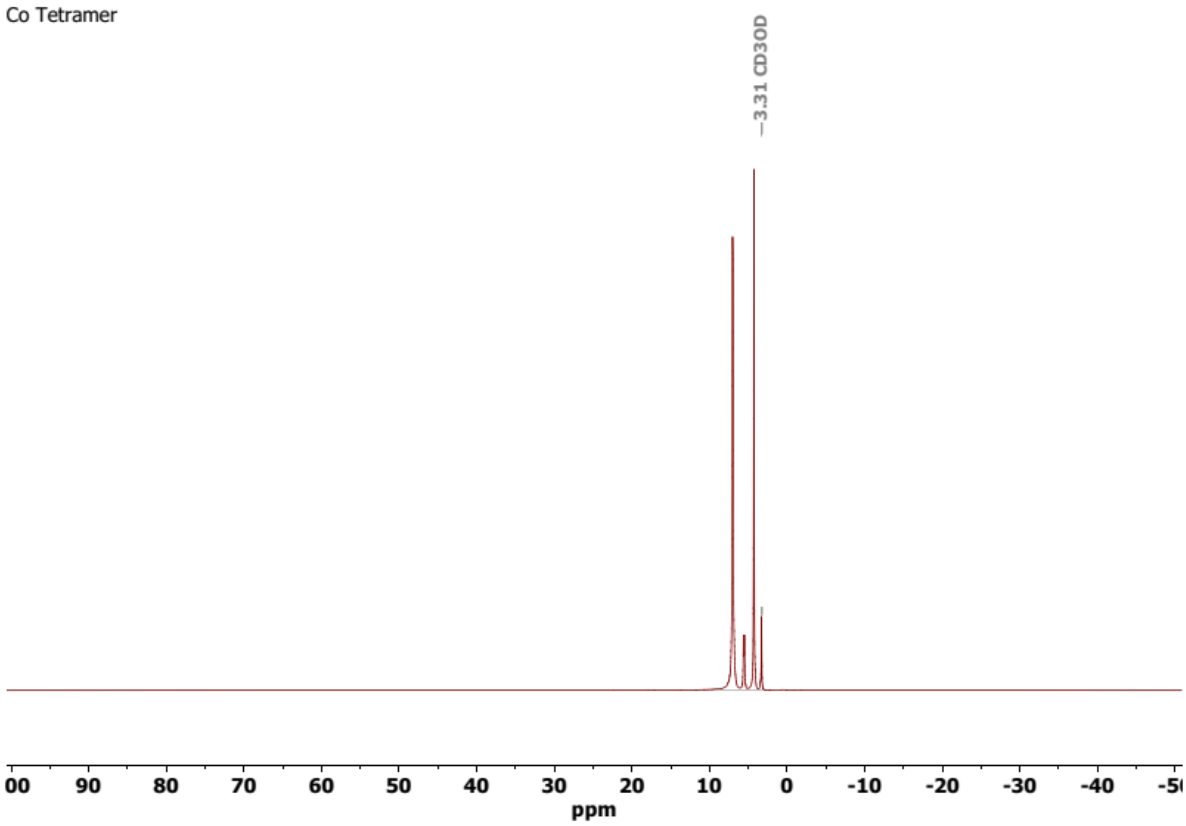
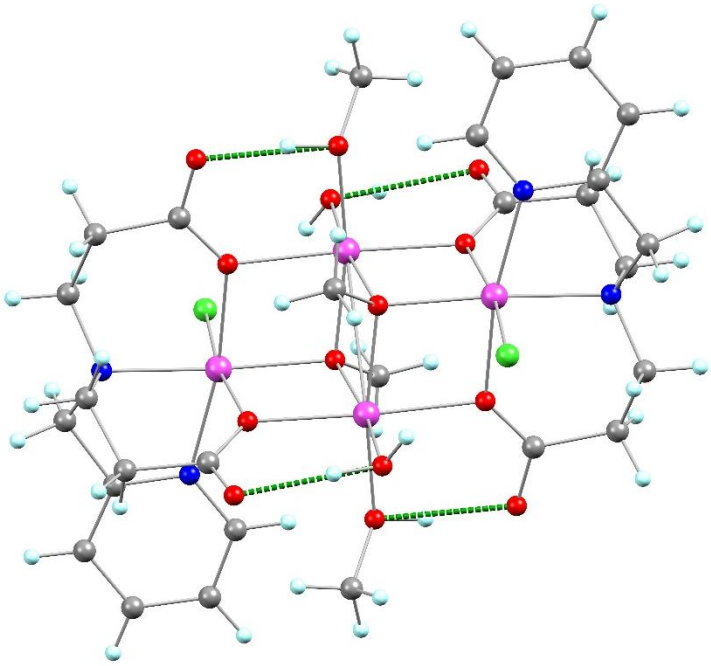


Fig. S2 ^{1}H NMR spectrum of **1** in CD_3OD.

(a)



(b)

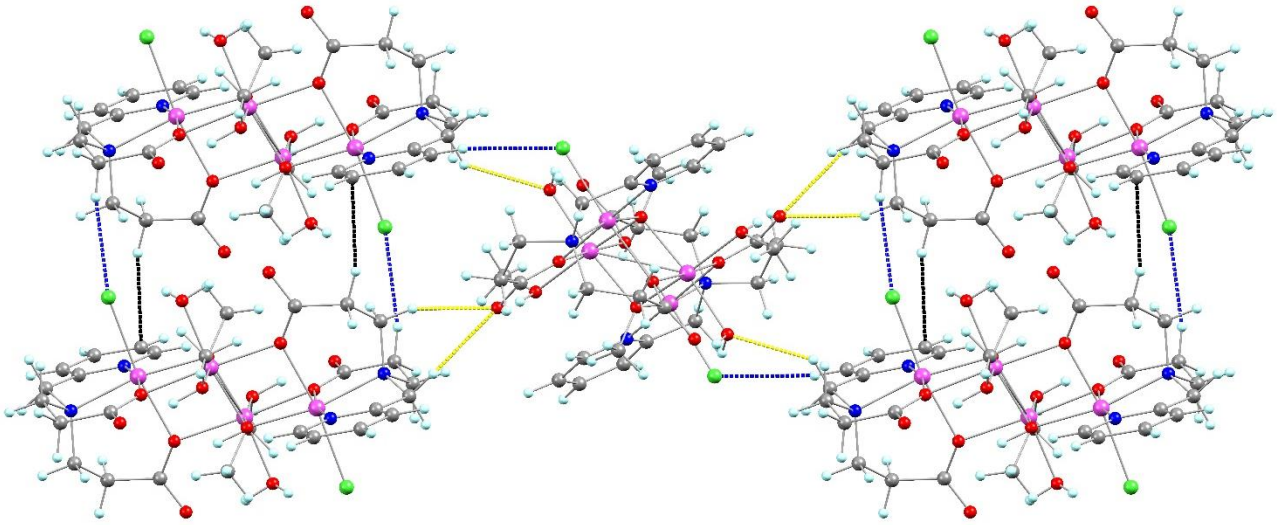


Fig. S3 Crystal packing diagram, (a) showing intramolecular O–H···O (in green) and (b) intermolecular C–H···O (in yellow) and C–H···Cl (in blue) C–H···π (in black) interactions of $[Co^{II}_4\{L^3\text{-}(CO_2^-)_2\}_2(\mu_3\text{-}OCH_3)_2(CH_3OH)_2(H_2O)_2Cl_2]$ (**1**).

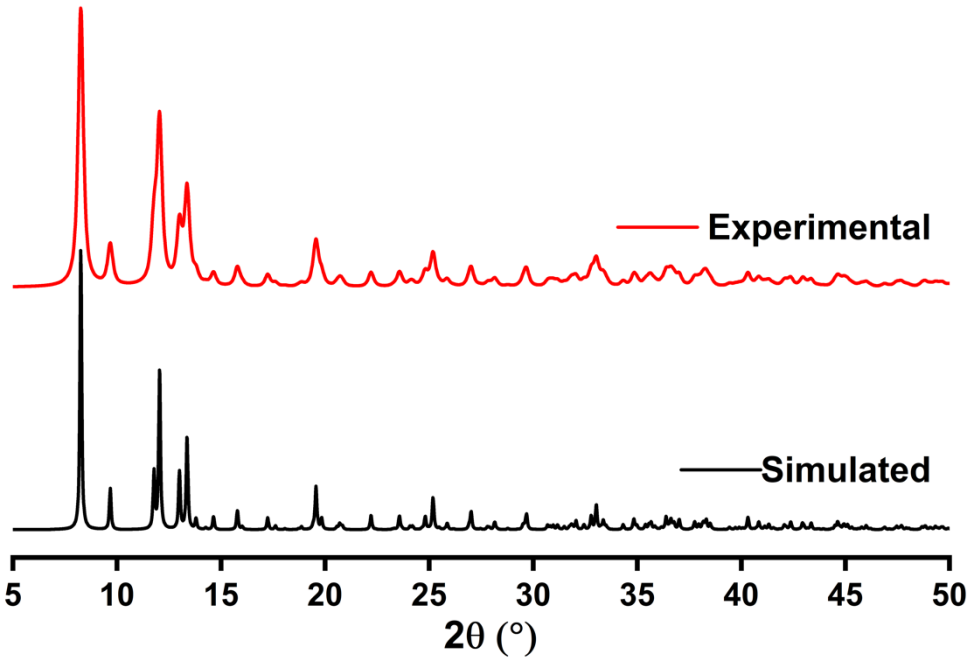


Fig. S4 XPRD spectra of $[Co^{II}_4\{L^3\text{-}(CO_2^-)_2\}_2(\mu_3\text{-}OCH_3)_2(CH_3OH)_2(H_2O)_2Cl_2]$ (**1**).

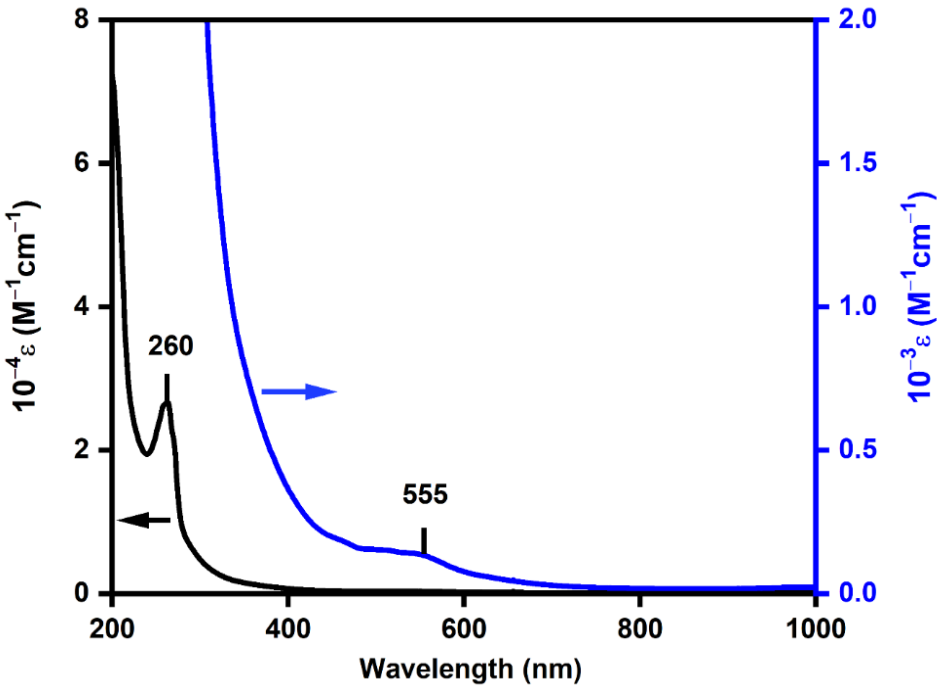


Fig. S5 UV-Vis spectrum of $[Co^{II}_4\{L^3\text{-}(CO_2^-)_2\}(\mu_3\text{-}OCH_3)_2(CH_3OH)_2(H_2O)_2Cl_2]$ **1** in CH_3CN-CH_3OH (2:1; v/v).

Table S1. Data Collection and Structure Refinement Parameters for $[Co_4\{L^3\text{-}(CO_2^-)_2\}(\mu_3\text{-}OCH_3)_2(CH_3OH)_2(H_2O)_2Cl_2]$ (**1**)

1	
Formula	$C_{28}H_{46}Cl_2Co_4N_4O_{14}$
Formula weight	969.31
Crystal colour, habit	red, block
T / K	100(2)
Crystal system	Monoclinic
Space group	$P2_1/n$ (no. 14)
a/Å	7.694(5)
b/Å	13.188(5)
c/Å	18.365(5)
α/°	90.0
β/°	96.099(5)
γ/°	90.0
V/Å^3	1852.9(15)
Z	2
D_c/g cm^{-3}	1.737
μ/mm^{-1}	1.973
Reflections measured	9843
Unique reflections/R_{int}	3436/0.0383
Reflections used $I > 2\sigma(I)$]	2712
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	$R_1 = 0.0404^a$ $wR_2 = 0.0975^b$
$R_1{}^a$, $wR_2{}^b$ (all data)	$R_1 = 0.0546^a$ $wR_2 = 0.1075^b$
GOF on F^2	1.037

$^aR_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$. $^bwR_2 = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2]/\Sigma[w(|F_o|^2)^2]\}^{1/2}$

Table S2. Hydrogen-bonding parameters in **1**

D–H···A	H···A, Å	D···A, Å
O7–H7···O4	1.646	2.563
O6–H6D···O2	1.820	2.690
C11–H11B···Cl1	2.852	3.816
C4–H4···Cl1	2.834	3.736
C6–H6A···O6	2.539	3.273
C7–H7A···O4	2.437	3.382
C6–H6B···O4	2.690	3.542
C8–H8B···π	2.753	3.715

Table S3 Calculated spin configurations and their relative energies as a function of different J_i constants. The spin configuration used as a reference is that with the maximum multiplicity generated from the parallel alignment of all local spin moments of the Co^{II} ions. Only the centres with an antiparallel (negative) alignment of their spin moment are noted.

Spin conf.	**S**	J_1	J_2	J_3	**Energy**[a]
{Co2,Co2$^{\#}$}	0	12	12	0	–52.53
{Co1$^{\#}$,Co2}	0	12	0	6	+78.94
{Co1$^{\#}$,Co2$^{\#}$}	0	0	12	6	–1.55
{Co2$^{\#}$}	3	6	6	6	+38.57
{Co1}	3	6	6	0	–26.10

[a]In cm^{-1}.