STRUCTURAL
CHEMISTRY

Volume 74 (2018)

Supporting information for article:

Structural investigation of one- and two-dimensional coordination polymers based on cobalt–bis(dioxolene) units and 1-hydroxy-1,2,4,5-tetrakis(pyridin-4-yl)cyclohexane

Olga Drath, Robert Gable and Colette Boskovic

Table S1 Experimental data for **1**·2 EtOH·15H_2O collected at 275 K.

Crystal data	
Chemical formula	$C_{54}H_{64}CoN_4O_5·C_2H_6O·5H_2O$
M_r	1044.017
Crystal system, space group	Triclinic, $\bar{P}1$
Temperature (K)	275
a, *b*, *c* (Å)	10.066 (2), 16.124 (3), 18.205 (4)
α, β, γ (°)	75.36 (3), 83.11 (3), 78.68 (3)
V (Å3)	2795.5 (11)
Z	2
Radiation type	Synchrotron, λ = 0.71073 Å
μ (mm−1)	0.37
Crystal size (mm)	0.1 × 0.04 × 0.02
Data collection	
Diffractometer	ADSC Quantum 210r
Absorption correction	Multi-scan SADABS2012/1 (Bruker,2012)
No. of measured, independent and observed [I > 2σ(I)] reflections	110832, 17440, 11405
Rint	0.073
(sin θ/λ)max (Å−1)	0.753
Refinement	
R[F2 > 2σ(F2)], wR(F2), S	0.087, 0.270, 1.04
No. of reflections	17440

No. of parameters	683
No. of restraints	74
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e Å−3)	1.58, −0.82

Computer programs: ShelXT (Sheldrick, 2015), *SHELXL* (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

Table S2 Experimental data for **2**·EtOH·3H_2O collected at 315 K.

Crystal data	
Chemical formula	$C_{54}H_{64}CoN_4O_5\cdot 3H_2O$
M_r	1008.13
Crystal system, space group	Triclinic, $\bar{P}1$
Temperature (K)	315
a, *b*, *c* (Å)	10.168 (2), 16.321 (3), 18.515 (4)
α, β, γ (°)	75.33 (3), 82.77 (3), 78.77 (3)
V (Å^3)	2906.0 (11)
Z	2
Radiation type	Synchrotron, λ = 0.71073 Å
μ (mm^{-1})	0.35
Crystal size (mm)	0.1 × 0.04 × 0.02
Data collection	
Diffractometer	ADSC Quantum 210r
Absorption correction	Multi-scan *SADABS2012*/1 (Bruker,2012)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	194018, 17669, 10358

R_{int}	0.101
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.746
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.099, 0.323, 1.03
No. of reflections	17669
No. of parameters	680
No. of restraints	128
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.16, −0.52

Computer programs: *SHELXL* (Sheldrick, 2015), Olex^2 (Dolomanov *et al.*, 2009).

Table S3 SHAPE[a] (for O_h) and metrical oxidation state (MOS)[b] indices.

	1·2 EtOH·15H_2O	**2**·EtOH·5H_2O	**2**·EtOH·5H_2O	**2**·EtOH·3H_2O
	100 K	100 K	275 K	315 K
SHAPE	0.212	0.103	0.159	0.258
MOS[c]	-1.25	-1.68	-1.90	-1.61
MOS[d]	-1.86	-1.26	-1.31	-1.22

[a] (Alvarez *et al.*, 2002). [b](Brown, 2012). [c] Dioxolene 1 (O1, O2). [d]Dioxolene 2 (O3, O4).