1D magnetic chain built from vanadyl ions and pyrazine-2,5-dicarboxylate

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Supplementary Material

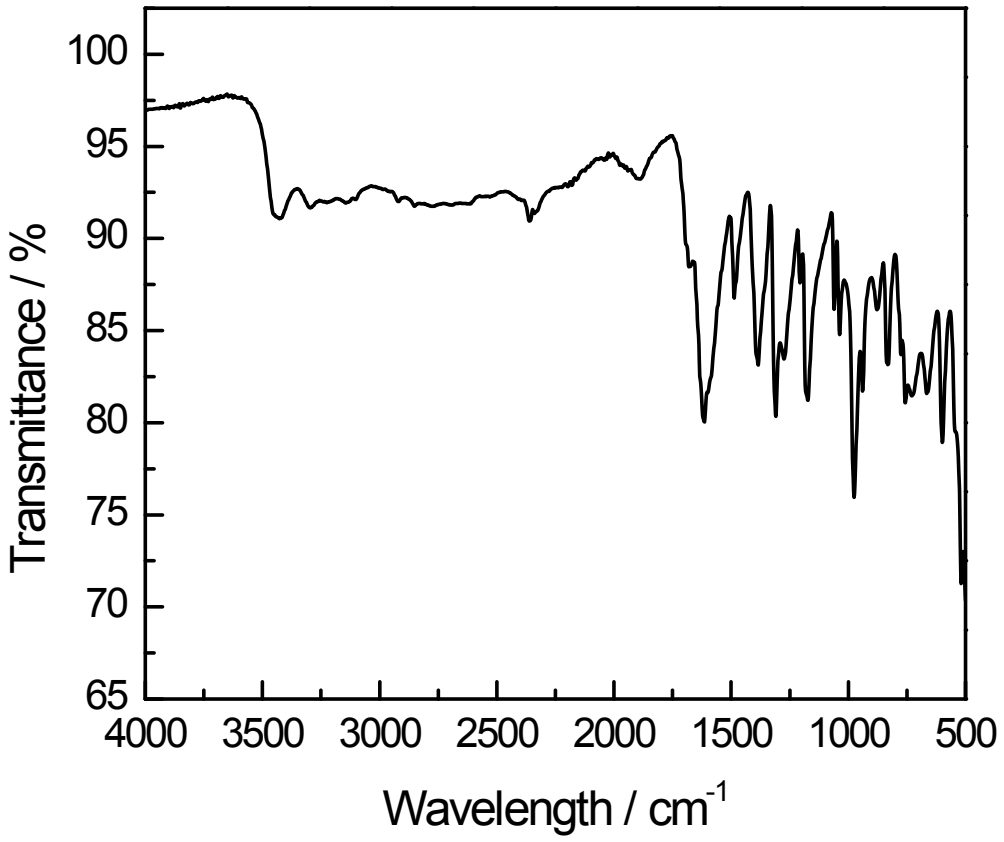

Figure S1. IR spectrum of $\{[VO(pzdc)(H_2O)_2]\ H_2O\}_n$.

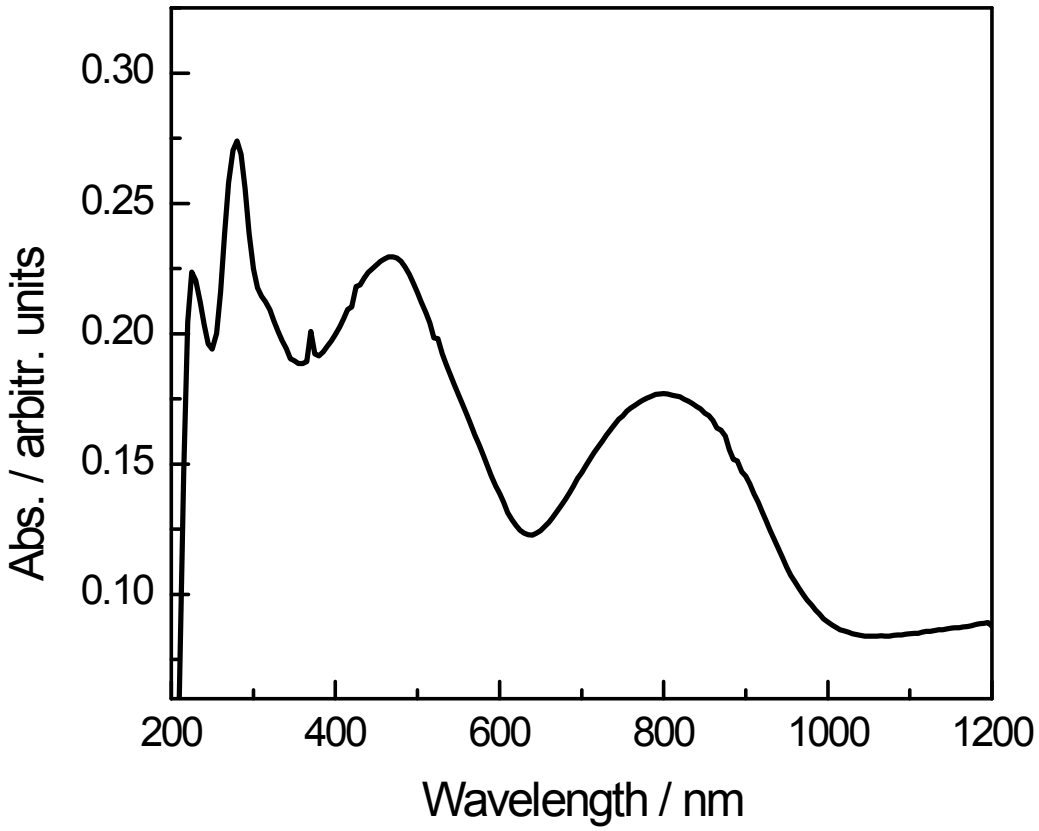

Figure S2. The UV–Vis spectrum of $\{[VO(pzdc)(H_2O)_2]\ H_2O\}_n$.

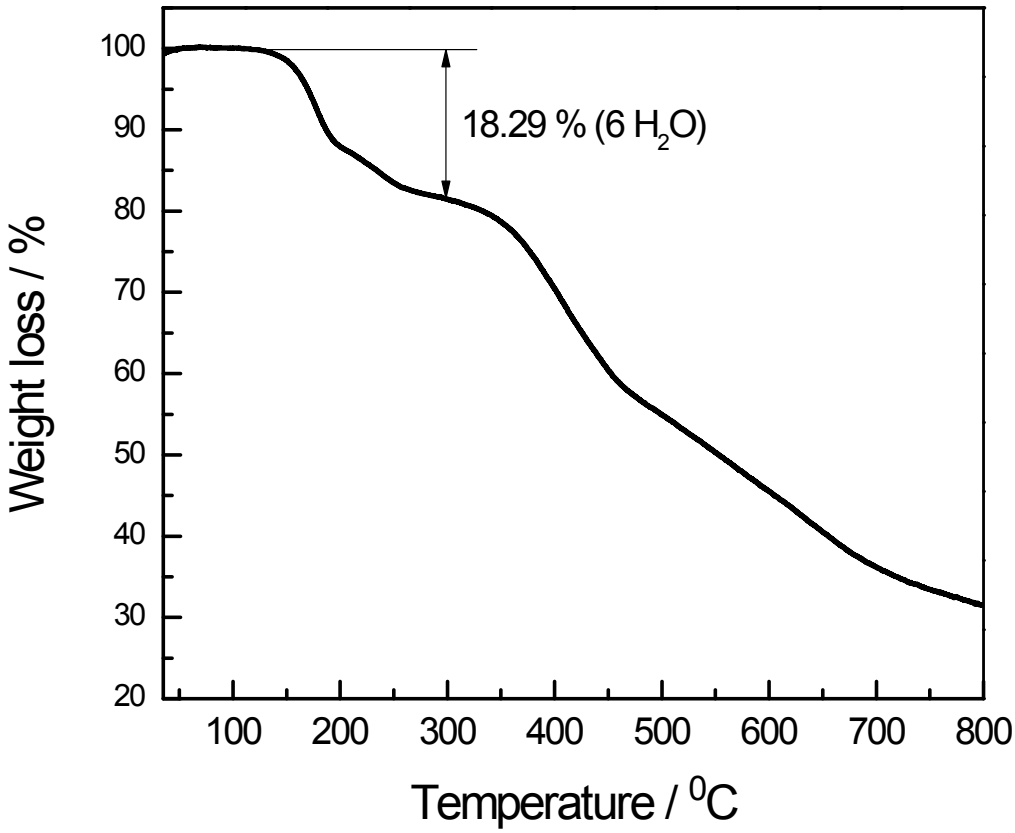

Figure S3. The TGA curve of $\{[VO(pzdc)(H_2O)_2]\ H_2O\}_n$ recorded at 5 °C/min and in argon atmosphere

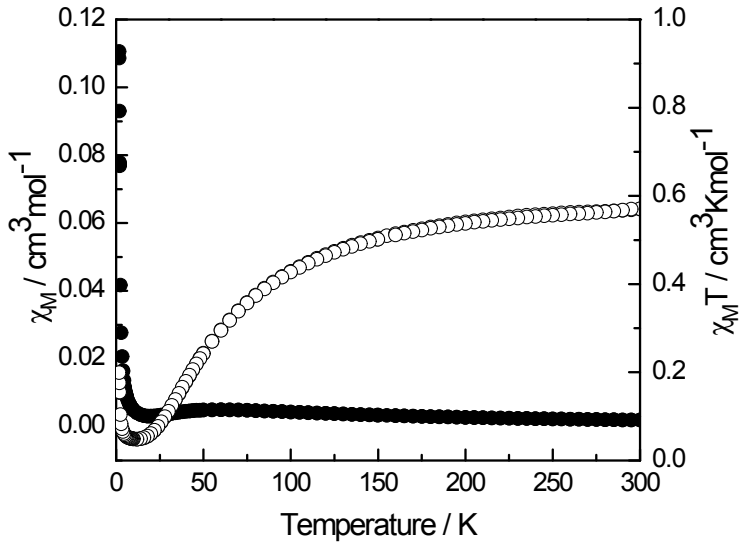

Figure S4. Temperature dependence of the magnetic susceptibility of $\{[VO(pzdc)(H_2O)_2]\cdot H_2O\}_n$: χ_M *vs* T (●)and $\chi_M T$ *vs* T (○).

Table S1. Crystal data for compound $\{[VO(pzdc)(H_2O)_2]\ H_2O\}_{2n}$

Empirical Formula	$C_{12}H_{16}N_4O_{16}V_2$
Formula Weight	574.16
Crystal Color, Habit	Red brown, block
Crystal Dimensions	5.000 × 0.050 × 0.050 mm
No. of Reflections Used for Unit Cell Determination (2q range)	5180 6.0 - 55.0°
Omega Scan Peak Width at Half-height	0.00°
Lattice Parameters	a = 6.7612(8) Å b = 8.792(1) Å c = 9.346(2) Å α = 65.850(5)° β = 87.775(6)° γ = 84.909(6)° V = 504.9(1) Å^3
Space Group	P-1 (#2)
Z value	1
Space Group	P-1 (#2)
D_{calc}	1.888 g/cm^3
F_{000}	290.00
μ(MoK_a)	10.187 cm^{-1}
D_{calc}	1.888 g/cm^3

Table S2. Bond lengths (Å) and angles (°) of the hydrogen bonding

Donor	– H –	Acceptor	D···A	D - H	H···A	D - H···
O1	H4	O7	2.700(3)	0.81	1.89(4)	178(4)
O1	H5	O8	2.569(4)	0.72	1.88(5)	159(4)
O3	H7	O2	2.935(3)	0.66	2.51(5)	124(4)
O3	H7	O7	2.833(3)	0.66	2.22(5)	156(4)
O3	H8	O5	2.660(3)	0.78	1.88(5)	177(3)
O8	H1	N2	2.875(3)	0.90	1.98(5)	170(5)
O8	H2	O4	2.866(3)	0.88	2.02(5)	161(4)