

## Supplementary Information

### A cyanide-bridged Fe-Co pearl-like single chain magnet containing 4-coordinate cobalt(II) ions

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**Table S1** Selected Bond lengths [Å] and angles [deg] for **1**.

<b>Fe1</b> Fe1–C1 Fe1–C2 Fe1–C3 Fe1–N4 Fe1–N6 Fe1–N8	1.908(7) 1.923(6) 1.926(7) 1.963(5) 1.949(5) 1.962(5)	<b>Co1</b> Co1–N1 Co1–N3 <sup>2</sup> Co1–Cl1 Co1–Cl2	2.026(6) 2.042(6) 2.233(3) 2.250(3)
<b>Co2</b> Co2–N2 Co2–N2 <sup>1</sup> Co2–O1 Co2–O2 Co2–O1 <sup>1</sup> Co2–O2 <sup>1</sup>	2.103(6) 2.103(6) 2.079(6) 2.075(7) 2.079(6) 2.075(7)		
<b>Fe1</b> C1–Fe1–C2 C1–Fe1–C3 C1–Fe1–N6 C1–Fe1–N8 C2–Fe1–C3 C2–Fe1–N4 C2–Fe1–N8 C3–Fe1–N4 C3–Fe1–N6 N4–Fe1–N6 N4–Fe1–N8 N6–Fe1–N8	90.1(3) 84.1(3) 91.0(3) 95.9(2) 88.8(3) 89.3(2) 91.1(2) 91.6(2) 92.2(3) 89.6(2) 88.4(2) 87.9(2)	<b>Co1</b> N1–Co1–N3 <sup>2</sup> N1–Co1–Cl1 N1–Co1–Cl2 N3 <sup>2</sup> –Co1–Cl1 N3 <sup>2</sup> –Co1–Cl2 Cl1–Co1–Cl2	104.5(3) 107.0(2) 112.5(3) 109.7(2) 107.4(3) 115.18(14)
<b>Co2</b> N2–Co2–O1 N2–Co2–O1 <sup>1</sup> N2–Co2–O2 N2–Co2–O2 <sup>1</sup> O1–Co2–O2 O1–Co2–O2 <sup>1</sup>	87.4(3) 91.7(2) 91.6(3) 88.4(3) 87.4(3) 92.6(3)		

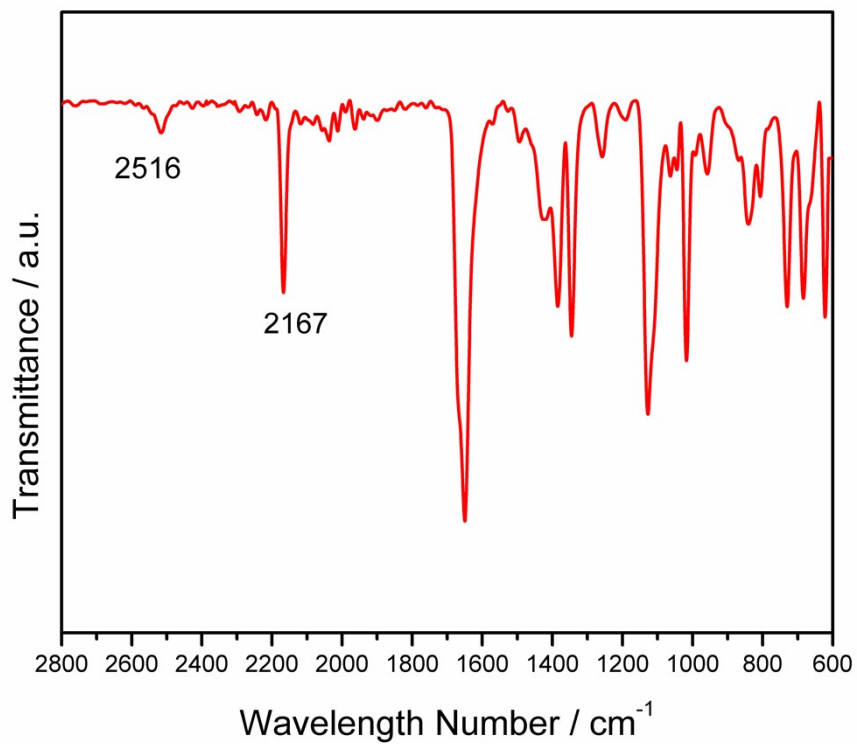
**Table S2** Selected Bond lengths [Å] and angles [deg] for **2**.

<b>Fe1</b> Fe1–C1 Fe1–C2 Fe1–C3 Fe1–N6 Fe1–N8 Fe1–N10	1.928(7) 1.931(8) 1.923(8) 2.004(7) 2.002(6) 1.979(7)	<b>Co1</b> Co1–N1 Co1–N3 <sup>1</sup> Co1–Cl1 Co1–Cl2	1.987(6) 1.989(7) 2.294(5) 2.195(4)
<b>Co2</b> Co2–N2 Co2–N2 <sup>2</sup> Co2–O1 Co2–O2 Co2–O1 <sup>2</sup> Co2–O2 <sup>2</sup>	2.107(6) 2.107(6) 2.100(7) 2.061(7) 2.100(7) 2.061(7)		
<b>Fe1</b> C1–Fe1–C2 C1–Fe1–C3 C1–Fe1–N6 C1–Fe1–N10 C2–Fe1–C3 C2–Fe1–N6 C2–Fe1–N8 C3–Fe1–N8 C3–Fe1–N10 N6–Fe1–N8 N8–Fe1–N10 N6–Fe1–N10	90.9(3) 87.1(3) 90.7(3) 90.0(3) 89.8(3) 90.2(3) 88.7(3) 92.5(3) 90.5(3) 89.7(3) 90.3(3) 89.6(3)	<b>Co1</b> N1–Co1–N3 <sup>1</sup> N1–Co1–Cl1 N1–Co1–Cl2 N3 <sup>1</sup> –Co1–Cl1 N3 <sup>1</sup> –Co1–Cl2 Cl1–Co1–Cl2	103.2(3) 109.0(3) 111.9(3) 105.1(2) 115.0(2) 112.0(2)
<b>Co2</b> N2–Co2–O1 N2–Co2–O1 <sup>2</sup> N2–Co2–O2 N2–Co2–O2 <sup>2</sup> O1–Co2–O2 O1–Co2–O2 <sup>2</sup>	88.4(3) 91.6(3) 88.4(3) 91.6(3) 89.5(3) 90.5(3)		

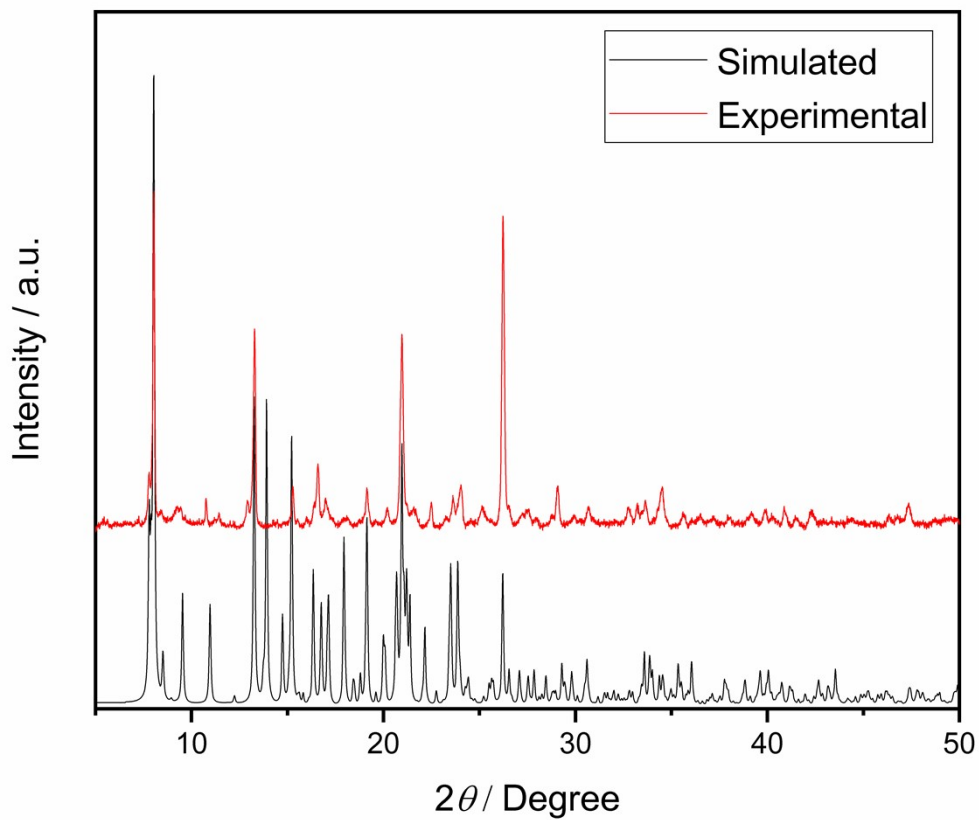
**Table S3.** Continuous Shape Measures (CShM) calculated by *SHAPE*<sup>1</sup> Software for **1** and **2**.

Compound	Metal ion	Symmetry	CShM
<b>1</b>	Co1	$T_d$	0.493
	Co2	$O_h$	0.068
	Fe1	$O_h$	0.140
<b>2</b>	Co1	$T_d$	0.550
	Co2	$O_h$	0.050
	Fe1	$O_h$	0.047

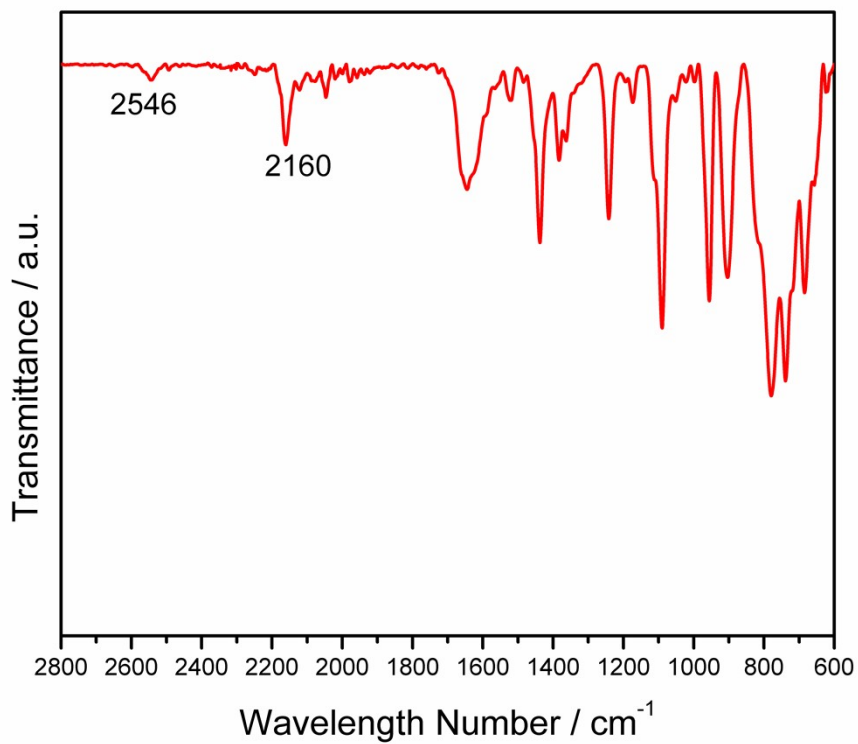
1. *SHAPE*, version 2.0: continuous shape measures calculation; Electronic Structure Group, Universitat de Barcelona: Barcelona, Spain, 2010.



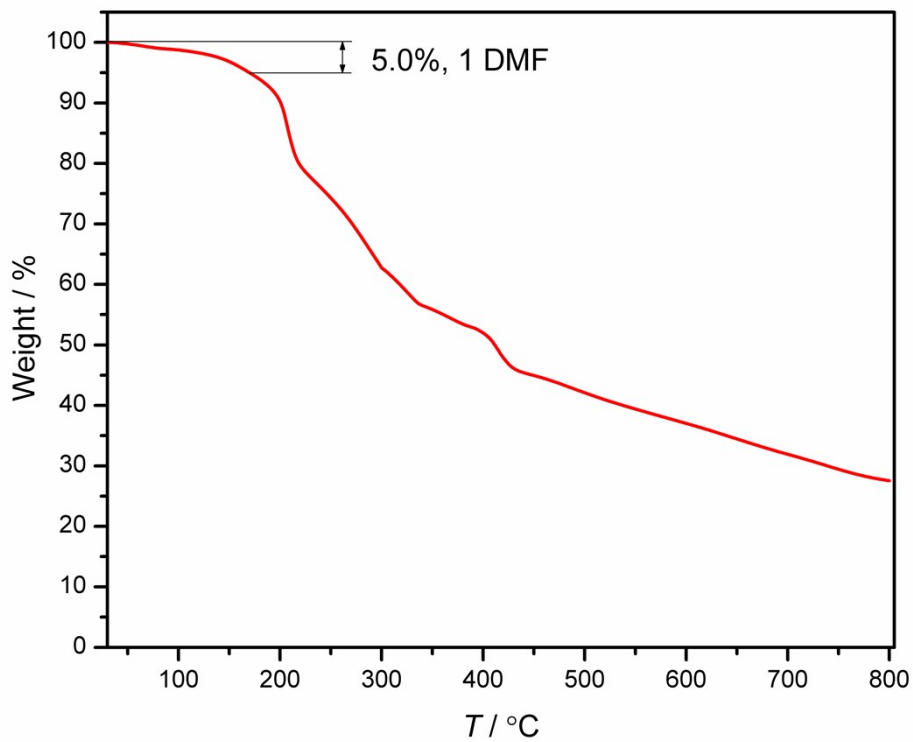
**Fig. S1** IR spectrum of compound **1**.



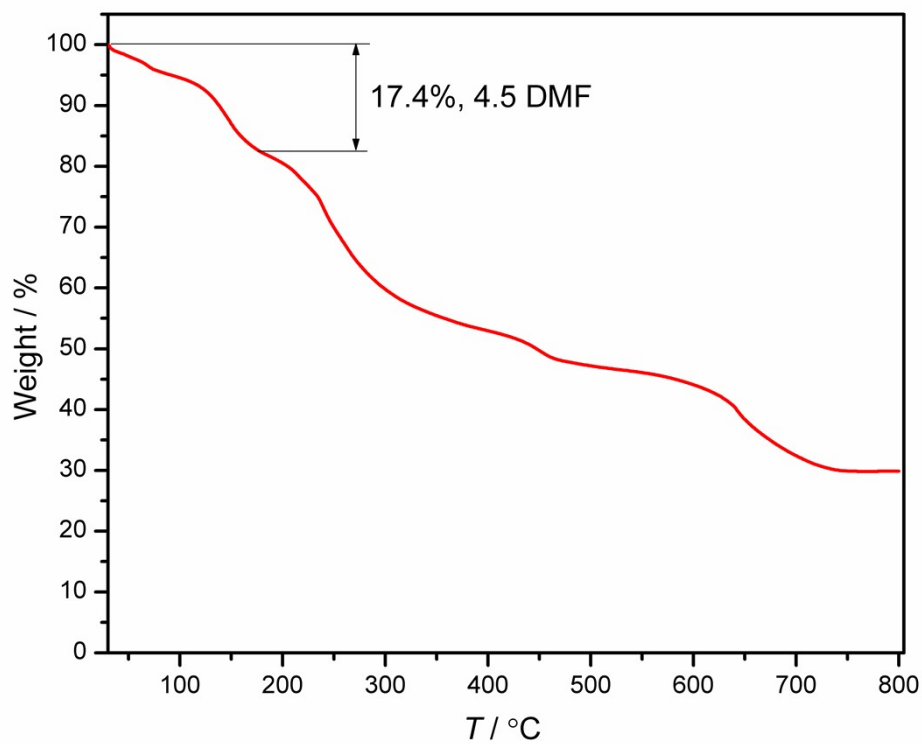
**Fig. S2** Experimental and simulated PXRD patterns of **1**.



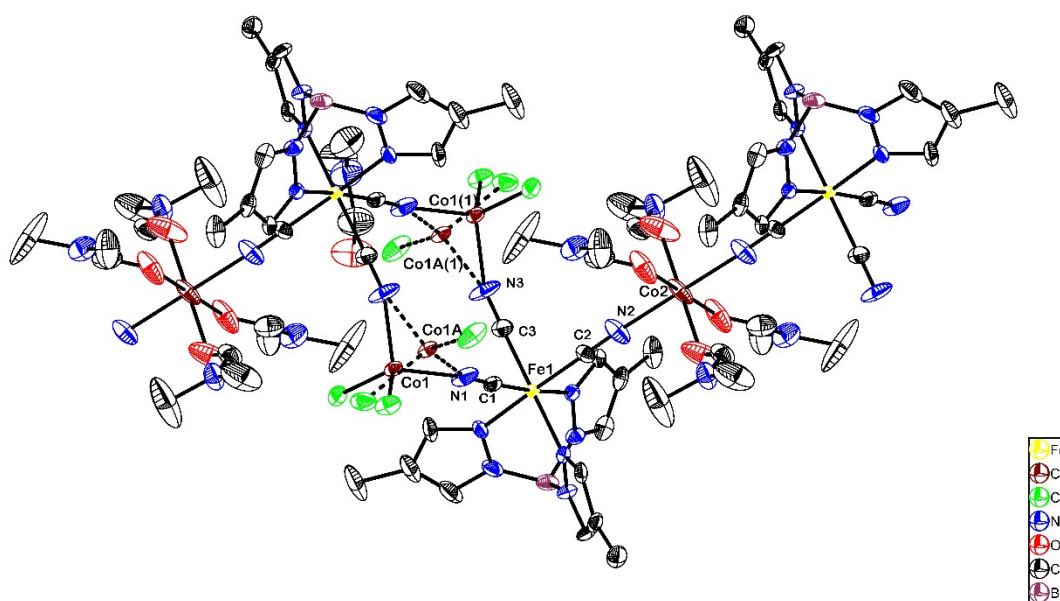
**Fig. S3** IR spectrum of compound **2**.



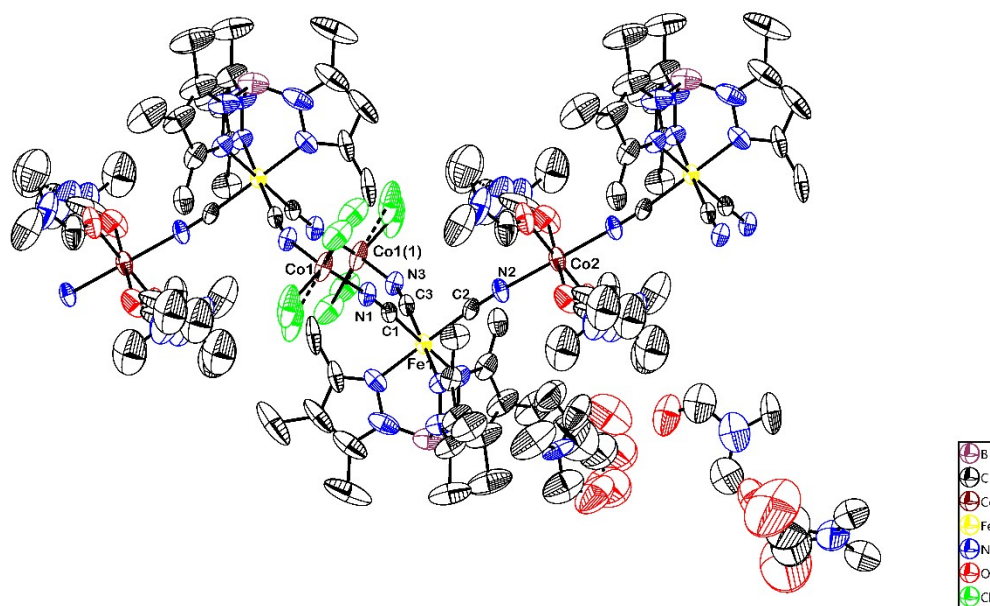
**Fig. S4** Thermo-gravimetric curve of **1**.



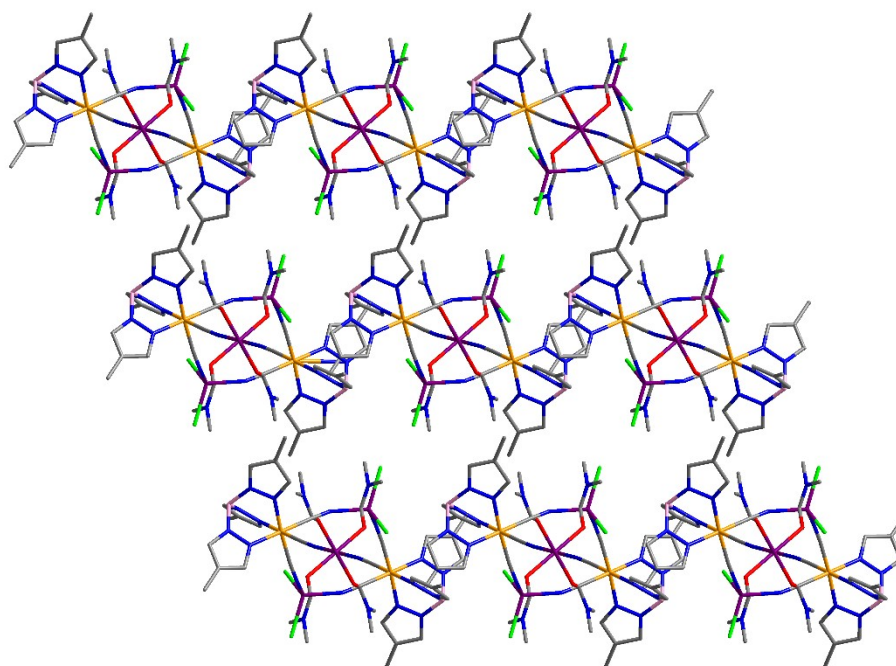
**Fig. S5** Thermo-gravimetric curve of **2**.



**Fig. S6** Crystal structure of **1** drawn with ellipsoids at the 50% probability level. The hydrogen atoms have been omitted for the sake of clarity.

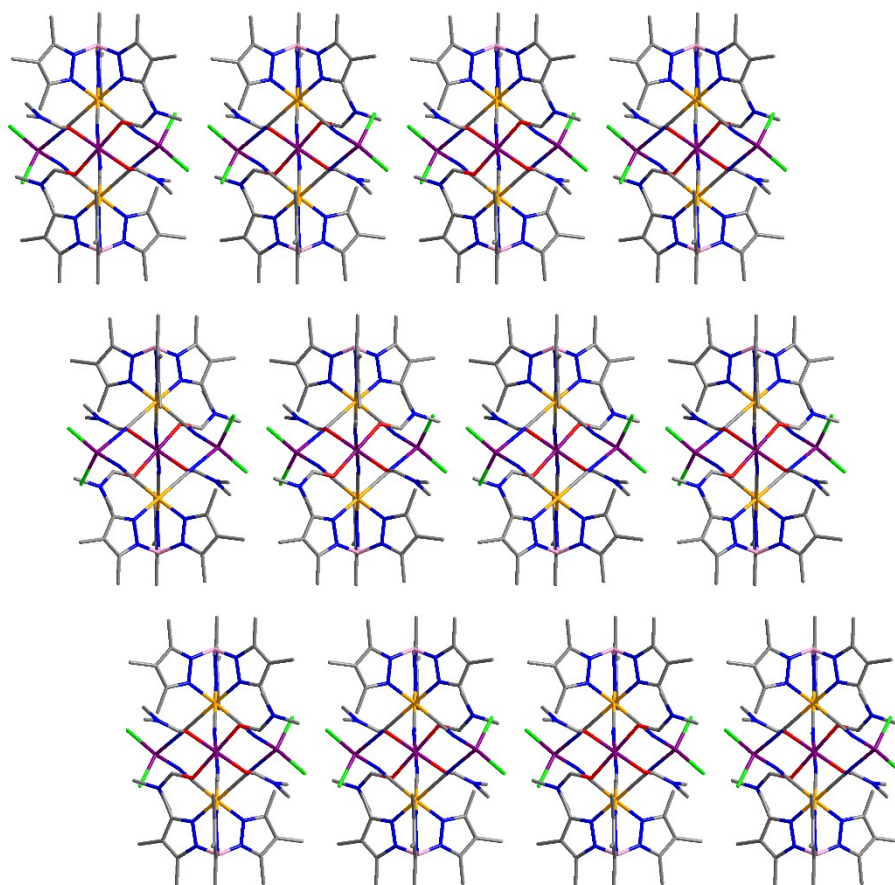


**Fig. S7** Crystal structure of **2** drawn with ellipsoids at the 50% probability level. The hydrogen atoms have been omitted for the sake of clarity.

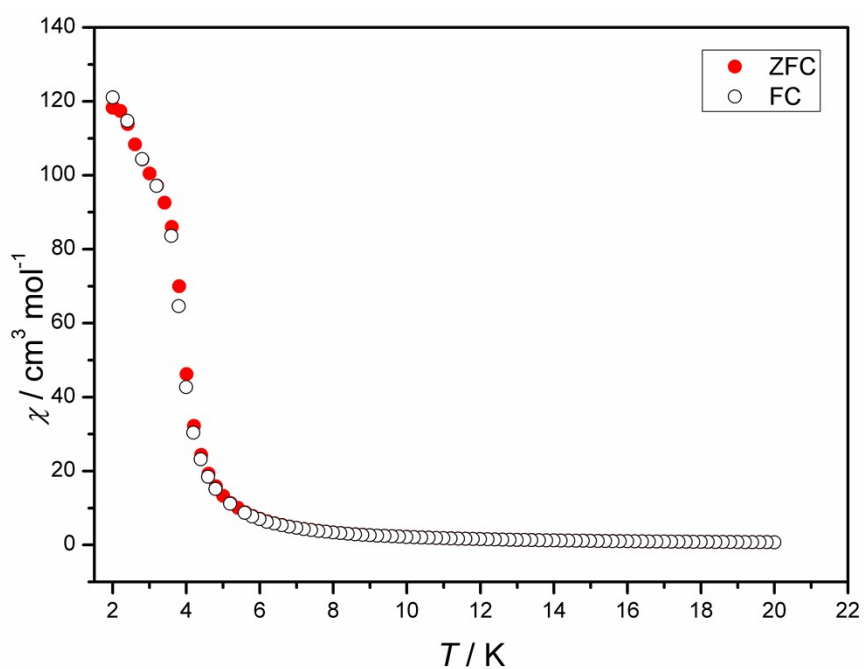


**Fig. S8** The packing diagram of **1** view along the crystallographic b axis.

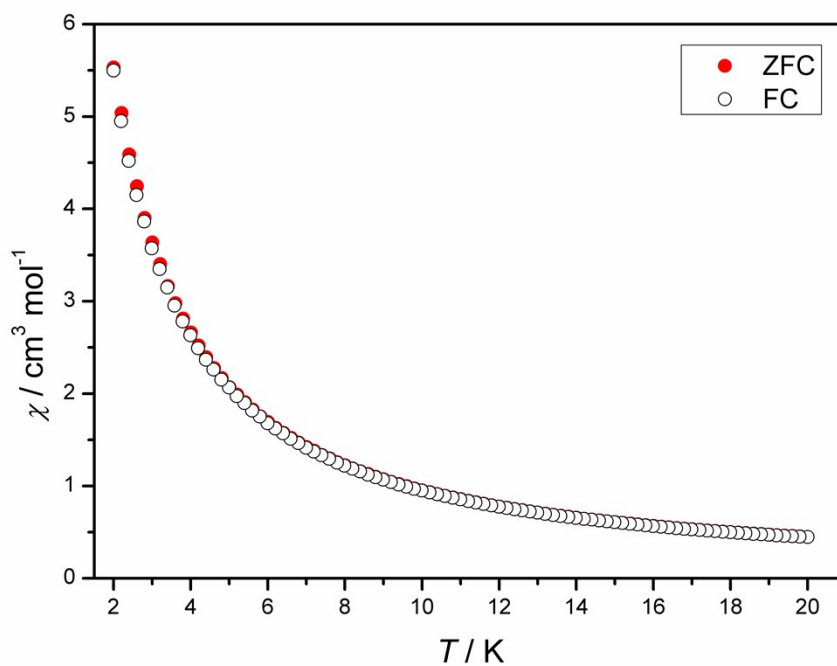




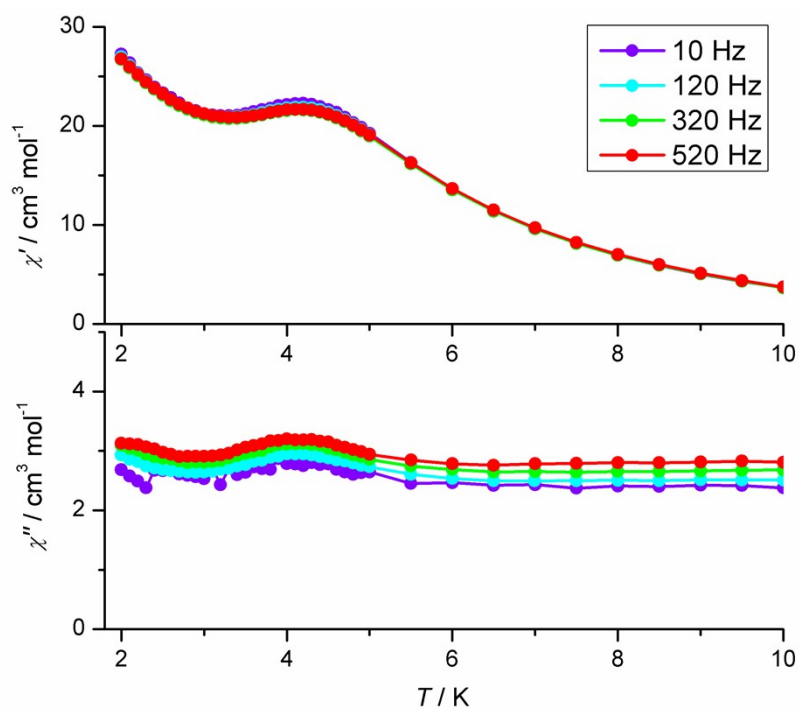
**Fig. S9** The packing diagram of **2** view along the crystallographic b axis.



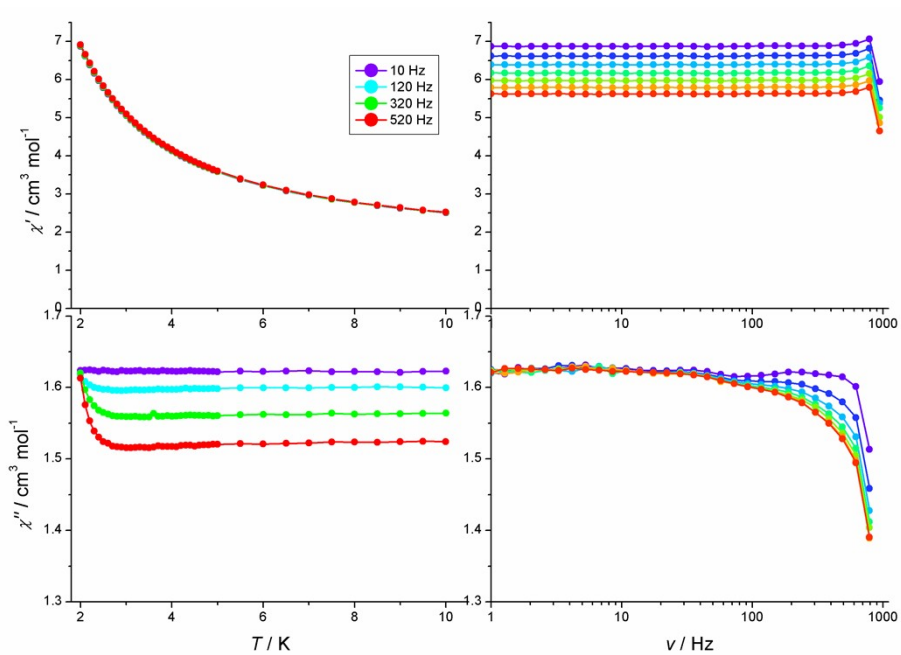
**Fig. S10** Zero-field cooled and field-cooled magnetization data of **1** at 2–20 K.



**Fig. S11** Zero-field cooled and field-cooled magnetization data of **2** at 2–20 K.



**Fig. S12** Temperature dependence of the in-phase ( $\chi'$ ) and out-of-phase ( $\chi''$ ) ac magnetic susceptibilities for **1** under 1 kOe dc field.



**Fig. S13** Temperature (left) and frequency (right) dependence of the in-phase ( $\chi'$ ) and out-of-phase ( $\chi''$ ) ac magnetic susceptibilities for **2** under zero dc field.