

## Electronic Supplementary Information (ESI)

How to Force a Classical Chelating Ligand to a Metal Non-Chelating  
Bridge: the Observation of a Rare Coordination Mode of Diethanolamine  
in the 1D Complex  $\{[\text{Cu}_2(\text{Piv})_4(\text{H}_3t\text{BuDea})](\text{Piv})\}_n$

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**Table S1.** Selected geometrical parameters (distances/Å and angles/°) for **1**.

Cu1–O1	2.159(2)	Cu2–O2	2.192(2)
Cu1–O11	1.961(3)	Cu2–O31	1.957(3)
Cu1–O12 <sup>a</sup>	1.957(3)	Cu2–O32 <sup>b</sup>	1.974(3)
Cu1–O21	1.950(3)	Cu2–O41	1.951(3)
Cu1–O22 <sup>a</sup>	1.969(3)	Cu2–O42 <sup>b</sup>	1.945(3)
Cu1…Cu1 <sup>a</sup>	2.5776(8)	Cu2…Cu2 <sup>b</sup>	2.5959(8)
O1–Cu1–O11	91.11(10)	O2–Cu2–O31	94.74(10)
O1–Cu1–O12 <sup>a</sup>	99.31(10)	O2–Cu2–O32 <sup>b</sup>	95.96(10)
O1–Cu1–O21	93.58(10)	O2–Cu2–O41	93.02(10)
O1–Cu1–O22 <sup>a</sup>	96.94(10)	O2–Cu2–O42 <sup>b</sup>	97.69(10)
O11–Cu1–O12 <sup>a</sup>	169.56(11)	O31–Cu2–O32 <sup>b</sup>	169.28(11)
O11–Cu1–O21	89.70(12)	O31–Cu2–O41	89.95(13)
O11–Cu1–O22 <sup>a</sup>	89.50(12)	O31–Cu2–O42 <sup>b</sup>	89.66(13)
O12 <sup>a</sup> –Cu1–O21	90.27(12)	O32 <sup>b</sup> –Cu2–O41	88.82(12)
O12 <sup>a</sup> –Cu1–O22 <sup>a</sup>	88.62(12)	O32 <sup>b</sup> –Cu2–O42 <sup>b</sup>	89.57(12)
O21–Cu1–O22 <sup>a</sup>	169.45(11)	O41–Cu2–O42 <sup>b</sup>	169.28(11)

Symmetry transformations used to generate equivalent atoms: <sup>a</sup>  $-x, -y, 2-z$ ; <sup>b</sup>  $1-x, -y, 2-z$ .

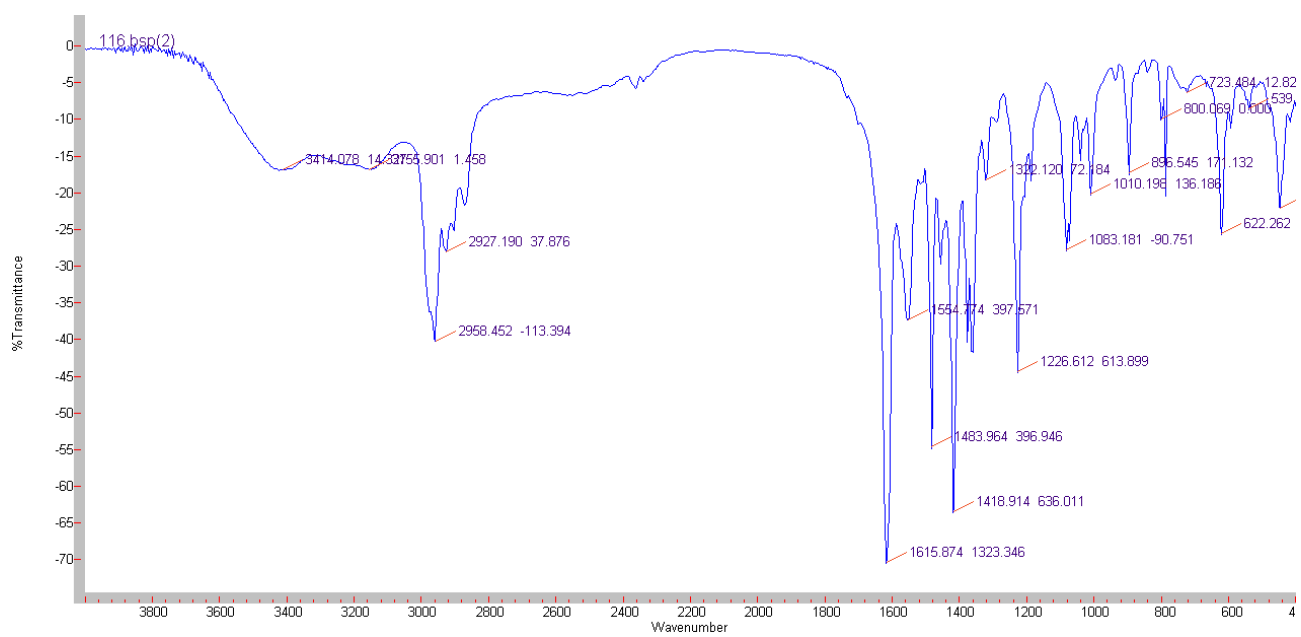
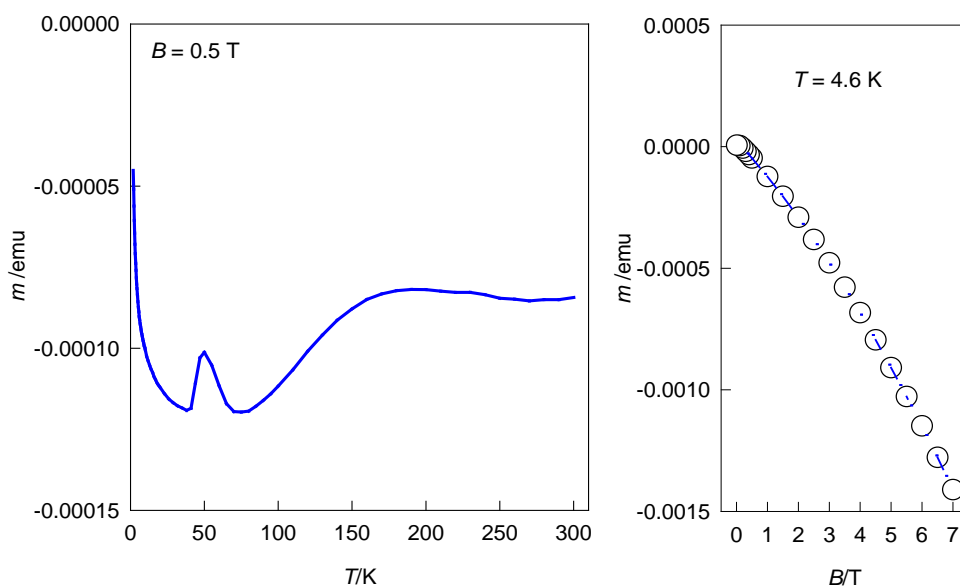
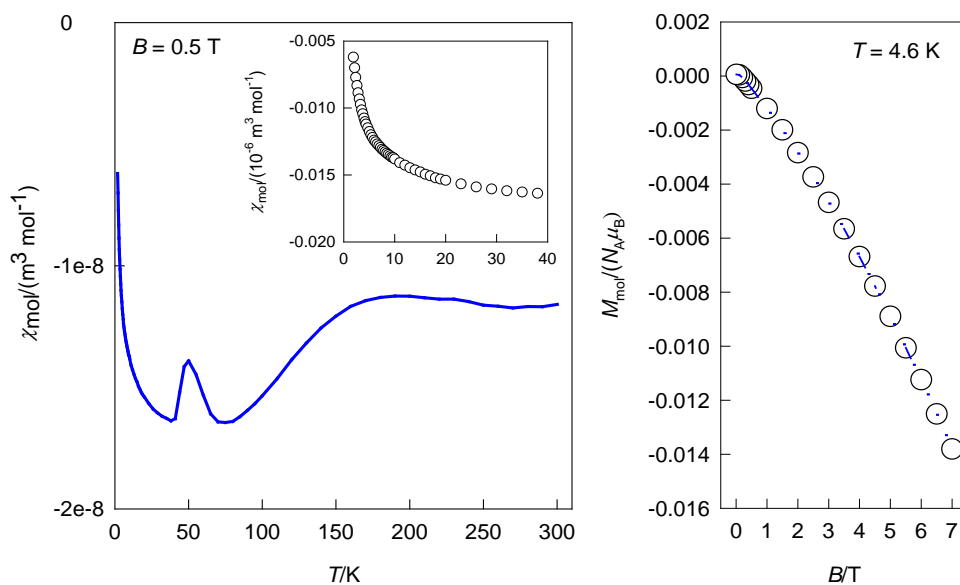


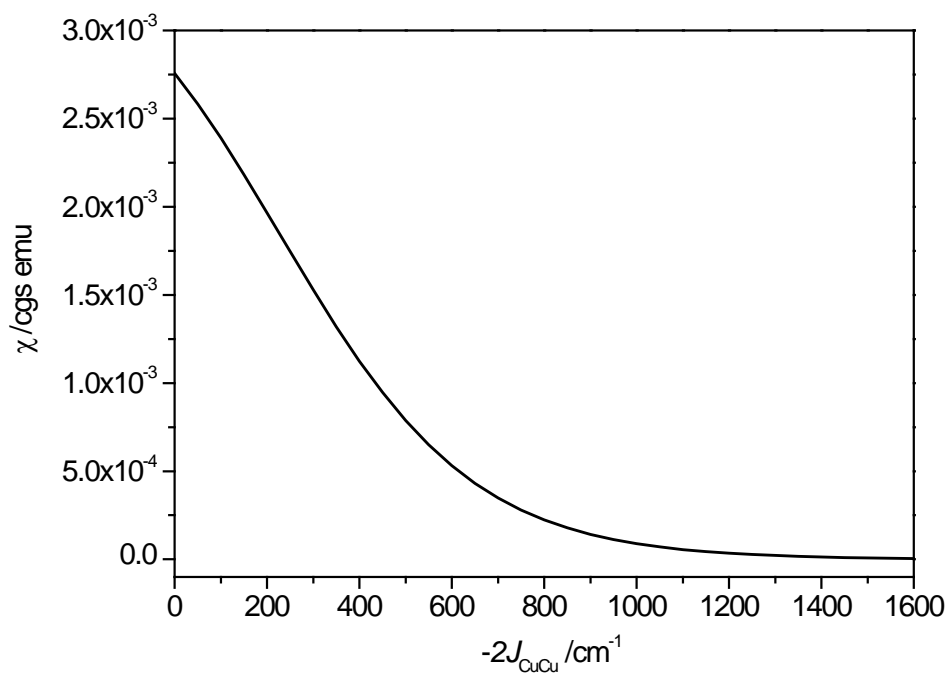
Figure S1. IR spectrum of **1** (in KBr).



**Figure S2.** Raw magnetic data for **1**: left – temperature dependence of the magnetic moment of the specimen; right – field dependence of the magnetic moment.



**Figure S3.** Magnetic data for **1**: left – temperature dependence of the molar magnetic susceptibility; right – field dependence of the magnetization per formula unit. Estimate of the net diamagnetic contribution is  $\chi_{\text{dia}} = -(5 \cdot M_r) \cdot 10^{-9}$ ; using  $M_r = 794.94/1000$  one gets  $\chi_{\text{dia}} = -3.97 \times 10^{-9} \text{ m}^3 \text{ mol}^{-1}$  (SI units are applied). A temperature-independent paramagnetic correction is  $\chi_{\text{TIP}} = +2 \cdot 0.75 \times 10^{-9} \text{ m}^3 \text{ mol}^{-1}$ .



**Figure S4.** The dependence of the molar magnetic susceptibility (per two copper centres) on the exchange coupling constant  $J_{\text{CuCu}}$  calculated from the Bleaney–Bowers equation. The magnitude of  $\chi$  becomes neglectable only for  $|J| \gg 1000 \text{ cm}^{-1}$ .