Supplementary Material (ESI) for Chemical Communications

Supplementary Material

Conversion of a Porous Material Based on a Mn^{II}-$TCNQF_4$ Honeycomb Net to a Molecular Magnet Upon Desolvation

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Figure S1-S5.

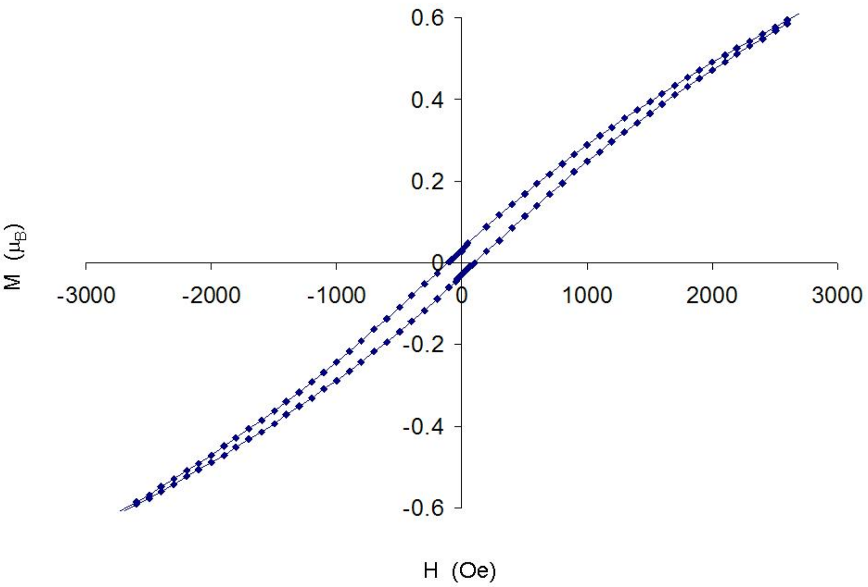
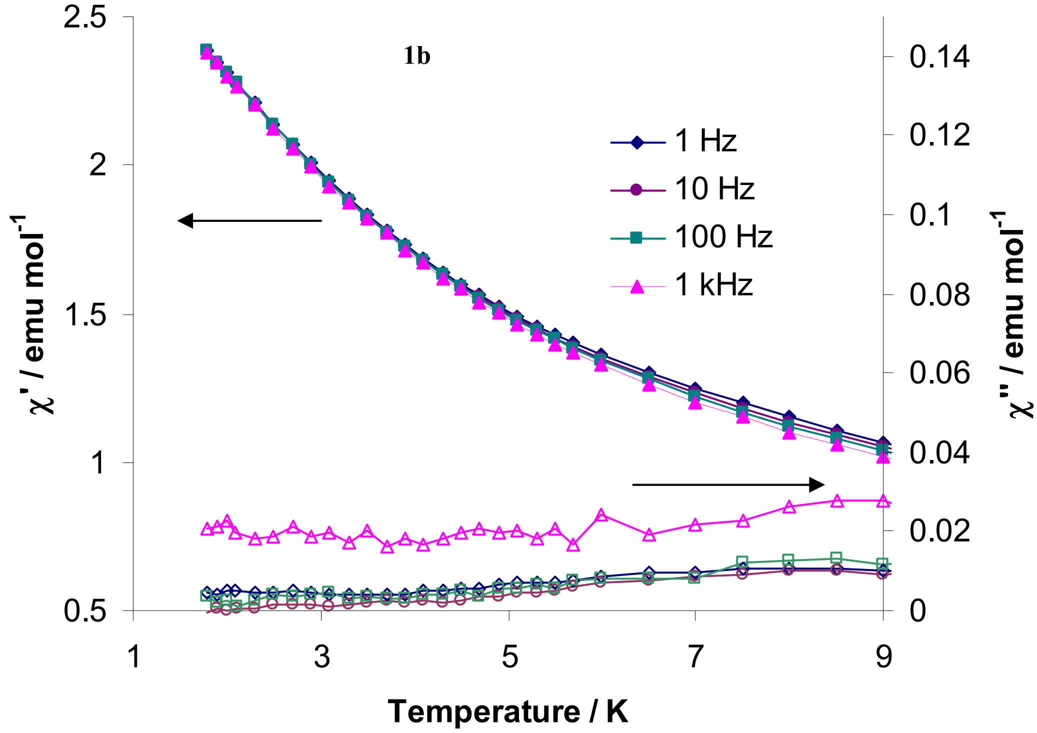


Figure S1. Hysterisis loop for **1a** at 1.8K.



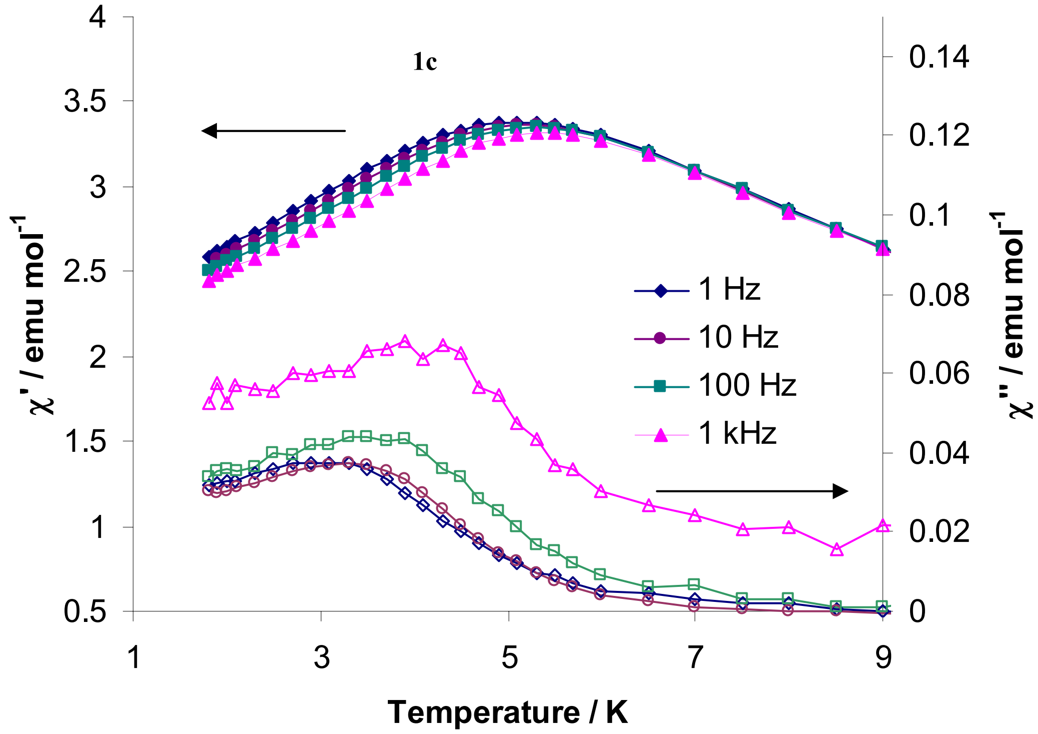


Figure S2. Temperature dependences of the real χ' and imaginary χ'' components of the AC magnetic susceptibility of **1b** (top) and **1c** (bottom) measured in an oscillating field of 3 Oe at different frequencies.

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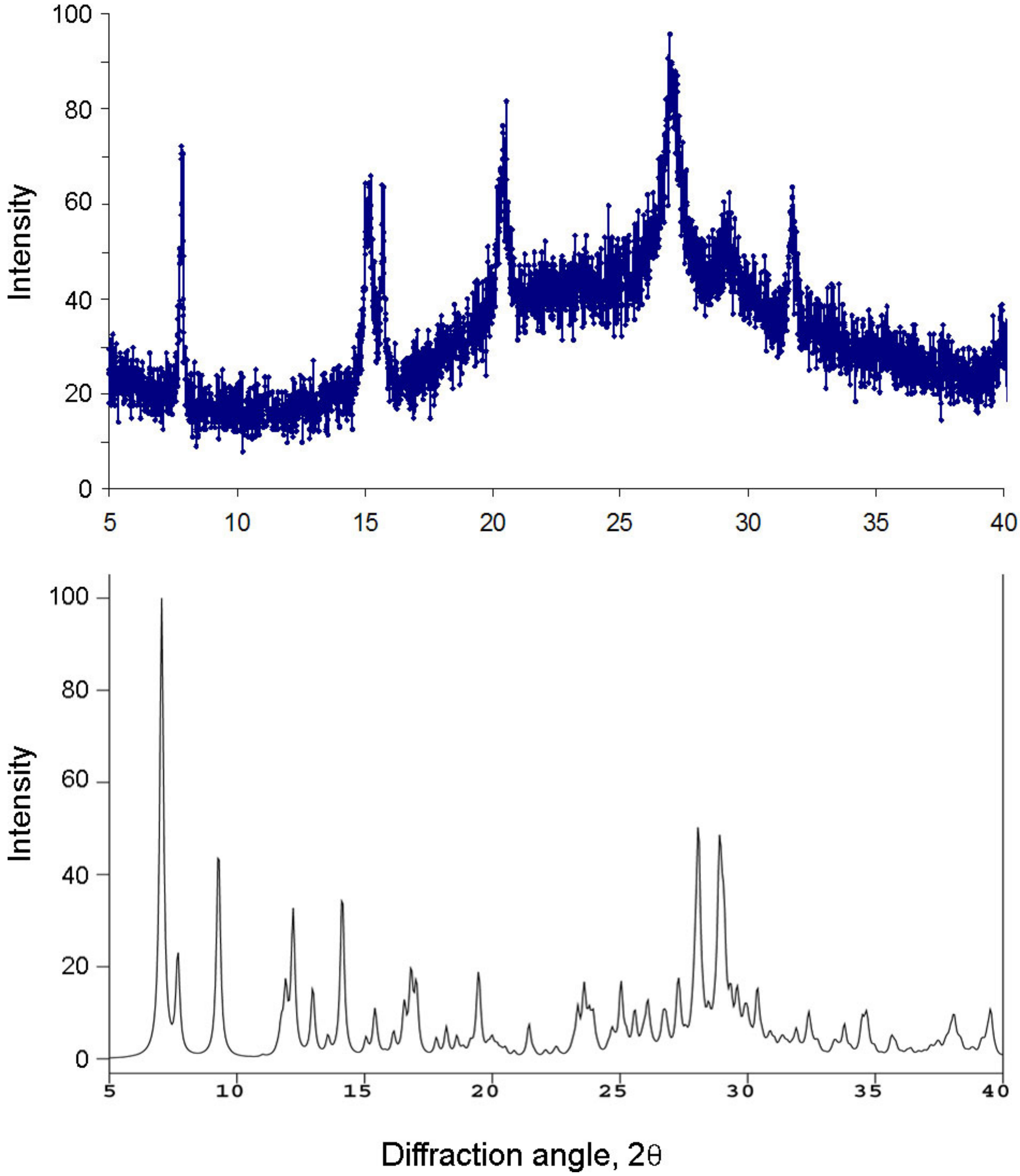

Figure S3. X-ray powder diffraction pattern of **1a** (top) and simulated X-ray powder diffraction pattern of **1**$\supset$7.5CH_3OH (bottom) Cu Kα radiation (λ = 1.54096Å).

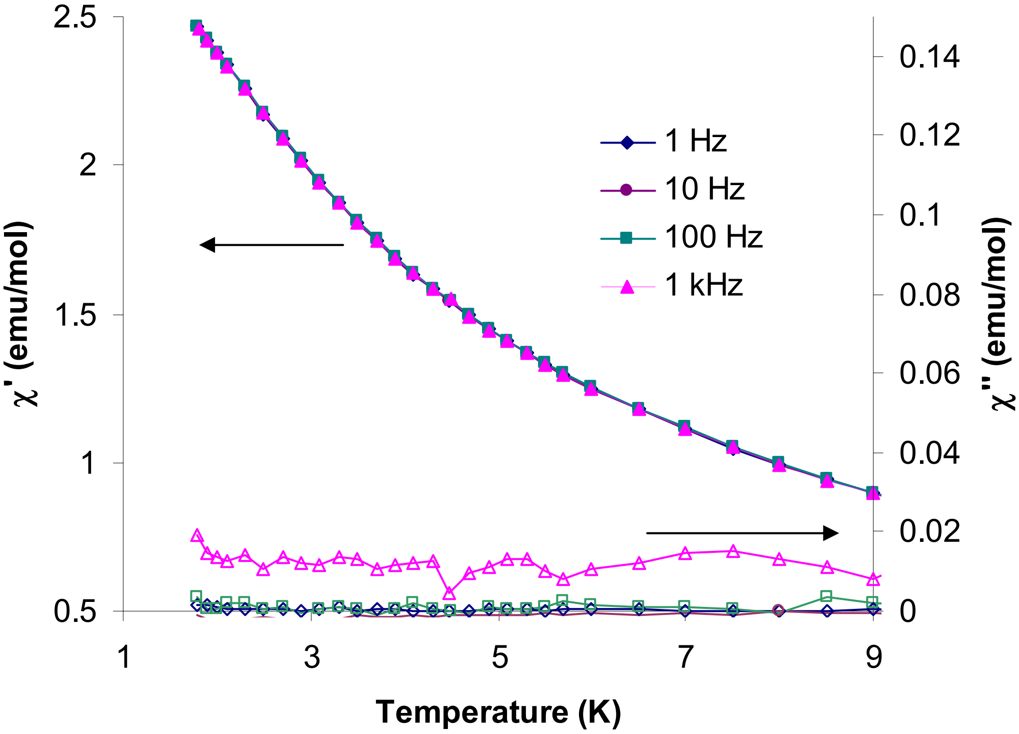

Figure S4. Temperature dependences of the real χ' and imaginary χ'' components of the AC magnetic susceptibility of **1**⊃7.5CH_3OH measured in an oscillating field of 3 Oe at different frequencies.

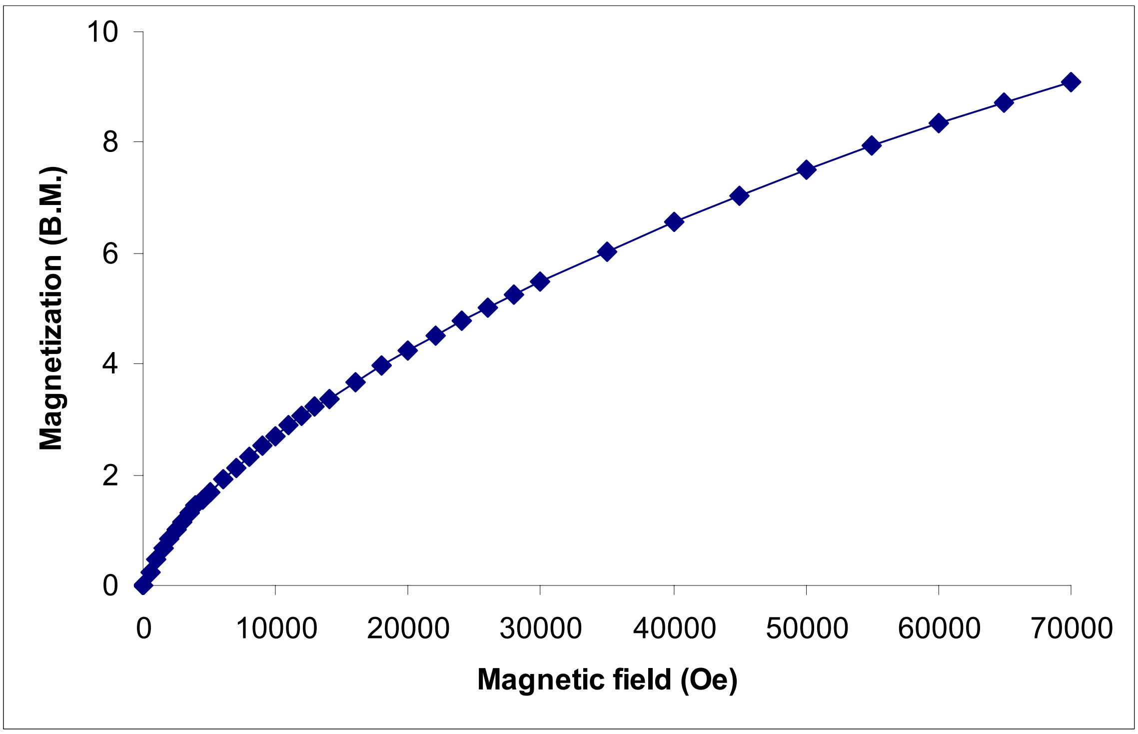

Figure S5. Field dependent magnetization curve of **1a** measured at 1.8 K.

The parameters that indicate the degree of spin-glass like behavior for **1a** were obtained in several ways. The relaxation time (τ) was obtained from the Arrhenius law:

$$\tau(T) = \tau_0 \cdot \exp\left(\frac{U}{k_B T}\right) \qquad \text{(S1)}$$

The best-fit parameters are U = 102.8 cm^{-1}; $\tau_0 = 6.4*10^{-21}$ s^{-1}. The obtained U and τ_0 values are in the range previously reported for spin glasses (U >100 cm^{-1}; τ_0 < 10-10 s^{-1}).[1-5]
The disorder parameter (ϕ) was obtained from Eq. S2

$$\phi = \Delta T_m/T_g/\Delta log\ \omega \qquad \text{(S2)}$$

where ΔT_m is the shift of the peak in χ', log ω is the logarithm of the applied frequency, and T_g the position of the peak at zero frequency. The value $\phi = 0.023$ places this compound in the range of canonical spin-glasses which have the typical value $\phi < 0.1$. Moreover, the data are very well described by assuming critical dynamics of a spin-glass with a finite static glass temperature T_g[1-5] as described by:

$$\tau = \tau_0((T_m\text{-}T_g)/T_g)^{-z\nu} \qquad \text{(S3)}$$

where $\tau = 1/2\pi\omega$ and $z\nu$ is the dynamical critical exponent which varies between 4 and 12 for different spin-glasses. The best fit yields T_g = 4 K, $\tau_0 = 7.3*10^{-6}$ s and $z\nu = 9.9$, which is within the realm of the conventional spin glass phases.[1-5]

1. D. Li, L. Zheng, Y. Zhang, J. Huang, S. Gao and W. Tang, *Inorg. Chem*. 2003, **42**, 6123.
2. R. Clérac, S. O'Kane, J. Cowen, X. Quyang, R. Heintz, H. Zhao, M. J. Bazile and K. R. Dunbar, *Chem. Mater*. 2003, **15**, 1840.
3. M. Hagiwara, *J. Magn. Magn. Mater.* 1998, **177**, 89.
4. S. Sahoo, O. Petracic, W. Kleemann, S. Stappert, G. Dumpich, P. Norblad, S. Cardoso and P. P. Freitas, *Appl. Phys. Lett*. 2003, **82**, 4116.
5. T. Mori, and H. Mamiya, *J. Phys. Condens. Mater.* 2004, **16**, S743.