Electronic supplementary information

| Table S1. Crystal data and results of refi | nement for 1 . |
|--|---|
| Empirical formula | $C_{10}H_9CoN_7$ |
| Formula weight [g mol-1] | 286.17 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Unit cell dimensions [Å, °, Å ³] | a = 11.8865(9) |
| | b = 16.4090(8) |
| | c = 6.0486(4) |
| | $\beta = 96.452(6)$ |
| | V = 1172.28(13) |
| Ζ | 4 |
| Calculated density [Mg m ⁻³] | 1.621 |
| Absorption coefficient [mm ⁻¹] | 11.436 |
| Crystal form, colour, size [mm] | Deep blue, needle, |
| | $0.32 \times 0.12 \times 0.08$ |
| Temperature [K] | 100(1) |
| Radiation [Å] | 1.54186 |
| Diffractometer | Stoe StadiVari |
| θ range for data collection [°] | 7.484 to 142.898 |
| Index ranges | $-14 \le h \le 13$, $-7 \le k \le 19$, $-7 \le l \le 7$ |
| Reflections coll. / indep. / parameters. | 10729 / 2212 / 197 |
| GooF (S) all/ind. | 0.950 |
| Final R indices $[I > 2\sigma(I)]$ | R1 = 0.0770, wR2 = 0.1887 |
| R indices (all data) | R1 = 0.1017, $wR2 = 0.2007$ |
| Largest diff. peak and hole [e Å ⁻³] | 0.92 / -0.32 |

‡ Crystallographic data: dark blue single-crystal of **1** was mounted on Eulerian-cradle diffractometer Stoe StadiVari possessing PILATUS3R 300K HPAD detector and CuKα radiation microfocus source Xenocs Genix3D ($\lambda = 1.54186$ Å) at 100K. The structure of **1** was solved by SHELXT, refined by SHELXL (ver. 2018/3) and drawn using OLEX2 and MERCURY programs.¹ Crystal data for **1**: C₁₀H₉CoN₇, $M_r = 286.17$, monoclinic $P2_1/c$, a = 11.8865(9), b = 16.4090(8), c = 6.0486(4) Å, $\alpha = 90$, $\beta = 96.452(6)$, $\gamma = 90$ deg, V = 1172.28(13) Å³, Z = 4, $D_c = 1.621$ g cm⁻³, $\mu = 11.436$ mm⁻¹, F(000) = 580, T = 100(1) K, 20max = 142.898° (-14 ≤ h ≤ 13, -7 ≤ k ≤ 19, -7 ≤ l ≤ 7). Final results (164 parameters): R1 = 0.0770 and wR2 = 0.1887 [I > 2 σ (I)], and R1 = 0.1017, wR2 = 0.2007 and S = 0.950 for all 10729 reflections. CCDC reference number 1859501.

Table S2. Selected geometric parameters [Å,°] for 1.

| Tuble Sal Sciected Scome | file parameters [11,] for 1. | | | |
|---|-------------------------------|---------------------------------------|------------|--|
| Co1–N1 | 2.068(6) | Co1–N2 | 2.032(5) | |
| Co1–N2 ⁱ | 2.152(5) | Co1–N5 | 2.020(5) | |
| Co1–N5 ⁱⁱ | 2.176(6) | Co1…Co1 ⁱ | 3.2340(7) | |
| Co1…Co1 ⁱⁱ | 3.2340(7) | | | |
| | | | | |
| Col ⁱ –Col–Col ⁱⁱ | 138.51(6) | Co1–N2–Co1 ⁱⁱ | 101.2(2) | |
| Co1–N2–Co1 ⁱ | 100.8(2) | N1–Co1–N2 ⁱ | 95.5(2) | |
| N1–Co1–N5 ⁱⁱ | 94.0(2) | N1-Co1-N2 | 109.3(2) | |
| N2-Co1-N2 ⁱ | 96.5(2) | N2 ⁱ -Co1-N5 ⁱⁱ | 170.33(19) | |
| N2-Co1-N5 ⁱⁱ | 78.6(2) | N1-Co1-N5 | 127.5(2) | |
| N2-Co1-N5 | 123.2(2) | N2 ⁱ -Co1-N5 | 79.4(2) | |
| N5–Co1–N5 ⁱⁱ | 96.1(2) | | | |

Symmetry codes: (i) x, 1/2-y, 1/2+z; (ii) x, 1/2-y, -1/2+z

| Table S3. Possible hydro | gen bonds (Å, °) for 1. | | | | |
|------------------------------|-------------------------|------------------|-----------------|--------|--|
| D–H···A | d(D-H) | <i>d</i> (H···A) | $d(D \cdots A)$ | <(DHA) | |
| C1-H1N2 | 0.95 | 2.84 | 3.455(8) | 123 | |
| C1-H1···N3 ⁱⁱ | 0.95 | 2.71 | 3.626(8) | 163 | |
| C1-H1···N4 ⁱⁱ | 0.95 | 2.71 | 3.556(6) | 149 | |
| C6-H6N5 | 0.95 | 2.64 | 3.528(9) | 156 | |
| C8–H8····N7 ⁱⁱⁱ | 0.95 | 2.49 | 3.407(11) | 163 | |
| C10-H10A····N4 ^{iv} | 0.98 | 2.69 | 3.645(12) | 164 | |
| C10-H10BN7v | 0.98 | 2.70 | 3.558(11) | 146 | |
| C10–H10C…N4vi | 0.98 | 2.60 | 3.405(12) | 139 | |

Symmetry code: (ii) x, 1/2-y, -1/2+z; (iii) 1-x, 1/2+y, 3/2-z; (iv) -x, 1/2+y, -1/2-z; (v) 1-x, 1/2+y, 1/2-z; (vi) -x, 1/2+y, 1/2-z.



Figure S1. View of the hydrogen bonding system in 1.

|--|

| Tuble 51: Tizido offuged eo(ii) Tz | enam complexes as sing | Bie enam magnets | |
|---|------------------------|---------------------------------|------------|
| Complex | Chromophore | SHAPE analysis agreement factor | Ref., CCDC |
| $[Co(N_3)_2(mqu)]_n$ | $\{CoN_5\}$ | TBPY-5 = 1.117 | this work |
| | | | 1859501 |
| $[Co(N_3)(L) \cdot H_2O]_n$ | $\{CoN_4O\}$ | TBPY-5 = 2.239 | a, 715892, |
| $[CoNa(N_3)_2(L)]_n$ | $\{CoN_4O_2\}$ | OC-6 = 1.544 | 715893 |
| ${[Co(N_3)_2(bib)](H_2O)}_{\infty}$ | $\{CoN_6\}$ | OC-6 = 1.046 | b, 791132 |
| $\{[Co(N_3)(bib)_2](NO_3)\}_{\infty}$ | $\{CoN_6\}$ | OC-6 = 0.083 | c, 870007 |
| $[Co(N_3)_2(H_2O)_2] \cdot (bpeado)$ | $\{CoN_4O_2\}$ | OC-6 = 0.831 | d, 677366 |
| $[Co_3(L)_2(N_3)_4(H_2O)_2]_n \cdot 2nH_2O$ | $\{CoN_2O_4\}$ | OC-6 = 0.118 | e, 792985 |
| | $\{CoN_3O_3\}$ | OC-6 = 0.173 | |
| $[Co(L)(N_3)]_n \cdot nH_2O$ | $\{CoN_2O_4\}$ | OC-6 = 0.026 | f, 797005 |

(a) B-W. Hu, J-P. Zhao, Q. Yang, X-F. Zhang, M. Evangelisti, E. C. Sañudo and X-H. Bu, *Dalton Trans.*, 2010, **39**, 11210; (b) Z-X. Li, Y-F. Zeng, H. Ma and X-H. Bu, *Chem. Commun.*, 2010, **46**, 8540; (c) Z-X. Li, W. Jie, G. Zha, T. Wang, and Y. Xu, *Eur. J. Inorg. Chem.*, 2012, **22**, 3537; (d) H-L. Sun, Z-M. Wang and S. Gao, *Chem. Eur. J.*, 2009, **15**, 1757; (e) Y-Q. Wang, W-W. Sun, Z-D. Wang, Q-X. Jia, E-Q. Gao and Y. Song, *Chem. Commun.*, 2011, **47**, 6386; (f) X-M. Zhang, Y-Q. Wang, K. Wang, E-Q. Gao and C-M. Liu, *Chem. Commun.*, 2011, **47**, 1815.

| | $(\Delta_{\tau}/k)/K$ | τ_0/s | ref. |
|---|-----------------------|------------------------|------|
| $[Co^{II}(btaz)(N_3)_2]$ | 94 | 3×10^{-12} | a |
| $[\{[Co^{II}_{2}(L)(N_{3})_{4}]\cdot 2DMF\}_{n}$ | 35 | 2×10^{-9} | b |
| $[\mathrm{Co}^{\mathrm{II}}_{2}(\mathrm{N}_{3})_{4}(\mathrm{DMF})_{3}]$ | 202 | $2 	imes 10^{-18}$ | с |
| $[\mathrm{Co}^{\mathrm{II}}_{4}(\mathrm{N}_{3})_{8}(\mathrm{DEF})_{5}]$ | 60 | 2×10^{-9} | с |
| $[\mathrm{Co^{II}}_{2}(\mathrm{N}_{3})_{4}(\mathrm{DIPF})_{2}]$ | 72 | 7×10^{-12} | с |
| $[Co^{II}_{5}(pic)_{6}(N_{3})_{4}]$ | 66 | 4×10^{-11} | d |
| | 51 | 2×10^{-9} | |
| [Co ^{II} (hfac)2NaphNN] _n | 398 ± 14 | $4\pm3	imes10^{-12}$ | e |
| | 344 ± 36 | $2-40 \times 10^{-10}$ | |
| [Co ^{II} (hfac) ₂ (NITPhOMe) ₂] | 154 | 3×10^{-11} | f |
| $[Co^{II}Cu^{II}(tmpa)_2(H_2O)_2]\cdot 4H_2O$ | 24 | 4×10^{-9} | g |

 $Co^{II}(H_2L)(H_2O)$

Table S5. Calculated activation energy barriers and extrapolated relaxation time in some of azido-bridged Co(II) 1D-chain complexes as single chain magnets

(a) T-F. Liu, D. Fu, S. Gao, Y-Z. Zhang, H-L. Sun, G. Su and Y-J. Liu, J. Am. Chem. Soc., 2003, 125, 13976; (b) Y-Q.
Wang, X-M. Zhang, X-B. Li, B-W. Wang, and E-Q. Gao, Inorg. Chem., 2011, 50, 6314; (c) X-H. Zhao, L-D. Deng, Y.
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Zhang, and Rodolphe Clérac, Inorg. Chem., 2014, 53, 7870; (e) R. A. Allão Cassaro, S. G. Reis, T. S. Araujo, P. M. Lahti, M. A. Novak and M. G. F. Vaz. Inorg. Chem., 2015, 54, 9381; (f) A. Caneschi, D. Gatteschi, N. Lalioti, C. Sangregorio, R.
Sessoli, G. Venturi, A. Vindigni, A. Rettori, M. G. Pini and M. A. Novak. Angew. Chem. Int. Ed., 2001, 40, 1760; (g) E.
Pardo, R. Ruiz-Garcia, F. Lloret, J. Faus, M. Julve, Y. Journaux, F. Delgado and C. Ruiz-Perez. Adv. Mater., 2004, 16, 1597; (h) Z-M. Sun, A. V. Prosvirin, H-H. Zhao, J-G. Mao and K. R. Dunbar. J. Appl. Phys., 2005, 97, 10B305.

27-29

8-34 ×10⁻¹⁰

h

Quantum-chemical calculations

Main problem of the quantum chemical calculations is a selection of an appropriate model fragment of the real chain-like structure. Therefore the results has to be accepted with reservation.

DFT and *ab initio* calculations were performed with ORCA 4.0.0 computational package at the truncated experimental geometries.^{S1} The relativistic effects were included in the calculations with zero order regular approximation (ZORA) together with the scalar relativistic contracted version of def2-TZVPP basis function for Co atom and def2-SV(P) function for other elements.

The *ab initio* calculations were based on state average complete active space self-consistent field (SA-CASSCF) wave functions complemented by N-electron valence second order perturbation theory (NEVPT2).^{S2} Active space comprised of seven electrons in five metal-based d-orbitals. The state averaged approach was used, in which 10 quartet and 40 doublet states were equally weighted. The calculations utilized the RI approximation with appropriate decontracted auxiliary basis set and the chain-of-spheres (RIJCOSX) approximation to exact exchange. Increased integration grids (Grid4 and GridX5) and tight SCF convergence criteria were used for all calculations. Energies of multiplets were calculated through quasi-degenerate perturbation theory in which an approximation to the Breit-Pauli form of the spin-orbit coupling operator (SOMF) was utilized. The ZFS parameters were calculated using the effective Hamiltonian theory.

The magnetic parameters of a monomeric moiety $[Co(mqu)(N_3)_4]^{2-}$ (model **1b**) were evaluated by using CASSCF/NEVPT2/QDPT method (Table S5). Geometry of this structure is rather close to the trigonal bipyramid (according to the SHAPE analysis) thus its ground state corresponds to 4A_1 ' in the ideal D_{3h} symmetry. This assumption is confirmed by the results according to which the two lowest Kramers doublets are well separated from the remaining excited ones and their energy gap is $\Delta = 2D$.

Table S6. Calculated *ab initio* magnetic parameters for model 1b

| | | - |
|---|--|---|
| Calculated six lowest Kramers doublets | 0, 107, 1117, 1497, 2090, 2347 | |
| (SOC corrected) /cm ⁻¹ | | |
| Ground term | ${}^{4}A_{1}$ ', D _{3h} | |
| NEVPT2 transition energies | 1375, 1863 | |
| (quartet-quartet) /cm ⁻¹ | | |
| $D_{\rm calc}/{\rm cm}^{-1}$ | 50.06 | |
| E/D | 0.21 | |
| g-factors | 1.981, 2.351, 2.593 | |
| (SOC corrected) /cm ⁻¹ Ground term NEVPT2 transition energies (quartet-quartet) /cm ⁻¹ D_{calc} /cm ⁻¹ E/D g-factors | ⁴ A ₁ ', D _{3h} 1375, 1863 50.06 0.21 1.981, 2.351, 2.593 | |

DFT calculations of the exchange coupling constant *J* were based on B3LYP functional and utilized the RIJCOSX approximation with the auxiliary SARC/J Coulomb fitting basis set. The *J* values have been calculated using the broken-symmetry solution for low-spin wave function through the Yamaguchi formula.^{S3} DFT calculation of the isotropic exchange parameter *J* has been done for $[Co_2(\mu-N_3)_2(mqu)_2(N_3)_4]^{2-}$ dimer. Calculation predicts a relatively marked ferromagnetic interaction $J_{calc} = +16.58 \text{ cm}^{-1}$) for such a model system.

- (S1) (a) F. Neese, The ORCA program system, Wiley Interdiscip. Rev. Comput. Mol. Sci., 2012, 2, 73; (b) F. Neese, ORCA – An Ab Initio, Density Functional and Semi-empirical Program Package, Version 4.0.0, 2017.
- (S2) (a) M. Atanasov, D. Ganyushin, D. A. Pantazis, K. Sivalingam and F. Neese, *Inorg. Chem.*, 2011, 50, 7460; (b) C. Angeli, S. Borini, M. Cestari and R. Cimiraglia, J. *Chem. Phys.*, 2004, 121, 4043; (c) C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger and J.-P. Malrieu, *J. Chem. Phys.*, 2001, 114, 10252; (d) C. Angeli, R. Cimiraglia and J.-P. Malrieu, *J. Chem. Phys.*, 2002, 117, 9138; (e) F. Neese, *J. Chem. Phys.*, 2005, 122, 34107; (f) D. Ganyushin and F. Neese, *J. Chem. Phys.*, 2006, 125, 24103; (g) F. Neese, *J. Chem. Phys.*, 2007, 127, 164112.
- (S3) (a) K. Yamaguchi, Y. Takahara, T. Fueno in: V. H. Smith (Ed.) Applied Quantum Chemistry, Reidel, Dordrecht, 1986, p. 155. (b) F. Neese, Coord. Chem. Rev. 2009, 253, 526.

Magnetic experiments

- All magnetic measurements were performed using a SQUID magnetometer (Quantum Design, MPMS-XL7).
- The DC susceptibility data was taken at $B_{DC} = 0.1$ in the RSO mode of detection; they were corrected for the underlying diamagnetism and transformed to the effective magnetic moment μ_{eff} .
- The magnetization data was taken until B = 7 T at T = 3.0 and 4.6 K, respectively; they are presented in the form of the magnetization per formula unit and bohr magneton: $M_1 = M_{\text{mol}}/N_A\mu_B$.
- The AC susceptibility data was taken at the oscillating magnetic field $B_{AC} = 0.38$ mT under the applied B_{DC} as indicated throughout for 25 frequencies between f = 0.025 and 1500 Hz. Ten scan were averaged and the data spanning outside the 1σ interval was ignored and the rest again averaged and analyzed.



Figure S2. DC magnetization data fitted with (a) and without (b) molecular-field correction (*zj*). The MF correction is based upon formula $\chi_{corr} = \chi_{mol} / [1 - (zj / N_A \mu_0 \mu_B^2) \chi_{mol}] + \chi_{TIM}$ where χ_{TIM} is a temperature-independent magnetism.

AC magnetic data

Fitting of the AC susceptibility data is based upon 48 data points (24 in-phase and 24 out-of phase) using the formula for the two- or three-set Debye model

$$\chi(\omega) = \chi_S + \sum_{k=1}^{3} \frac{\chi_{T,k} - \chi_{T,k-1}}{1 + (\mathrm{i}\omega\tau_k)^{1-\alpha_k}}$$

This equation decomposes into two explicit formulae for

a) the in phase component

b) the out of phase component

with the constraint for the isothermal susceptibilities $\chi_S < \chi_{T1} < \chi_{T2} < \chi_{T3}$ in order to get positive contributions from each primitive component. Seven (ten) free parameters can be retrieved reliably by using 48 experimental data points.

The functional to be minimized accounts to the relative errors of both susceptibility components

 $F = w \cdot E(\chi') + (1 - w) \cdot E(\chi'')$ with the typical weight w = 0.07, and

$$E(\boldsymbol{\chi}) = (1/N) \left[\sum_{i}^{N} \left| (\boldsymbol{\chi}_{i}^{e} - \boldsymbol{\chi}_{i}^{c}) / \boldsymbol{\chi}_{i}^{e} \right| \right]$$

The optimization routine refers to the genetic algorithm of D. L. Carroll, Univ. Illinois, Urbana, USA, 1998.

The quality of the fit is expressed by

a) discrepancy factors for the in-phase and out-of phase susceptibilities $R(\chi')$ and $R(\chi'')$ defined as

$$R(\boldsymbol{\chi}) = \sqrt{\left[\sum_{i} (\boldsymbol{\chi}_{i}^{\mathrm{e}} - \boldsymbol{\chi}_{i}^{\mathrm{c}})^{2}\right]} / \left[\sum_{i} (\boldsymbol{\chi}_{i}^{\mathrm{e}})^{2}\right]}$$

b) by the standard deviation for each optimized parameter; this is given in parentheses, e.g. 12.3(45) means 12.3 ± 4.5 (at 95% probability level).

The retrieved parameters should follow a systematic trend along a smooth dependence.

AC susceptibility data

| Table | S7. Para | ameters | of the thre | e- (two-) | set Debye | model fo | $r \mathbf{I}$ at $T =$ | = 1.9 K. | | | | | | |
|----------------------|------------|-------------|----------------|----------------|---------------|----------------|-------------------------|---------------|----------------|----------------|---------------|--------------|--------------|--------------|
| $B_{\rm DC}/{\rm T}$ | $R(\chi')$ | $R(\chi'')$ | $\chi_{ m LF}$ | $lpha_{ m LF}$ | $	au_{ m LF}$ | $\chi_{ m IF}$ | $lpha_{ m IF}$ | $	au_{ m IF}$ | $\chi_{ m HF}$ | $lpha_{ m HF}$ | $	au_{ m HF}$ | $x_{\rm LF}$ | $x_{\rm IF}$ | $x_{\rm HF}$ |
| | /% | /% | | | / s | | | / ms | | | / μs | | | |
| 0.2 | 0.28 | 6.2 | 1.03(4) | 0.39(2) | 0.15(1) | - | | | 6.18(2) | 0.40(3) | 1.5(3) | .17 | - | .83 |
| 0.4 | 0.38 | 2.9 | 2.80(6) | 0.45(1) | 0.24(1) | - | | | 6.25(5) | 0.34(4) | 3.5(6) | .45 | - | .55 |
| 0.6 | 3.6 | 7.3 | 2.1(8) | 0.0(1) | 0.80(13) | 3.4(3) | 0.3(3) | 60(57) | 5.89(9) | 0.5(5) | 1.0(3) | .35 | .23 | .42 |
| 0.8 | 3.6 | 2.9 | 2.4(21) | 0.1(2) | 1.64(25) | 4.3(4) | 0.4(2) | 151 | 5.9(3) | 0.3 | 0.8 | .40 | .32 | .28 |
| 1.0 | 3.3 | 7.4 | 1.7(4) | 0.0(1) | 0.93(11) | 2.5(2) | 0.2(2) | 72(52) | 2.90(6) | 0.6(5) | 0.5 | .45 | .21 | .35 |

Table 67 D



Figure S3. Temperature dependence of the AC susceptibility components for 1.



Figure S4. Frequency dependence of the AC susceptibility components for 1. Full lines - calculated interpolation / extrapolation for the two-set Debye model; dotted – for the three-set Debye model with $\chi_S = 0$; dashed – visual guide.

| u) ui | DDC V | | | | | | | | | | | | | | |
|-------------|----------------|-------------|---------|----------------|----------------|---------------|----------|----------------|---------------|----------------|----------------|---------------|--------------|--------------|--------------|
| T/K | $R(\chi')$ | $R(\chi'')$ | χs | $\chi_{ m LF}$ | $lpha_{ m LF}$ | $	au_{ m LF}$ | Хıf | $lpha_{ m IF}$ | $	au_{ m IF}$ | $\chi_{ m HF}$ | $lpha_{ m HF}$ | $	au_{ m HF}$ | $x_{\rm LF}$ | $x_{\rm IF}$ | $x_{\rm HF}$ |
| | /% | /% | | | | / s | | | / ms | | | / μs | | | |
| 1.9 | 0.40 | 2.7 | 0 | 1.35(20) | .00(3) | 0.74(3) | 2.92(7) | .33(5) | 66(15) | 5.58(2) | .54(7) | 1.5(6) | .24 | .28 | .48 |
| 2.3 | 0.81 | 4.0 | 0 | 1.02(33) | .01(8) | 0.53(3) | 2.34(11) | .41(8) | 41(25) | 5.01(4) | .31(28) | 1.2 | .20 | .26 | .53 |
| 2.7 | 0.47 | 3.9 | 0 | 1.00(14) | .03(4) | 0.42(1) | 1.68(11) | .51(12) | 11(6) | 4.57(3) | .18 | 0.7 | .22 | .15 | .63 |
| 3.1 | 0.45 | 9.4 | 0 | 0.67(10) | .00(5) | 0.45(1) | 1.15(36) | .58(28) | 2.2 | 4.17(4) | .15 | 0.01 | .16 | .12 | .72 |
| | | | | . / | | | | | | . / | | | | | |
| 1.9 | 1.0 | 10 | 2.30(4) | 3.62(49) | .04 | 0.58(4) | 5.78(17) | .58(4) | 60(60) | - | - | - | .38 | .62 | - |
| 2.3 | 0.96 | 7.5 | 2.57(3) | 3.50(32) | .00(9) | 0.50(3) | 5.07(7) | .51(5) | 44(32) | | | | .37 | .63 | |
| 2.7 | 0.47 | 4.9 | 2.82(3) | 3.79(13) | .04(3) | 0.42(1) | 4.60(4) | .60(6) | 11(8) | | | | .54 | .46 | |
| 3.1 | 0.39 | 7.9 | 3.02(5) | 3.69(10) | .00(3) | 0.45(1) | 4.17(2) | .59(9) | 2.3(9) | | | | .58 | .42 | |
| 3.5 | 0.59 | 12 | 3.16(3) | 3.62(5) | .04(4) | 0.48(3) | 3.83(1) | .41(13) | 1.6(6) | | | | .68 | .32 | |
| 3.9 | 1.0 | 18 | 3.16(3) | 3.44(5) | .0(1) | 0.62(9) | 3.56(2) | .29(25) | 1.5(8) | | | | .69 | .31 | |
| 4.3 | 0.50 | 27 | 3.07(2) | 3.24(2) | .00(7) | 0.61(6) | 3.33(1) | .21(19) | 0.9(4) | | | | .66 | .34 | |
| 4.7 | 0.69 | 29 | 2.98(1) | 3.08(2) | .0(1) | 0.85(18) | 3.14(1) | .0(2) | 2.9(9) | | | | .60 | .40 | |
| 5.1 | 0.69 | 34 | 2.87(1) | 2.94(2) | .0(2) | 0.72(21) | 2.99(1) | .0(3) | 2.9(13) | | | | .60 | .40 | |
| | | | | ~ / | ~ ~ / | | | | | | | | | | |
| b) at | $B_{\rm DC}=0$ | .8 T | | | | | | | | | | | | | |
| <i>T</i> /K | $R(\chi')$ | $R(\chi'')$ | χs | χlf | $lpha_{ m LF}$ | $	au_{ m LF}$ | XIF | $lpha_{ m IF}$ | $	au_{ m IF}$ | χнf | $lpha_{ m HF}$ | $	au_{ m HF}$ | $x_{\rm LF}$ | $x_{\rm IF}$ | $x_{\rm HF}$ |
| | /% | /% | | | | / s | | | / ms | | | / μs | | | |
| 1.9 | 3.6 | 2.9 | 0 | 2.4(21) | .1(2) | 1.64(25) | 4.3(4) | .4(2) | 151 | 5.9(3) | .3 | 0.8 | .40 | .32 | .28 |
| 2.3 | 1.1 | 8.2 | 0 | 1.50(29) | .00(5) | 0.67(6) | 2.4(2) | .27(14) | 49(23) | 4.42(3) | .59(39) | 0.19 | .34 | .21 | .45 |
| 2.7 | 1.2 | 10 | 0 | 1.23(86) | .11 | 0.71(10) | 2.0(5) | .46 | 36 | 4.28(10) | .56 | 0.066 | .29 | .17 | .54 |
| 3.1 | 0.77 | 4.9 | 0 | 0.95(21) | .05(6) | 0.77(3) | 1.5(3) | .59(29) | 9.5 | 4.05(8) | .02 | 0.006 | .24 | .15 | .62 |
| | | | | . / | . / | | | . , | | | | | | | |
| 1.9 | 3.6 | 3.6 | 1.60(6) | 3.9(22) | .11 | 1.64(18) | 6.04(36) | .49(13) | 200 | - | - | - | .51 | .49 | - |
| 2.3 | 1.1 | 10 | 1.89(2) | 3.30(37) | .00(7) | 0.66(5) | 4.45(4) | .38(8) | 52(39) | - | - | - | .55 | .45 | - |
| 2.7 | 1.3 | 11 | 2.21(6) | 3.39(65) | .1(1) | 0.68(5) | 4.34(17) | .58(15) | 39`́ | | | | .55 | .45 | |
| 3.1 | 0.77 | 4.8 | 2.50(5) | 3.46(18) | .05(5) | 0.78(3) | 4.05(4) | .59(12) | 9.3 | | | | .62 | .38 | |
| 3.5 | 0.74 | 5.0 | 2.79(2) | 3.49(4) | .05(3) | 0.80(3) | 3.73(1) | .37(11) | 1.8(5) | | | | .75 | .25 | |
| 3.9 | 1.3 | 12 | 2.87(3) | 3.36(6) | .10(7) | 0.86(10) | 3.51(3) | .19 | 1.8(7) | | | | .77 | .23 | |
| 4.3 | 0.28 | 13 | 2.88(1) | 3.18(2) | .04(3) | 0.97(4) | 3.28(1) | .07 | 0.88 | | | | .72 | .28 | |
| 47 | 1 1 | 10 | 2 7000 | 2 01 (7) | ` ´ | 0.000 | | ~ . | 0.50 | | | | 7 | 22 | |
| 1./ | 1.1 | 19 | 2./9(6) | 3.01(7) | .09 | 0.96(18) | 3.12(2) | .31 | 0.52 | | | | .67 | .33 | |

Table S8. Results of the fitting procedure for AC susceptibility components of 1. a) at $B_{\rm DC} = 0.6$ T

In all cases: $\chi_{\rm S} < \chi_{\rm LF} < \chi_{\rm IF} < \chi_{\rm HF}$. Missing standard deviation means that it is greater than the mean value.