Supporting Information

Two 3*d*-4*f* nanomagnets formed via two-step *in-situ* reaction of picolinaldehyde

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1. Synthetic Procedures and Experimental Techniques.

Experimental Section

General Remarks:

All chemicals were commercially available and used as received without further purification. The C, H, and N microanalyses were carried out with an Elementar Vario-EL CHNS elemental analyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000—400 cm^{-1} with a Bruker-EQUINOX 55 FT-IR spectrometer.

Synthesis of *[$Dy^{III}_2Cu^{II}_7(OH)_2(\mathbf{L^2})_2(\mathbf{L^3})_2(OAc)_8(NO_3)_2(H_2O)_4](NO_3)_2\cdot 8.5H_2O$ (**1**)*: A mixture of picolinaldehyde ($\mathbf{L^1}$) (1.0 mmol), $Dy(NO_3)_3\cdot 6H_2O$ (0.5 mmol), $Cu(OAc)_2\cdot H_2O$ (1.0 mmol) and then triethylamine (0.5 mmol) in MeCN/MeOH (8mL/2mL) was stirred for 10 min, yielding blue solution. After that, the solution was filtered, and the filtrate was for evaporation. Blue crystals available for single crystal diffraction were obtained several days later (5 % yield based on picolinaldehyde). Anal. Calc. (%) for **1**: C, 25.41; H, 3.40; N, 5.70; Found (%): C, 25.27; H, 3.51; N, 5.88. Infra-red (KBr disc, cm^{-1}): 3386vs, 2848m, 1592vs, 1385vs, 1230m, 1134s, 1026s, 827w, 779s, 681m, 615m, 550w, 505m.

Synthesis of *[$Gd^{III}_6Cu^{II}_{12}(OH)_{12}(\mathbf{L^3})_6(NO_3)_7(OAc)_3(H_2O)_{12}](OH)_8\cdot 19H_2O\cdot MeCN$ (**2**)*: A mixture of $\mathbf{L^1}$ (0.2 mmol), $Gd(NO_3)_3\cdot 6H_2O$ (0.1 mmol), $Cu(OAc)_2\cdot H_2O$ (0.2 mmol) and then triethylamine (0.1 mmol) in MeCN/MeOH (8 mL/2 mL) was stirred for 10 min, yielding blue solution. After that, the solution was filtered, and the filtrate was for evaporation. Blue crystals available for single crystal diffraction were obtained several days later (2 % yield based on picolinaldehyde). Anal. Calc. (%) for **2**: C, 21.21; H, 3.16; N, 6.18. Found (%): C, 21.43; H, 3.18; N, 6.25. Infra-red (KBr disc, cm^{-1}): 3392s, 2922vs, 2852s, 1618m, 1556s, 1377vs, 1219w, 1103s, 980s, 775w, 654w, 586w, 498w.

Crystal data of **1** at 150(2) K: $C_{52}H_{83}Cu_7Dy_2N_{10}O_{52.50}$, M = 2458.06, triclinic, a = 11.6017(10) Å, b = 12.0819(9) Å, c = 15.5313(11) Å, α = 99.682(2) °, β = 102.582(2) °, γ = 105.718(3) °, V = 1984.6(3) $Å^3$, space group P-1, Z = 2, 15328 reflections measured, 7458 independent reflections (R_{int} = 0.1192). R_1 = 0.1141 for $I \geq 2\sigma(I)$ and wR_2 = 0.2636 for all data.

Crystal data of **2** at 150(2) K: $C_{80}H_{142}Cu_{12}Gd_6N_{20}O_{90}$, M = 4530.12, trigonal, a = 32.5859(19) Å, c = 13.4651(16) Å, V = 12382.2(18) $Å^3$, space group R-3, Z = 3, 17381 reflections measured, 5419 independent reflections (R_{int} = 0.0295). R_1 = 0.0732 for $I \geq 2\sigma(I)$ and wR_2 = 0.1549 for all data.

X-ray Crystallographic Study

Diffraction intensities were collected on a Rigaku R-AXIS SPIDE IP diffractometer and a Bruker SMART Apex CCD system with MoK_α radiation (λ = 0.71073 Å) at 150 K for **1** and **2**, respectively. The structures were solved by direct methods, and all non-hydrogen atoms were refined

anisotropically by least-squares on F^2 using the SHELXTL program. The program SQUEEZE,[1] a part of the PLATON package of crystallographic software, was used to calculate the solvent area and remove their contribution to the overall intensity data. Anisotropic thermal parameters were assigned to all non-hydrogen atoms. Hydrogen atoms on organic ligands were generated by the riding mode.[2] CCDC reference numbers 903918 (**1**) and 903919 (**2**).

Magnetic measurements

Magnetic susceptibility measurements were performed with a Quantum Design MPMS-XL7 SQUID. Polycrystalline samples were embedded in vaseline to prevent torqueing. Data were corrected for the diamagnetic contribution calculated from Pascal constants.

1 P. van der Sluis, A. L. Spek, *Acta Crystallogr*. 1990, **A46**, 194.

2 a) G. M. Sheldrick, *Acta Crystallogr*. 2008, **A64**, 112; b) G. M. Sheldrick, *SHELXTL 6.10*, Bruker Analytical Instrumentation, Madison, Wisconsin, USA, 2000.

3. Plots of Magnetic Measurements.

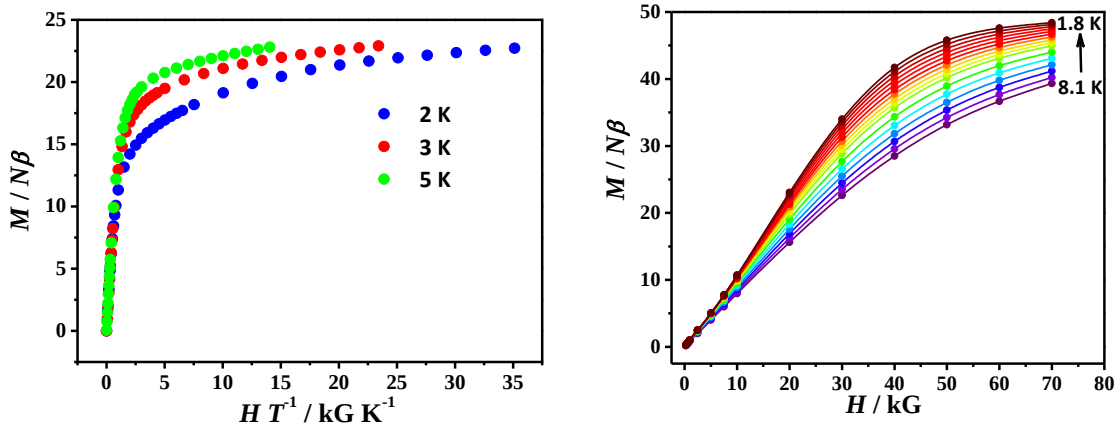

Figure S1. Molar magnetization ($M/N\beta$) *vs.* H/T at indicated temperatures for **1** (*left*) and $M/N\beta$ *vs.* H for **2** (*right*).

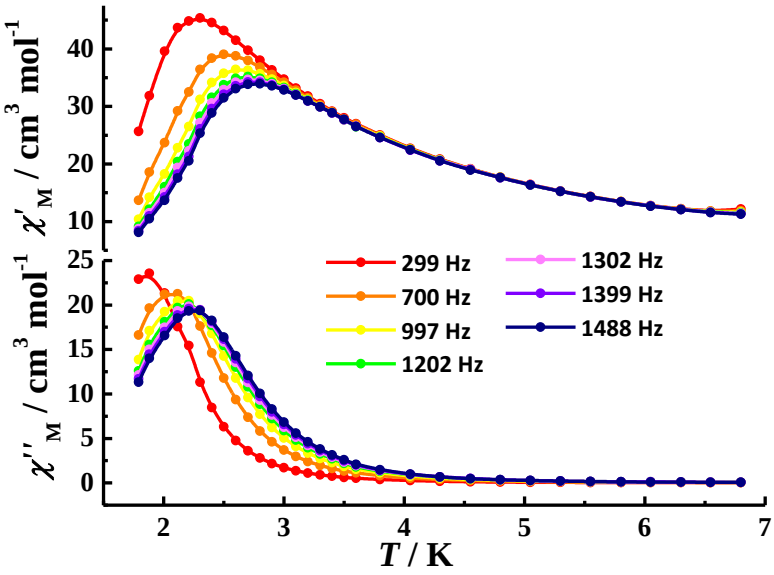

Figure S2. Plots of ac susceptibility *vs.* temperature oscillating at indicated frequencies at H_{ac} = 5 Oe and H_{dc} = 0 Oe for **1**.

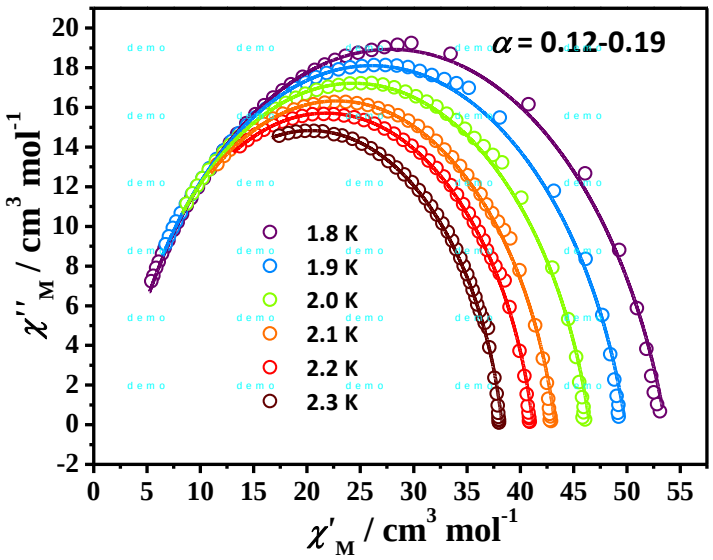

Figure S3. Cole-Cole plots at indicated temperature range for **1**. The solid lines represent the best fitting of the experimental data to a generalized Debye model.

4. Results of the Continuous Shape Measure Analysis.

Table S1. Results of the continuous shape measure analysis for **1** and **2**.

		CShM values (S_X) refer to		
		Capped Square Antiprism (CSAPR-9)	Tricapped Trigonal Prism (TCTPR-9)	Muffin (MFF-9)
Ln^{III}				
1	Dy1	1.153	2.213	1.142
2	Gd1	0.896	1.326	1.534
Cu^{II}				
		Trigonal Bipyramid (TBPY-5)	Square Pyramid (SPY-5)	Octahedron (OC-6)
1	Cu1	6.232	1.126	
	Cu2			4.209
	Cu3	6.922	3.456	
	Cu4			1.998
2	Cu1			2.532
	Cu2	6.992	1.776	

5. Computational Details.

Spin-orbit free states for fragments consisting in one Dy^{III} surrounded by its ligand coordination sphere were obtained by employing the RASSCF method and the effect of spin-orbit coupling was taken into account in a second step by the restricted active space state interaction method (RASSI).[3] The direction and magnitude of the magnetic moment of the final states were evaluated using the SINGLE_ANISO routine implemented in MOLCAS 7.8.[4] Cu-Cu coupling constants for **1** were obtained by DFT calculations using the ORCA package[5] by employing the usually called "broken-symmetry approach", as described elsewhere.[6] An estimation of the Dy-Cu coupling constant value was performed within the Lines model by means of the POLY_ANISO program.[7]

As the electronic structure of the ground state of Dy^{III} systems cannot be correctly described by single determinant DFT methods, reliable coupling constants of interactions involving Dy^{III} cannot be obtained within this framework. In this way, we focused on the CASSCF+RASSI study of the isolated Dy^{III} system, the Cu-Cu coupling constants calculated by DFT using the B3LYP functional[8] and the estimation of Dy···Cu interaction value by fitting from experimental susceptibility curves. From the X-ray structure of $[Dy_2Cu_7]$ we can identify three different Cu-Cu coupling constants with calculated values of J_1 = +107.6, J_2 = -14.2 and J_3 = +61.6 cm^{-1} ($\hat{H} = -J\ \hat{S}_1\ \hat{S}_2$), where J_1 corresponds to the coupling of the central copper with its symmetry-related neighbors, J_3 connects the first (or last) copper with its neighbor and J_2 links the second (or sixth) copper with one of the two symmetry-related copper centers interacting with the central Cu cation.

RASSCF Calculations:

Energies and Spin Hamiltonian parameters for low-energy states of Dy^{III} were obtained in a two-step procedure: (i) RASSCF(9,7) calculation of spin-free energies and wavefunctions for models considering Dy^{III} and their coordination environment. (ii) inclusion of spin-orbit coupling by a one-electron effective Hamiltonian considering the previously obtained spin-free states. We constructed mononuclear fragments (Figure S5) consisting in the center of interest, its connected ligands and the metals connected to these ligands, represented as *ab initio* model potentials (AIMP), were Dy atoms were replaced with La potentials (La.ECP.deGraaf.0s.0s.0e-La(LaMnO3)) and Cu centres with Zn potentials (Zn.ECP.Lopez-Moraza.0s.0s.0e-AIMP-KZnF3). A 8s7p5d4f2g1h ANO-RCC basis set was employed for Dy, 4s3p2d1f for O and N, 3s2p for C and 2s for H.

Table S2. Energies (cm^{-1}) and g_z values for the lowest eight Kramers' doublets for the Dy^{III} in $[Dy_2Cu_7]$ (see Figure 1).

Dy	E / cm^{-1}	0.0	138.4	273.6	388.1	480.2	534.7	632.6	674.0
	g_z	19.8	17.1	14.1	11.2	7.8	11.8	18.5	18.8

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7 a) M. E. Lines, *J. Chem. Phys.* 1971, **55**, 2977; b) L. F. Chibotaru and L. Ungur, *The computer programs SINGLE_ANISO and POLY_ANISO*, University of Leuven, 2006.

8 A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.

DFT Calculations:

In order to investigate the magnetic properties, electronic structure calculations based on Density Functional Theory (DFT) have been made for complex **2**. Due to the complexity of the structure, to obtain reasonable *J* values geometry optimization, Siesta code[9] were performed instead to use the X-ray structures. Numerical functions and PBE+U (U_{Cu} = 4.0 eV) functional[10] were employed, double-ζ basis set and triple-ζ for valence electron of the main group and Cu elements respectively and pseudopotencials generated according to the procedure of Troullier and Martins.[11] For Gd atoms a pseudopotencial previously tested have been employed.[12]

Description of the spin configurations employed in the Siesta calculations (PBE+U functional) together with the high spin solution to obtain *J* values for complex **2**.

	Inverted spins	2S
ds 1	Gd1, Gd2, Gd3, Cu7, Cu9, Cu11, Cu13, Cu15, Cu17	0
ds 2	Gd1, Gd4, Cu9, Cu10, Cu15, Cu16	18
ds 3	Gd1, Gd6, Cu7, Cu8	22
ds 4	Gd2, Cu11, Cu12	36
ds 5	Gd3, Gd4, Cu9, Cu11, Cu13	20
ds 6	Gd5, Gd6, Cu7, Cu8, Cu9, Cu10	18
ds 7	Gd5, Cu17	38
ds 8	Gd4, Gd5, Gd6, Cu7, Cu 9, Cu11, Cu14, Cu16, Cu18	0
ds 9	Cu7, Cu 9, Cu11, Cu13, Cu15, Cu17	42

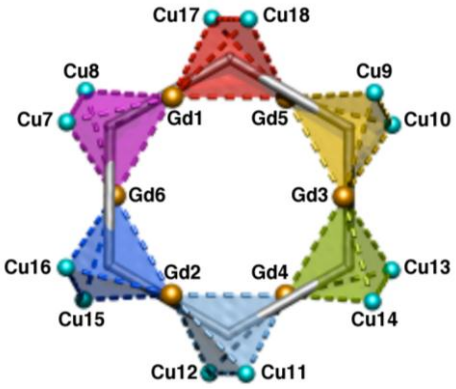

Figure S4. Topology of complex **2** with the numbers of the metal atoms used to assign the exchange coupling constants.

Table S3. DFT calculated *J* values (in cm^{-1}) for the optimized structure complex **2** (see Figure S4 for the atom labels).

	Atoms involved	**Bridging ligands**	J_{calc}
J_1	Cu7Cu8, Cu9Cu10, Cu11Cu12, Cu13Cu14, Cu15Cu16, Cu17Cu18	2(μ_3-OR)	7.7
J_2	Cu7Cu16, Cu8Cu17, Cu9Cu18, Cu10Cu13, Cu12Cu15, Cu11Cu14	(μ_3-$\mathbf{L}^3$)	-5.6
J_3	Gd1Cu7, Gd2Cu11, Gd3Cu9, Gd4Cu13, Gd5Cu17, Gd6Cu15	(μ_3-OH)(μ_3-OR) (μ_2-acetato)	-5.1
J_4	Gd1Cu17, Gd2Cu15, Gd3Cu13, Gd4Cu11, Gd5Cu9, Gd6Cu7	(μ_3-OH)(μ_3-OR)	4.1
J_5	Gd1Cu8, Gd2Cu12, Gd3Cu10, Gd4Cu14, Gd5Cu18, Gd6Cu16	(μ_3-OH)(μ_3-OR)	4.5
J_6	Gd1Cu18, Gd2Cu16, Gd3Cu14, Gd4Cu12, Gd5Cu10, Gd6Cu8	(μ_3-OH) (μ_3-OR)(OH···O)	-1.3
J_7	Gd1Gd5, Gd1Gd6, Gd2Gd4, Gd2Gd6, Gd3Gd4, Gd3Gd5	2(μ_3-OH) (μ_6-ONO_2)	-0.08

9 a) J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón and D. J. Sánchez-Portal, *Phys.: Condens. Matter*. 2002, **14**, 2745; b) E. Artacho, D. Sánchez-Portal, P. Ordejón, A. García, J. M. Soler, *Phys. Stat. Sol. A* 1999, **215**, 809; c) E. Artacho, E. Anglada, O. Dieguez, J. D. Gale, A. Garcia, J. Junquera, R. M. Martin, P. Ordejon, J. M. Pruneda, D. Sánchez-Portal and J. M. Soler, *J. Phys. Condes. Matter*. 2008, 20.
10 a) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865; b) V. I. Anisimov, F. Aryasetiawan and A. I. Lichtenstein, *J. Phys.: Condens. Matter*. 1997, **9**, 767.
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12 a) R. Pollet and D. Marx, *J. Chem. Phys.* 2007, **126**, 181102; b) A. Hosoi, Y. Yukawa, S. Igarashi, S. J. Teat, O. Roubeau, M. Evangelisti, E. Cremades, E. Ruiz, L. A. Barrios and G. Aromí, *Chem.-Eur. J.* 2011, **17**, 8264; c) E. Cremades, S. Gomez-Coca, D. Aravena, S. Alvarez and E. Ruiz, *J. Am. Chem. Soc.* 2012, **134**, 10532.

DFT Optimized geometry (Siesta PBE+U) for complex **2**.

Gd 19.78751950 -3.62786872 11.91823755
Gd 21.47170914 2.63237945 11.92632942
Gd 15.18608412 0.97161671 11.90819223
Gd 17.80483310 3.60418599 10.53286551
Gd 16.21520660 -2.66483137 10.52101651
Gd 22.46650043 -0.94533944 10.54017873
Cu 23.12864622 -3.61012610 12.77941010
Cu 22.36854984 -4.46693650 9.62995931
Cu 13.55862710 -1.92399779 12.77309261
Cu 13.19120492 -0.93731518 9.63558876
Cu 19.78843115 5.48933545 12.77942097
Cu 20.86162888 5.28067732 9.63870741
Cu 14.45568810 3.61839913 9.62642697
Cu 15.15150355 4.48054252 12.76614545
Cu 24.12415780 1.99493205 9.62655331
Cu 24.51584335 0.94199900 12.76600314
Cu 17.89278153 -5.57545648 9.62216177
Cu 16.73873100 -5.38316804 12.76550567
N 15.71890939 -7.12737093 12.68348668
N 11.83185946 -2.97440626 12.85512624
N 18.81232402 0.00349630 11.27675637
O 15.84640493 -5.05634328 11.00626686
O 13.78317649 -2.92242184 11.00229703
O 13.57005375 -5.20788762 11.62494490
O 17.44118055 -3.53204444 12.46935800
H 17.26737467 -2.95733953 13.26336302
O 18.30024834 -3.66903556 9.94675543
H 18.72395746 -3.39641385 9.07782697
O 18.49609500 -1.23105835 11.26779048
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H 16.62694622 -8.10565792 14.29831946
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H 8.85616248 -3.41525312 14.45371881
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H 26.87347382 2.21290817 14.34454591
C 28.75204136 1.66035226 13.29980677
H 29.40774138 2.25874576 13.96612099
C 29.27536012 0.90444324 12.22456142
H 30.36761362 0.90346804 12.01813292
C 28.39672837 0.13946846 11.42201450
H 28.77422381 -0.48050153 10.58161232
C 27.01530650 0.16955012 11.71387619
C 25.95774307 -0.67566588 10.98442011
H 26.24661936 -0.85522417 9.90796026
C 25.30216343 -3.01533579 11.04355878
H 25.67965089 -3.09287366 9.98163304
C 25.74820384 -4.22576385 11.88322313
C 26.99747642 -4.86698138 11.72620280
H 27.68200747 -4.55696955 10.90860284
C 27.35722933 -5.88615907 12.63840819
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C 26.46465074 -6.22427704 13.68303305
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O 20.48846048 1.61655360 14.05493887
H 19.74290989 2.00131567 14.57706216
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O 24.33996825 1.98931890 14.52571650
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C 21.90388562 4.52710454 14.73079375
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H 11.60836701 8.11465961 13.92777378
C 12.85995411 8.64942741 12.18689246
H 12.32729832 9.60135641 11.97223035
C 13.95929934 8.25014373 11.39055312
H 14.31700067 8.87627890 10.54584497
C 14.60734740 7.03231025 11.69336749
C 15.86298940 6.51689169 10.97093847
H 15.88055352 6.84800005 9.89203013
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