

Article

# Closing the Circle of the Lanthanide-Murexide Series: Single-Molecule Magnet Behavior and Near-Infrared Emission of the Nd<sup>III</sup> Derivative

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Supplementary

**Table S1.** Main crystallographic parameters for NdMurex.

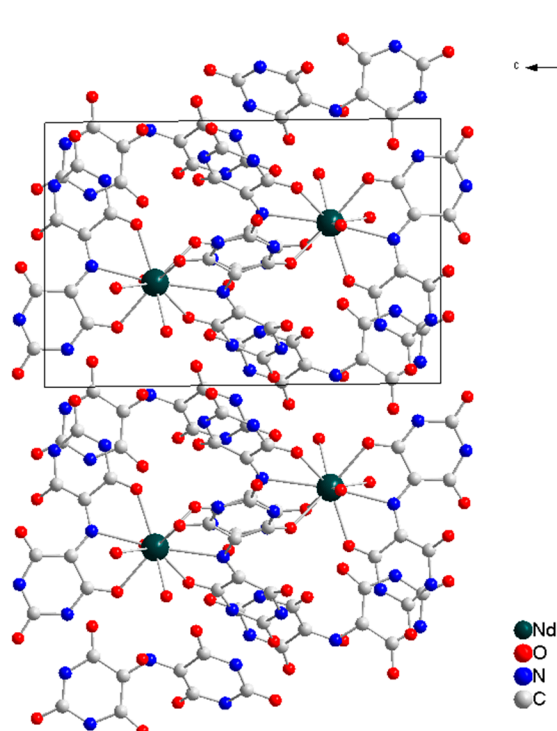
Formula	C <sub>48</sub> H <sub>64</sub> N <sub>30</sub> Nd <sub>2</sub> O <sub>56</sub>
M [g·mol <sup>-1</sup> ]	2245.77
Crystal system	triclinic
Space group	<i>P</i> -1( <i>N</i> <sup>o</sup> 2)
<i>a</i> (Å)	10.895(4)
<i>b</i> (Å)	11.095(6)
<i>c</i> (Å)	16.340(3)
$\alpha$ [°]	88.789(1)
$\beta$ [°]	82.016(2)
$\gamma$ [°]	76.973(1)
<i>V</i> (Å <sup>3</sup> )	1905.6(13)
<i>Z</i>	1
<i>T</i> (K)	150
2 $\theta$ range	2.03–27.490
Reflns collected	13625
Independent reflns	8692
Observed reflns	8246
Parameters	738
<i>R</i> 1/ $\omega$ <i>R</i> <sup>2</sup>	0.0196/0.0651
GofGoodness of fit	1.126

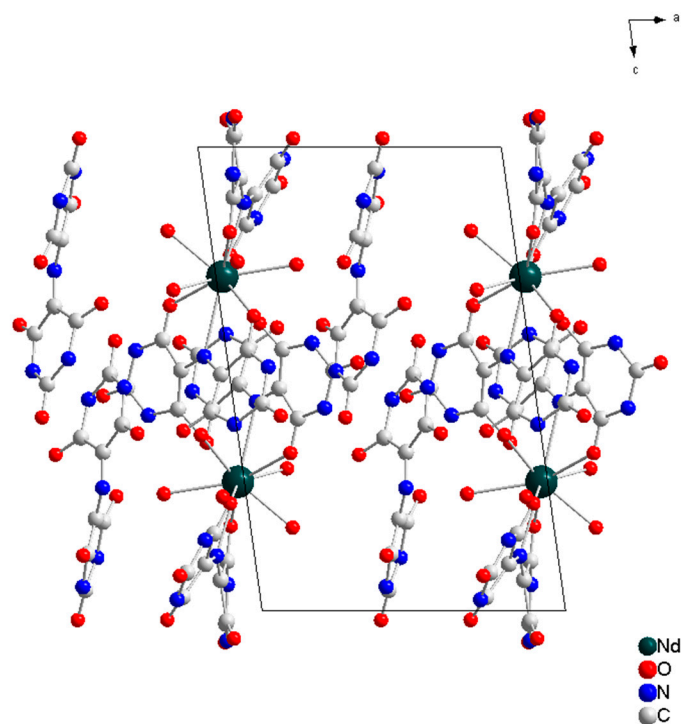
**Table S2.** Selected bond distances and angles of NdMurex.

Bond	Bond Lengths (Å)	Bonds	Angles (°)
Nd1-O1	2.4833(16)	O5-Nd1-O4	74.34(6)
Nd1-O2	2.5070(18)	O5-Nd1-O3	76.64(6)
Nd1-O3	2.4762(17)	O4-Nd1-O3	118.90(5)
Nd1-O4	2.4614(16)	O1-Nd1-O7	75.32(6)
Nd1-O5	2.4296(18)	O2-Nd1-O6	91.27(5)
Nd1-O6	2.678(2)	O7-Nd1-O2	79.11(5)
Nd1-O7	2.4985(18)	O1-Nd1-O2	122.26(5)
Nd1-O8	2.5052(15)	O3-Nd1-O6	151.85(5)
Nd1-N1	2.7440(19)	O4-Nd1-O6	61.52(5)
Nd1-N2	2.8659(19)	O8-Nd1-O6	72.76(5)
-	-	O5-Nd1-N1	120.02(6)
-	-	O4-Nd1-N1	122.16(5)
-	-	O3-Nd1-N2	59.33(5)
-	-	N1-Nd1-N2	173.22(5)

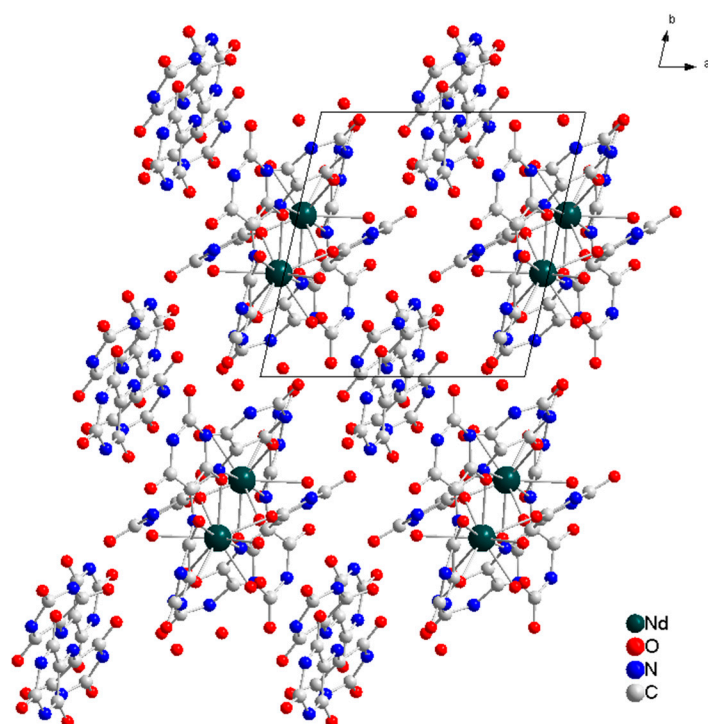
**Table S3.** Continuous Shape Measurements (CSM) extracted from analysis of NdMurex with SHAPE [1].

CSM Value	Capped Square Antiprism ( $C_{4v}$ )	Spherical Capped Square Antiprism ( $C_{4d}$ )	Spherical Tricapped Trigonal Prism ( $D_{3h}$ )
CSM	1.526	1.732	2.208

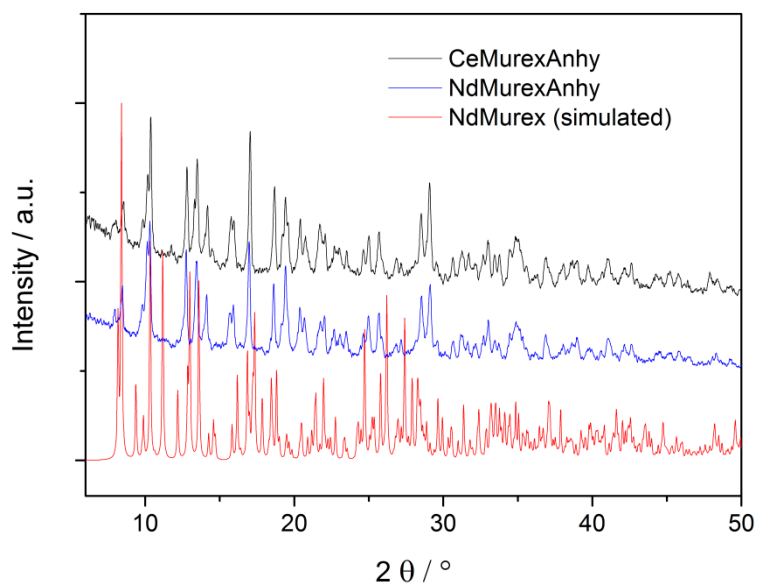
**Figure S1.** Representation of the crystal packing of NdMurex along the *a* axis. Water molecules and hydrogen atoms are omitted for clarity.



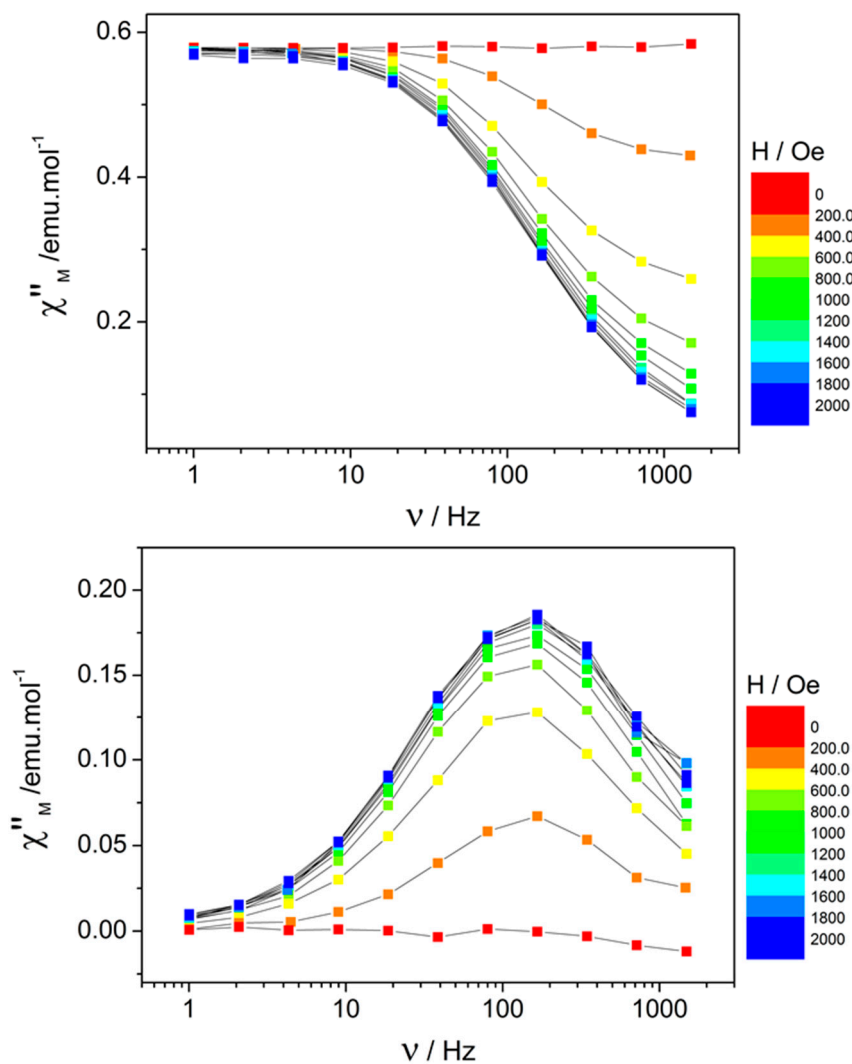
**Figure S2.** Representation of the crystal packing of NdMurex along the *b* axis. Water molecules and hydrogen atoms are omitted for clarity.



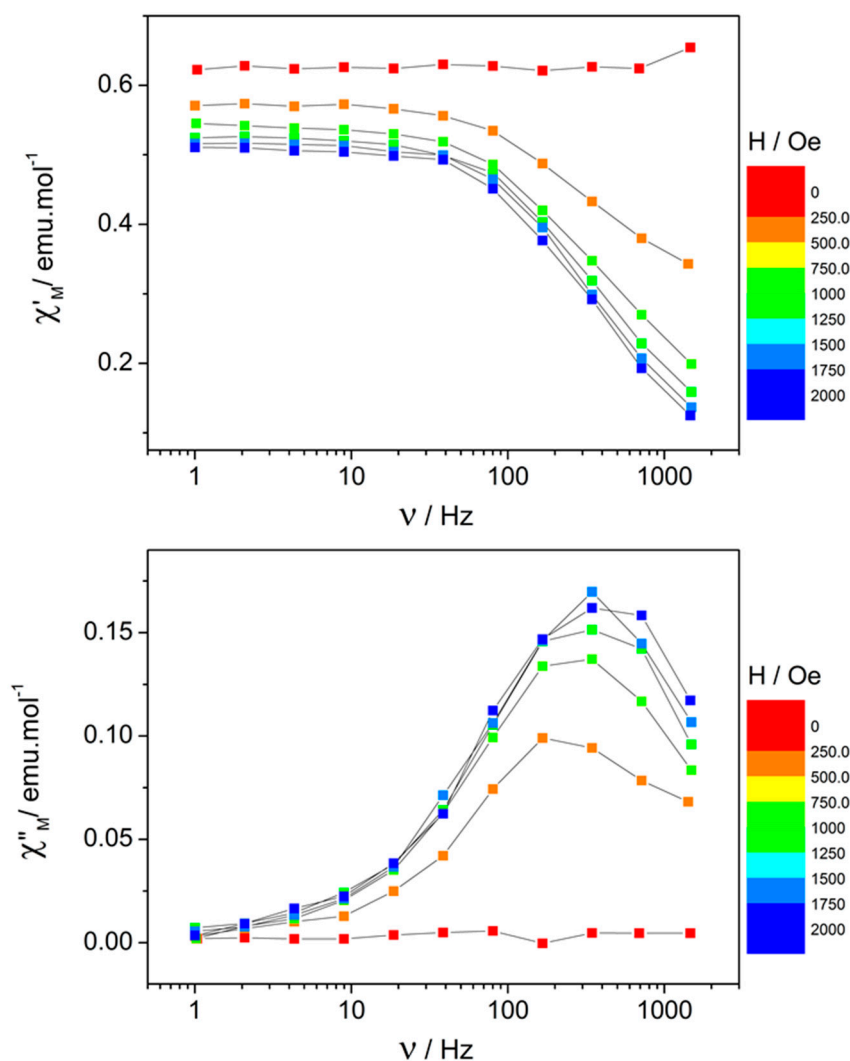
**Figure S3.** Representation of the crystal packing of NdMurex along the *c* axis. Water molecules and hydrogen atoms are omitted for clarity.



**Figure S4.** Powder X-ray diffraction pattern for NdMurexAnhy and CeMurexAnhy measured at 300 K with simulation from the structural data file of NdMurex at 150 K ( $\lambda_{\text{Cu}} = 1.5407 \text{ \AA}$ ).



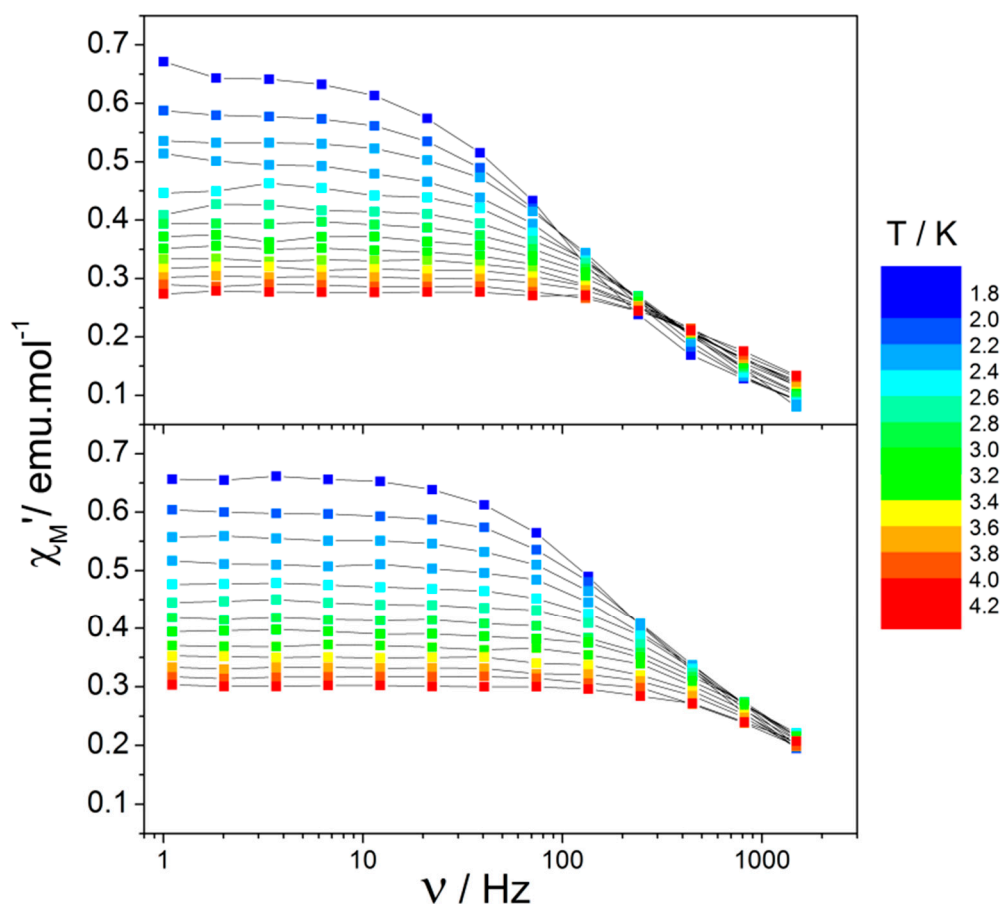
**Figure S5.** Field dependence of the in-phase (top) and out-of phase susceptibility (bottom) measured at 2 K for NdMurex.



**Figure S6.** Field dependence of the in-phase (top) and out of phase susceptibility (bottom) measured at 2 K for NdMurexAnhy.

**Table S4.** Table of the values extracted from the fitting of  $X''$  vs frequency curves for NdMurex.

T(K)	$\tau$ (s)
1.8	1343
2	1049
2.2	916
2.4	671
2.6	606
2.8	426
3	425
3.2	357
3.4	318
3.6	301
3.8	281
4	214
4.2	195
4.4	177



**Figure S7.** Frequency dependence of the in-phase susceptibility of NdMurex (top) and NdMurexAnhy (bottom) with  $H_{dc} = 1200$  Oe for temperatures from 1.8 (blue) to 4.4 K (red). Lines are guide to the eye.

**Table S5.** Table of the values extracted from the Argand plot for NdMurex.

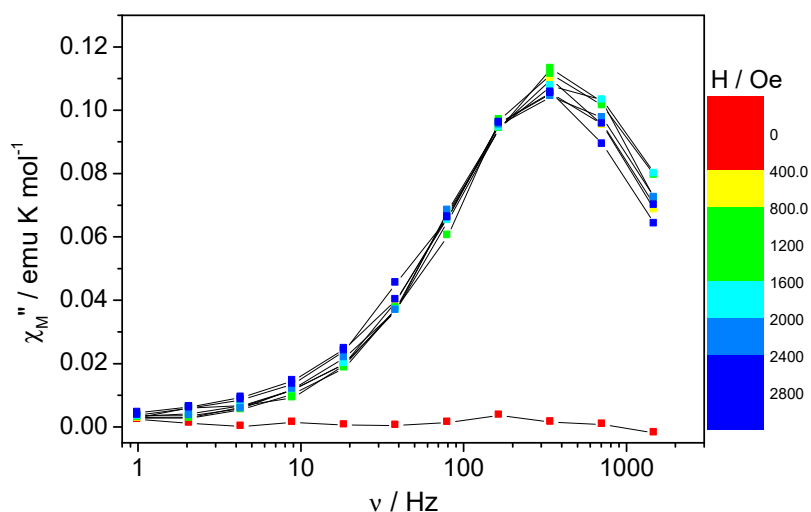
T (K)	$\chi_s$	$\chi_T$	$\alpha$	R <sup>2</sup>
1.8	0.057	0.651	0.22	0.98876
2	0.052	0.588	0.23	0.99244
2.2	0.055	0.540	0.21	0.98344
2.4	0.041	0.499	0.22	0.95589
2.6	0.035	0.463	0.27	0.93759
3.0	0.047	0.398	0.22	0.98236
3.2	0.045	0.375	0.21	0.97445
3.4	0.045	0.355	0.21	0.93707
3.6	0.066	0.335	0.15	0.98255
3.8	0.060	0.320	0.18	0.96585
4.0	0.056	0.304	0.16	0.98775
4.2	0.039	0.290	0.18	0.9872
4.4	0.055	0.278	0.14	0.95626

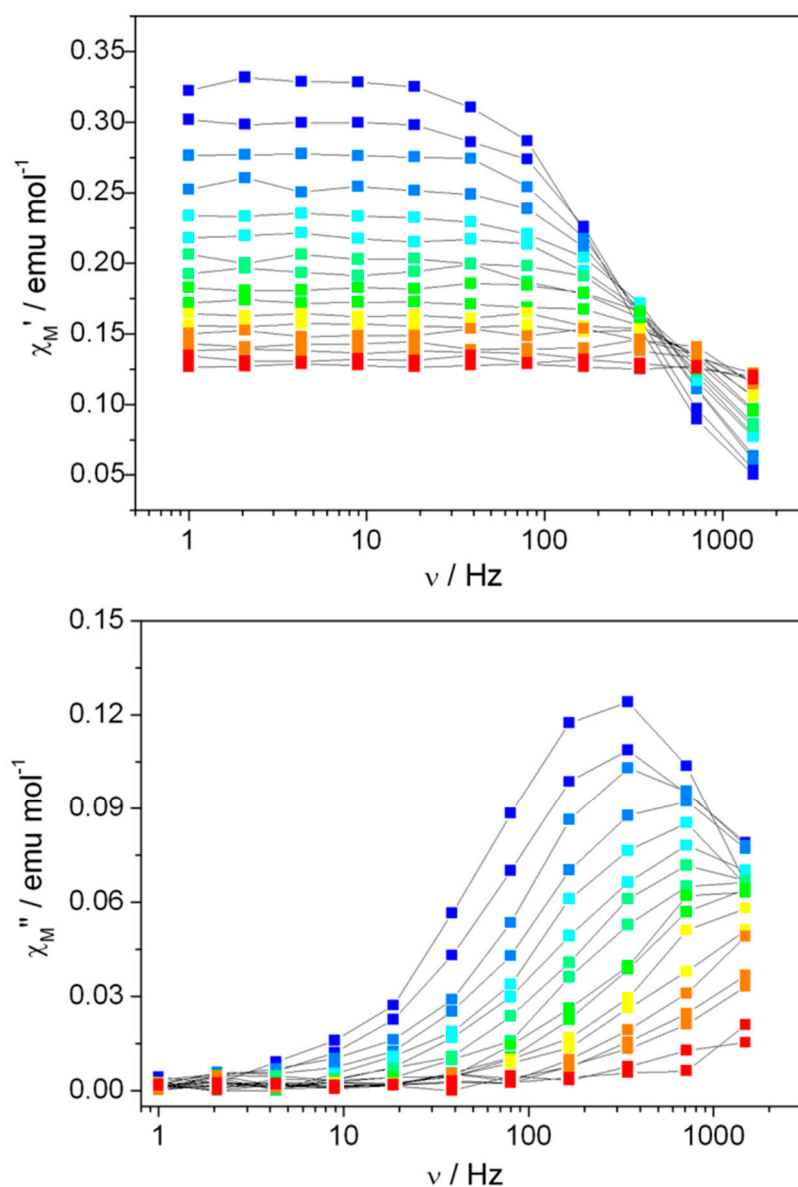
**Table S6.** Table of the values extracted from the fitting of  $X''$  vs frequency curves for NdMurexAnhy.

T (K)	$\tau$ (s)
1.8	608
2	453
2.2	385
2.4	318
2.6	266
2.8	223
3	176
3.2	158
3.4	143
3.6	120
3.8	112
4	97
4.2	83

**Table S7.** Table of the values extracted from the Argand plot for NdMurexAnhy.

T (K)	$\chi_s$	$\chi_T$	$\alpha$	R <sup>2</sup>
1.8	0.131	0.664	0.21	0.97681
2	0.120	0.606	0.22	0.98466
2.2	0.124	0.560	0.20	0.99076
2.4	0.121	0.516	0.21	0.98224
2.6	0.128	0.479	0.19	0.99352
2.8	0.117	0.449	0.21	0.98829
3.0	0.103	0.419	0.22	0.98909
3.2	0.100	0.397	0.22	0.98529
3.4	0.113	0.372	0.16	0.97344
3.6	0.085	0.353	0.21	0.98465
3.8	0.094	0.334	0.17	0.98716
4.0	0.097	0.319	0.18	0.97325

**Figure S8.** Field dependence of the out-of phase susceptibility measured at 2 K for CeMurexAnhy.



**Figure S9.** Frequency dependence of the in-phase (top) and out of phase (bottom) susceptibilities measured with  $H_{dc} = 400$  Oe for CeMurex for temperatures from 1.8 (blue) to 5 K (red).

**Table S8.** Table of the values extracted from the fitting of  $X''$  vs frequency curves for CeMurexAnhy.

T (K)	$\tau$ (s)
1.8	536
2	452
2.2	344
2.4	304
2.6	241
2.8	224
3	157
3.2	155
3.4	140
3.6	124
3.8	117



**Table S9.** Table of the values extracted from the Argand plot for CeMurexAnhy.

<b>T (K)</b>	<b><math>\chi_s</math></b>	<b><math>\chi_T</math></b>	<b><math>\alpha</math></b>	<b><math>R^2</math></b>
1.8	0.029	0.342	0.16	0.93186
2	0.013	0.302	0.14	0.97682
2.2	0.031	0.281	0.15	0.98825
2.4	0.037	0.255	0.12	0.99574
2.6	0.028	0.235	0.14	0.99118
2.8	0.039	0.218	0.10	0.99654
3.0	0.014	0.206	0.16	0.94575
3.2	0.028	0.191	0.11	0.99889

## References

1. Alvarez, S. Polyhedra in (inorganic) chemistry. *Dalton Trans.* **2005**, *13*, 2209–2233.



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