Electronic Supplementary Material (ESI) for Dalton Transactions.

Dy-based single ion magnet in the $SrLaGaO_4$ matrix: the enhanced parameters in an expanded crystal lattice

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Supporting Information

X-ray powder diffraction data

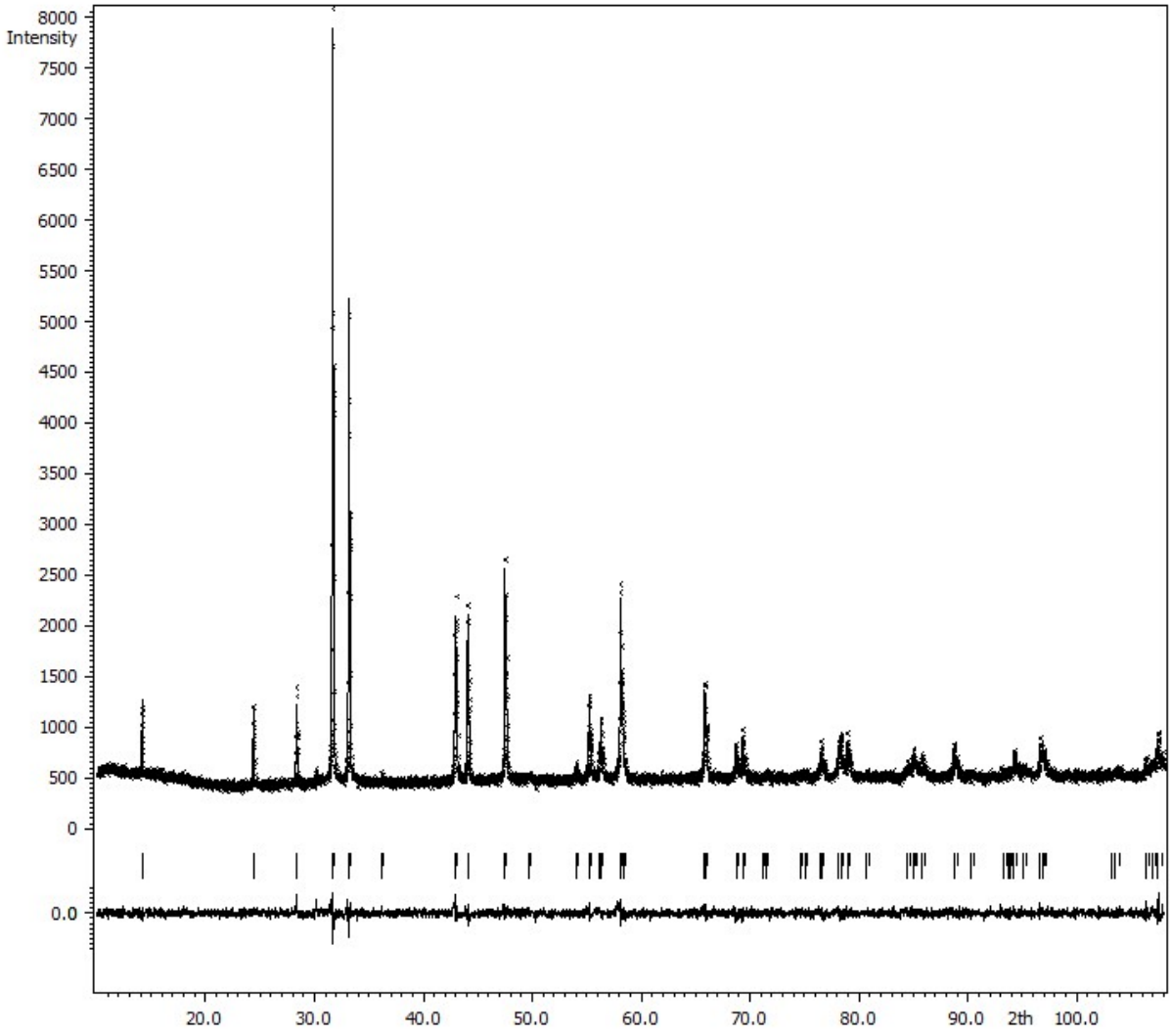


Figure S1. Powder X-ray diffraction pattern of $SrLa_{0.95}Dy_{0.05}GaO_4$. Observed (crosses), calculated (solid line) and difference (solid line below) plots. Positions of Bragg reflections are shown as strokes underneath.

Table S1. Crystal structure refinement data for $SrLa_{0.95}Dy_{0.05}GaO_4$.

Temperature (K)	293 K
Wavelength (Å)	1.54187
Space group	I4/mmm
a (Å)	3.8413(1)
c (Å)	12.6772(3)
V (Å^3)	187.06(1)
Z	2
2θ range (deg.)	10 – 108
R_{wp}	0.048
R_{all}	0.031
ΔF_{max}, ΔF_{min} (e Å^{-3})	2.2, -2.1

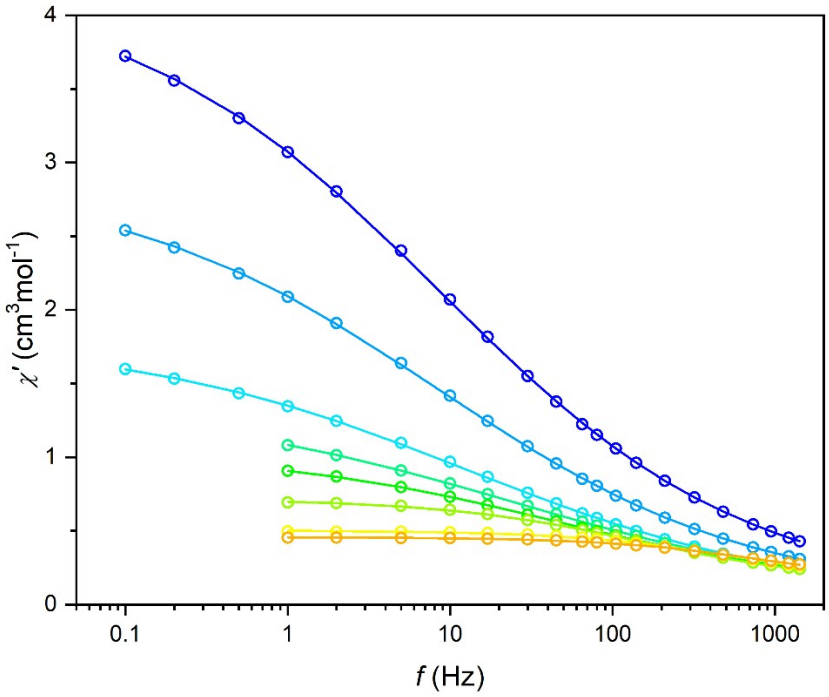
Table S2. Atomic parameters and thermal displacement parameters (Å^2) for $SrLa_{0.95}Dy_{0.05}GaO_4$.

Atom	Sr	La	Dy	Ga	O1	O2
Site	4e	4e	4e	2a	4c	4e
SOF	0.5	0.475	0.025	1	1	1
x	0	0	0	0	0	0
y	0	0	0	0	0	0.5
z	0.35888(16)	0.35888(16)	0.35888(16)	0	0.1674(9)	0
U_{iso}	0.0055(18)	0.0055(18)	0.0055(18)	0.010(2)	0.014(5)	0.008(5)

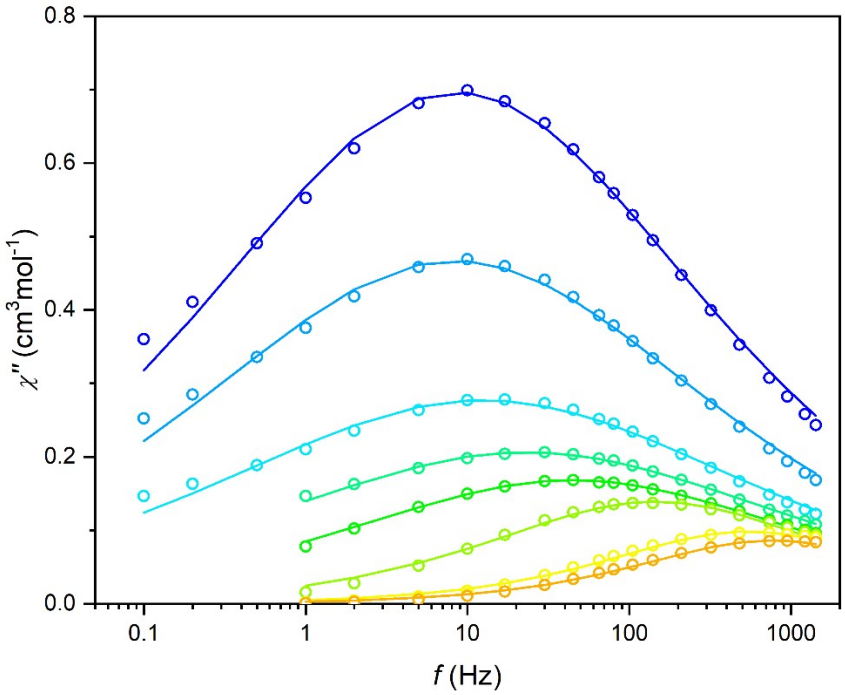
Table S3. Selected interatomic distances (Å) in the crystal structure of $SrLa_{0.95}Dy_{0.05}GaO_4$.

Sr,La,Dy-O1	2.427(12)	
Sr,La,Dy-O1	2.7366(15)	4x
Sr,La,Dy -O2	2.6248(14)	4x
Ga-O1	2.122(12)	4x
Ga-O2	1.92067(7)	2x

ac susceptibility data

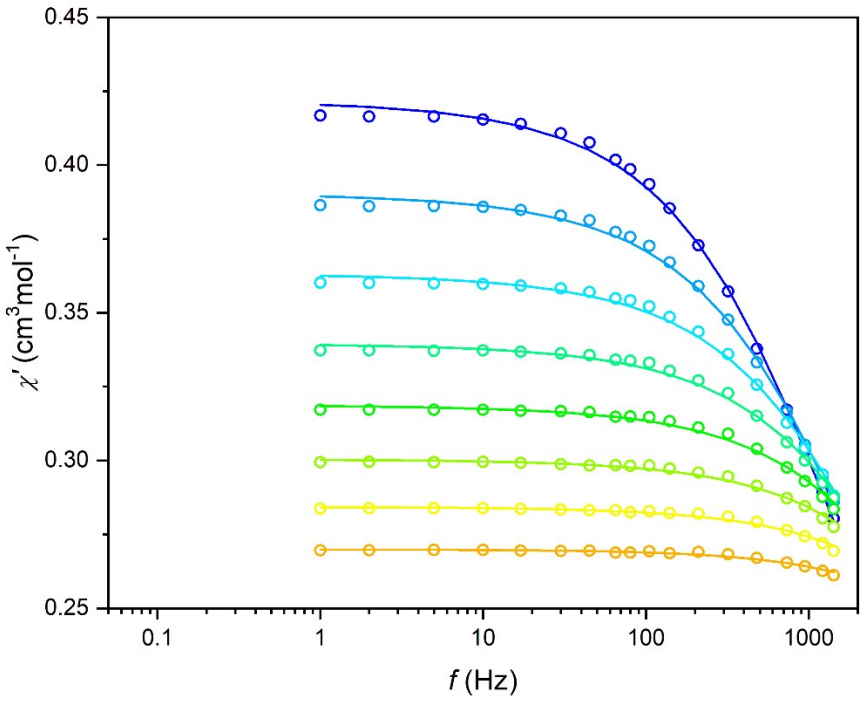


(a)

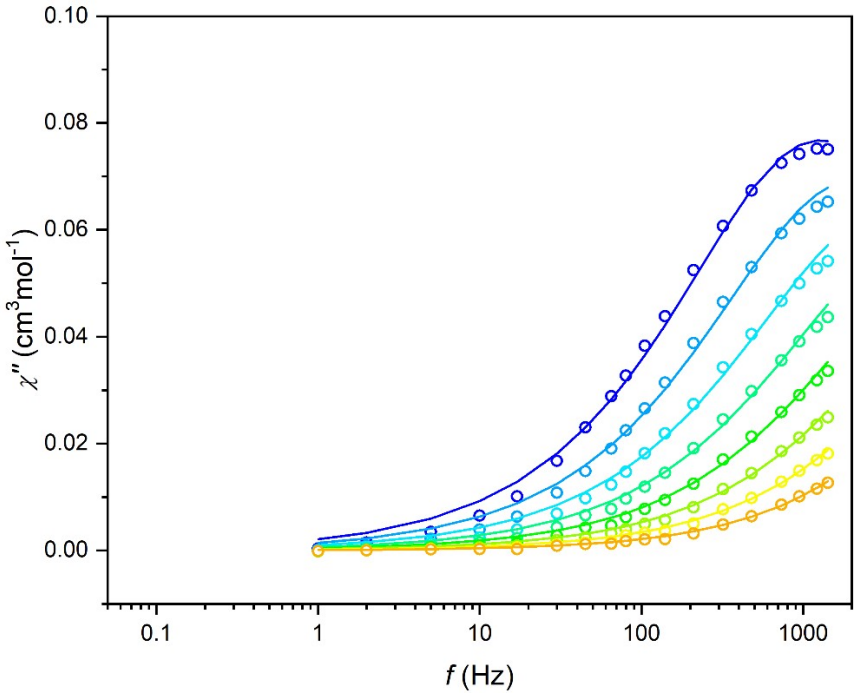


(b)

Fig. S2. Frequency dependence of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ at temperatures 2 – 22 K under a zero dc magnetic field. (a) – in-phase susceptibility χ', (b) – out-of-phase susceptibility χ''. Symbols – experimental points, lines – fitting. The color codes: from blue to orange – T = 2, 3, 5, 7, 10, 14, 20, 22 K.

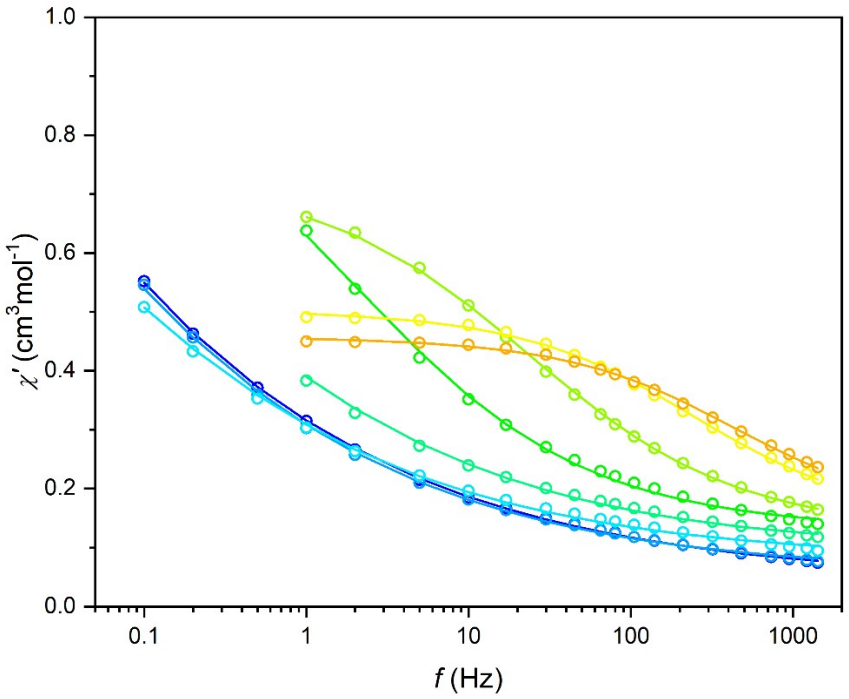


(a)

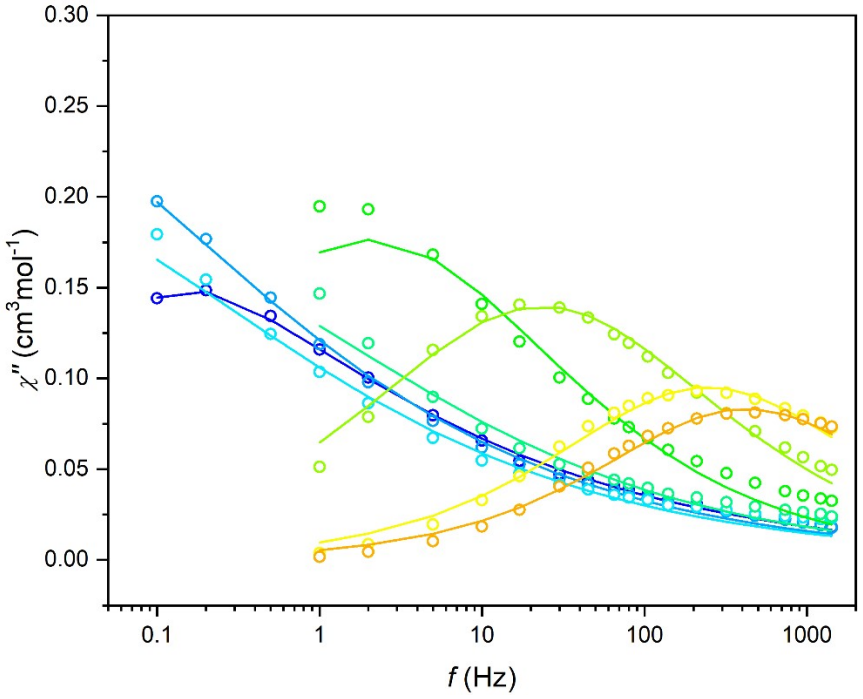


(b)

Fig. S3. Frequency dependence of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ at temperatures 24 – 38 K under a zero-dc magnetic field. (a) – in-phase susceptibility χ', (b) – out-of-phase susceptibility χ''. Symbols – experimental points, lines – fitting. The color codes: from blue to orange – T = 24 - 38 K, step 2 K.

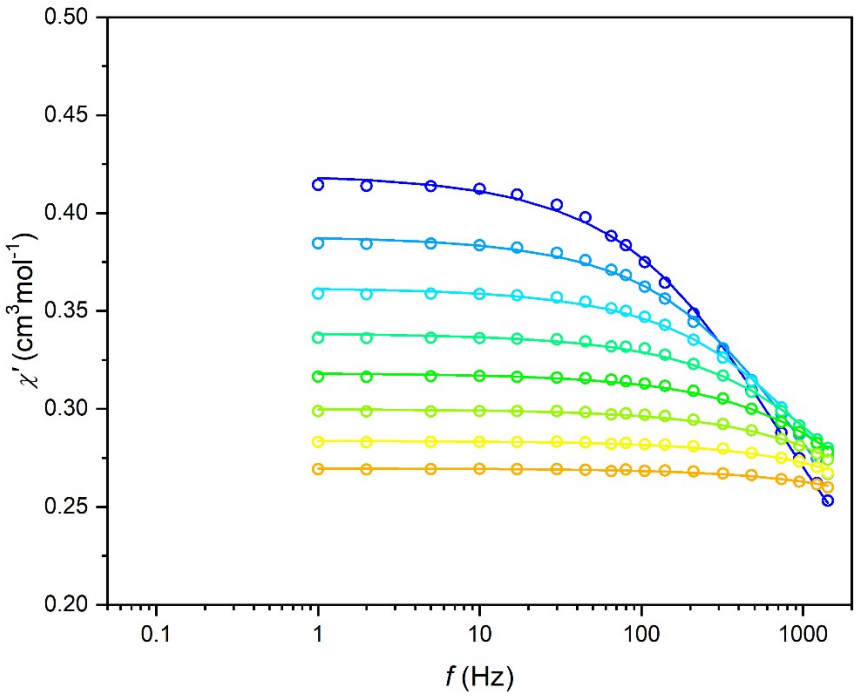


(a)

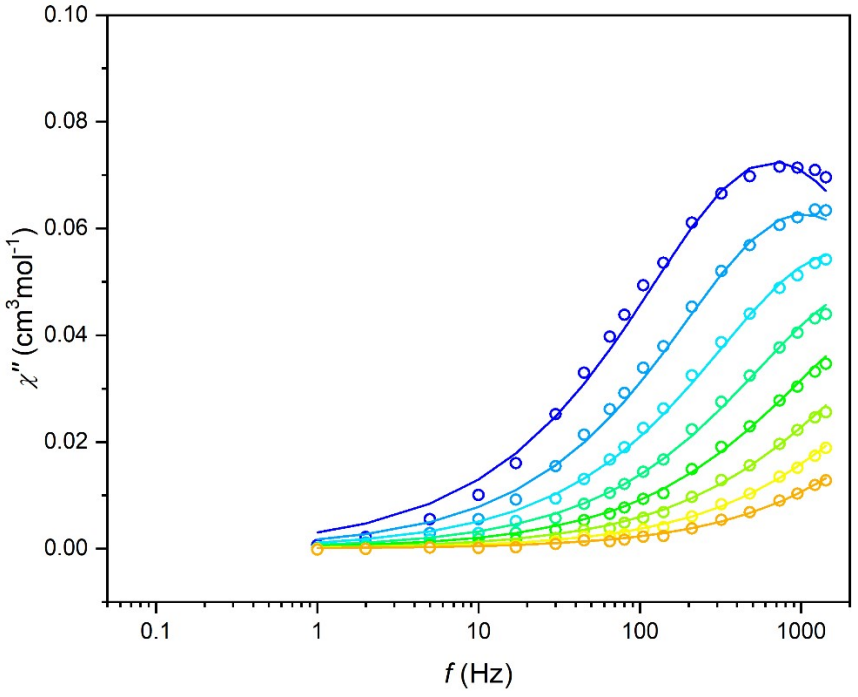


(b)

Fig. S4. Frequency dependence of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ at temperatures 2 – 22 K under a dc magnetic field of 4 kOe. (a) – in-phase susceptibility χ', (b) – out-of-phase susceptibility χ''. Symbols – experimental points, lines – fitting. The color codes: from blue to orange – T = 2, 3, 5, 7, 10, 14, 20, 22 K.

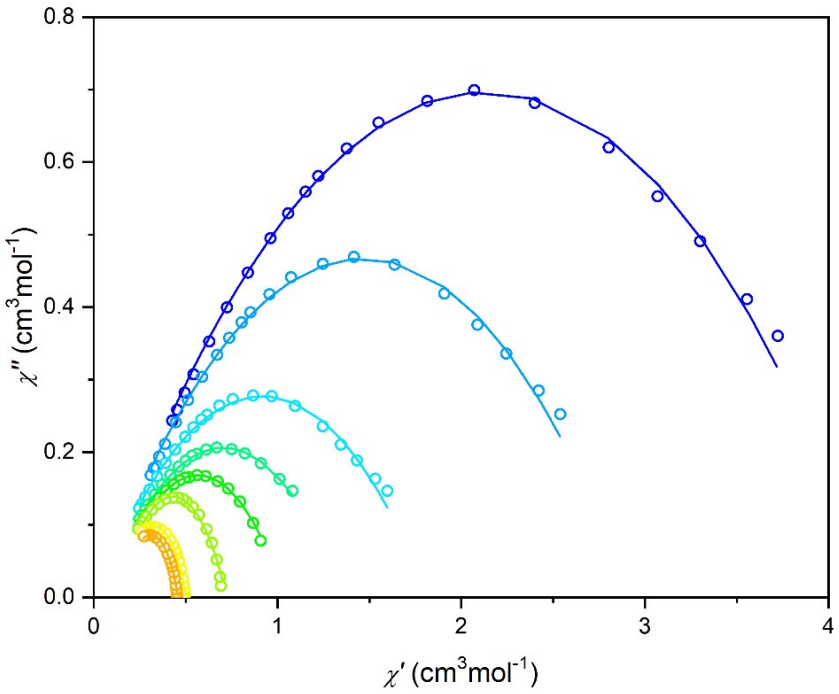


(a)

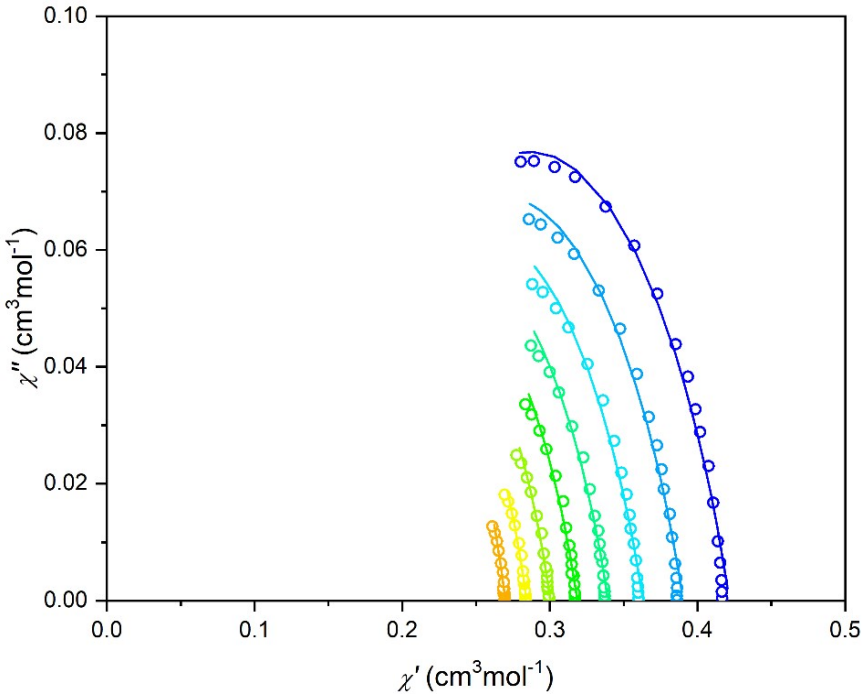


(b)

Fig. S5. Frequency dependence of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ at temperatures 24 – 38 K under a magnetic field of 4 kOe. (a) – in-phase susceptibility χ', (b) – out-of-phase susceptibility χ''. Symbols – experimental points, lines – fitting. The color codes: from blue to orange – T = 24 - 38 K, step 2 K.

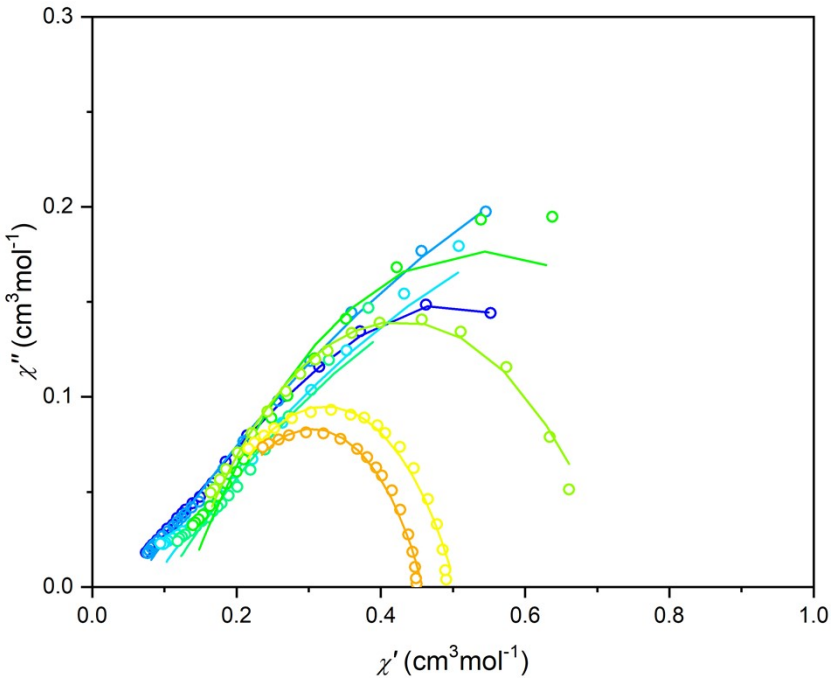


(a)

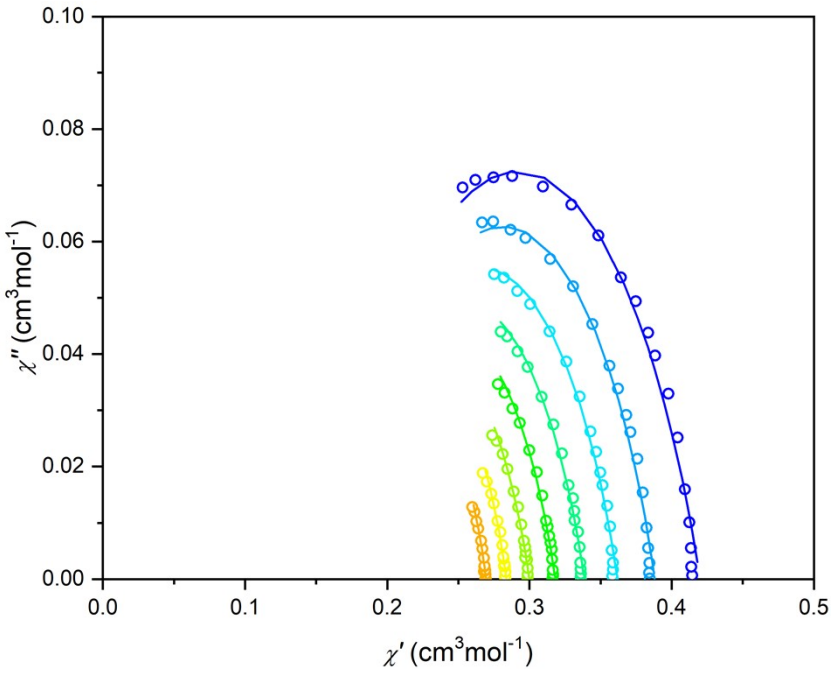


(b)

Fig. S6. Cole-Cole plots of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ under a zero dc magnetic field: (a) at temperatures 2, 3, 5, 7, 10, 14, 20, 22 K (from blue to orange); (b) at temperatures 24 – 38 K with a step of 2 K (from blue to orange). Symbols – experimental points, lines – fitting.



(a)



(b)

Fig. S7. Cole-Cole plots of ac susceptibility per mol of Dy for $SrLa_{0.95}Dy_{0.05}GaO_4$ under a dc magnetic field of 4 kOe: (a) at temperatures 2, 3, 5, 7, 10, 14, 20, 22 K (from blue to orange); (b) at temperatures 24 – 38 K with a step of 2 K (from blue to orange). Symbols – experimental points, lines – fitting.

Electronic structure data

Table S4. Crystal field parameters in Wybourne notation derived in the program CONCORD for Dy^{3+} using experimental atomic coordinates of the coordination polyhedron (from Table S2) and a partial charge on the oxygen atom of 0.95*e*.

Parameter	Value (cm^{-1})
B_{20}	454.533
B_{22}	0
B_{40}	77.045
B_{42}	0
B_{43}	0
B_{44}	-96.559
B_{60}	11.506
B_{62}	0
B_{63}	0
B_{64}	35.837
B_{66}	0

Table S5. Modeling of the Dy^{3+} electronic structure with the PHI program using crystal field parameters listed in Table SX1. The Kramers doublet energies of the ground term $^6H_{15/2}$ are shown only.

Kramer's doublet	Energy (cm^{-1})	M_J (%)
E_0	0	15/2 (99.92)
E_1	70.14	13/2 (99.65)
E_2	126.8	11/2 (99.14)
E_3	170.1	9/2 (97.89)
E_4	201.5	+7/2 (95.35), -1/2 (4.05)
E_5	220.8	+5/2 (79.75), -3/2 (19.60)
E_6	243.2	+3/2 (78.93), -5/2 (19.65)
E_7	247.3	+1/2 (94.01), -7/2 (4.35)