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Supplementary Material

Magnetic properties and neutron spectroscopy of lanthanoid-{tetrabromocatecholate/18-crown-6} single-molecule magnets

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Single crystal X-ray diffraction

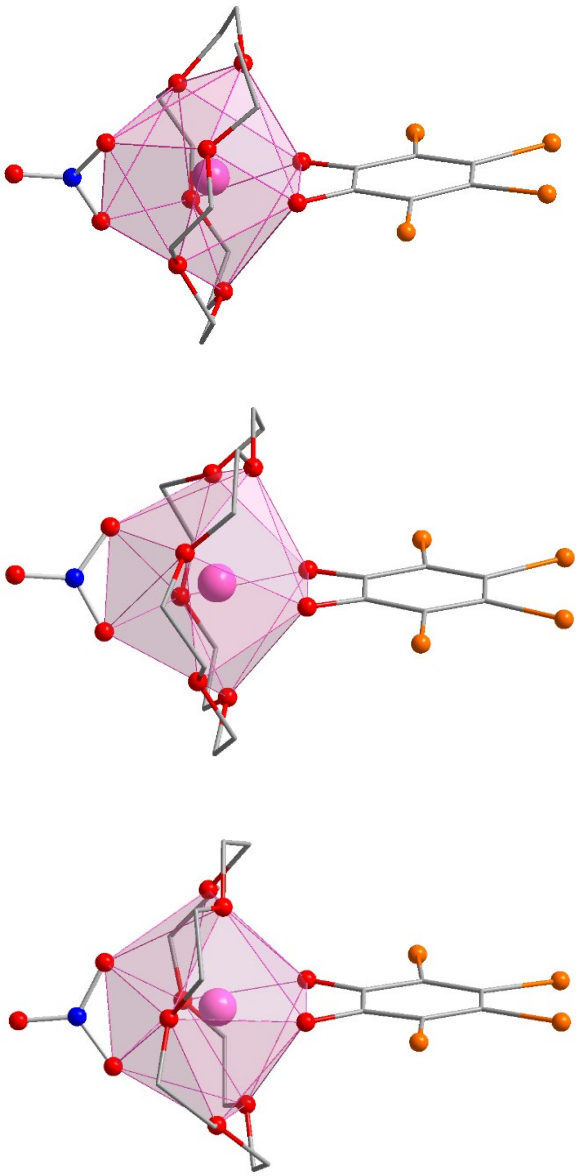

Figure S1: Structural representation of **1-Ln** (upper), **2-Ln** (middle) and **3-Ln** (lower) with the sphenocorona coordination polyhedra highlighted. Hydrogen atoms, disordered parts, and solvent molecules have been omitted for clarity. Colour code: Ln (pink), Br (orange), O (red), N (blue), C (grey).

Powder X-ray diffraction

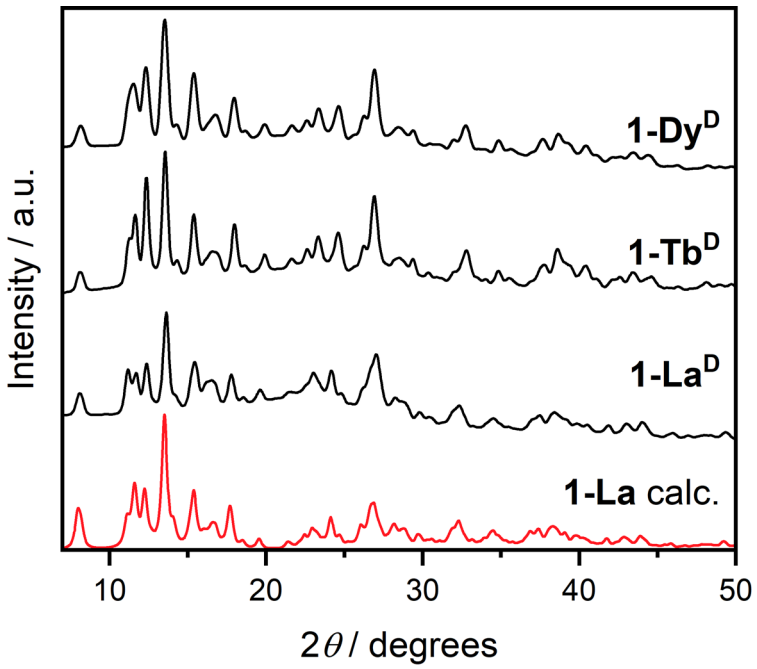

Figure S2: Powder X-ray diffraction data for **1-Ln^{D}**.

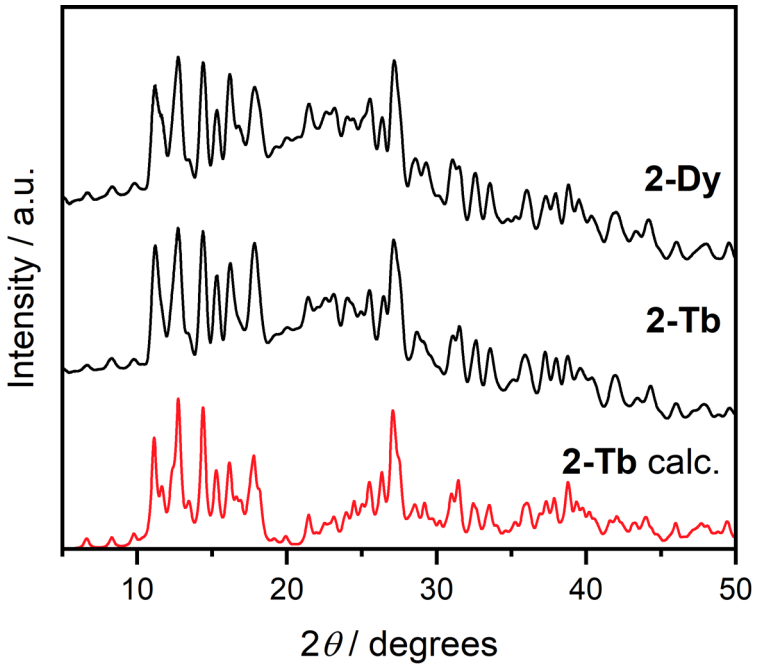

Figure S3: Powder X-ray diffraction data for **2-Ln**.

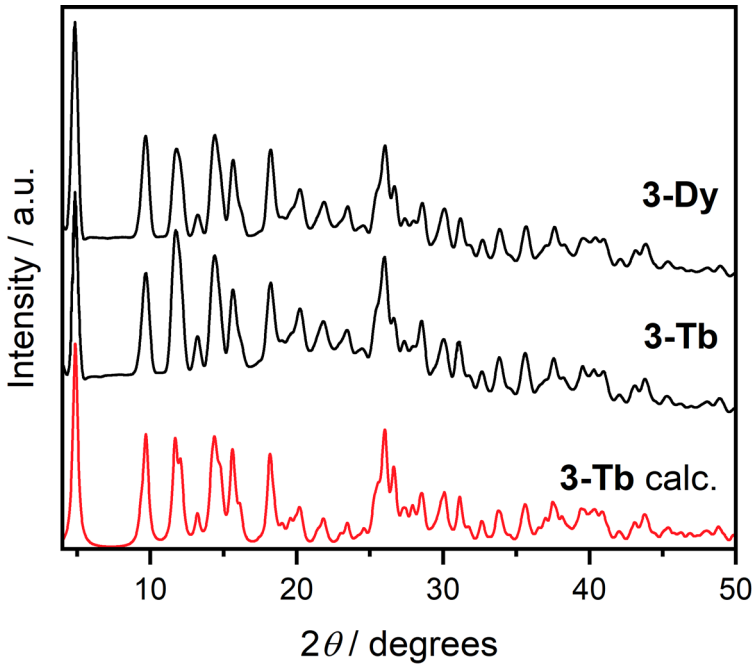

Figure S4: Powder X-ray diffraction data for **3-Ln**.

Infrared spectroscopy

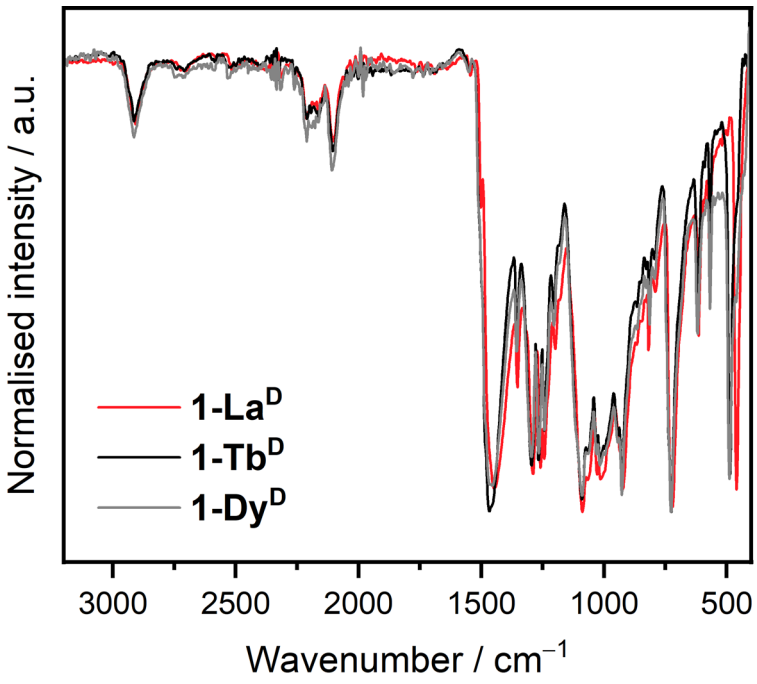

Figure S5: FT-IR (ATR) spectra of **1-Ln^{D}**.

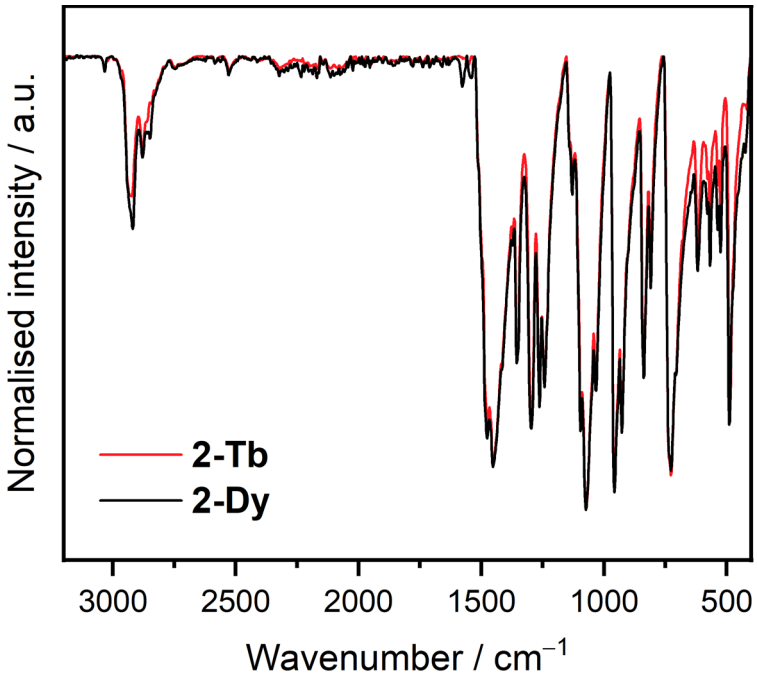

Figure S6: FT-IR (ATR) spectra of **2-Ln**.

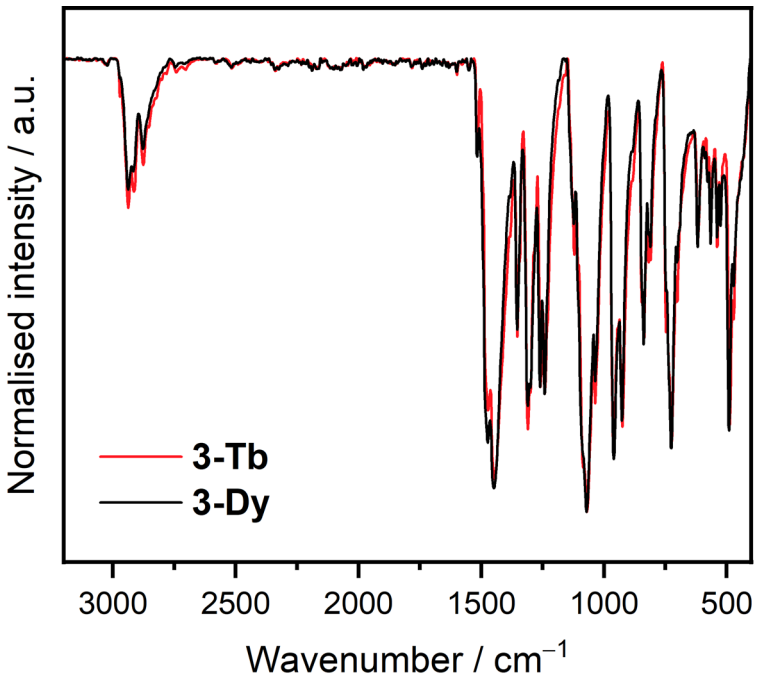

Figure S7: FT-IR (ATR) spectra of **3-Ln**.

Thermogravimetric analysis

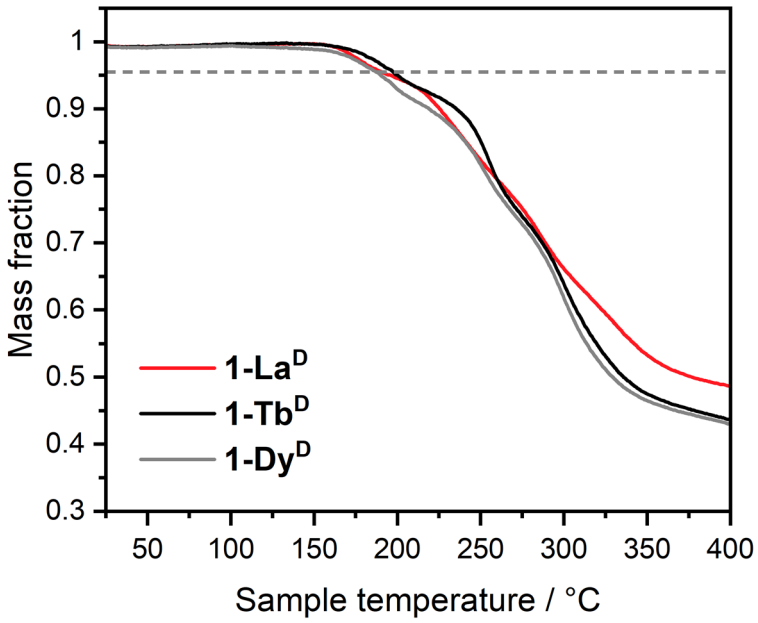

Figure S8: Thermogravimetric analysis of **1-Ln^{D}**.

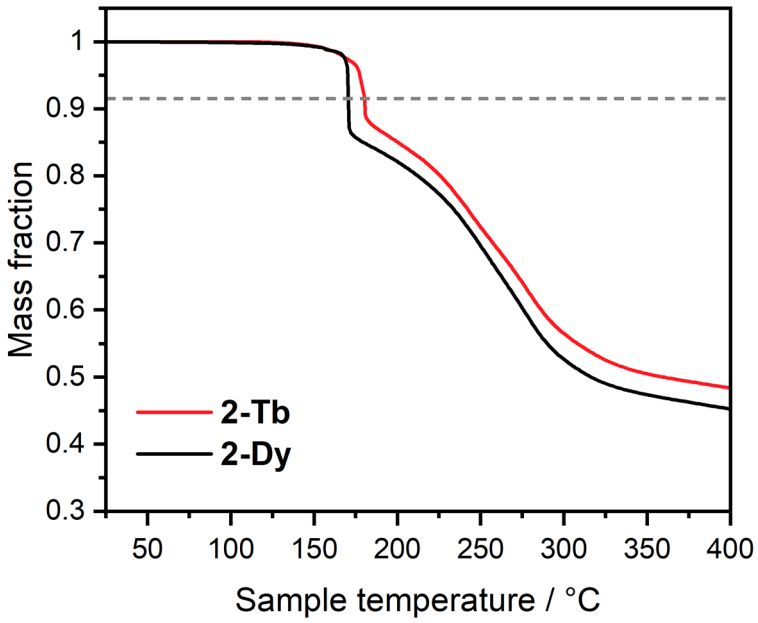

Figure S9: Thermogravimetric analysis of **2-Ln**.

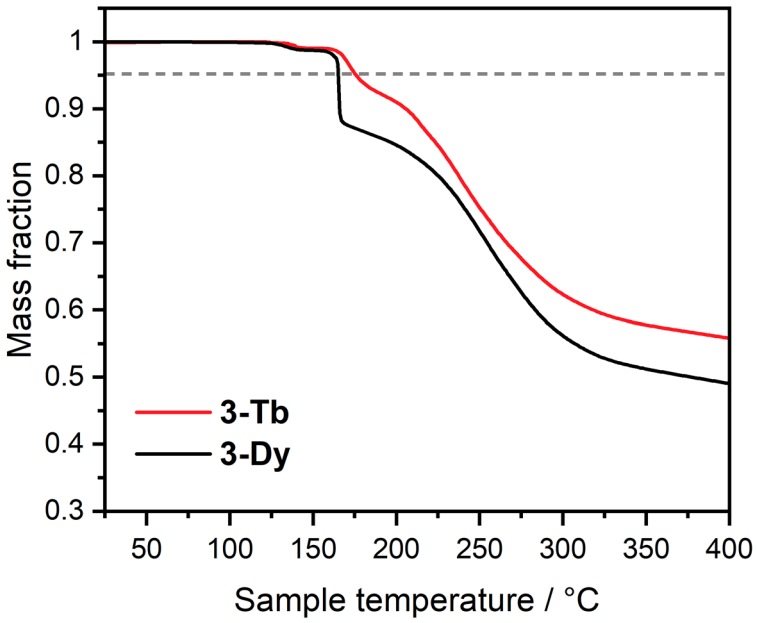

Figure S10: Thermogravimetric analysis of **3-Ln**.

Light field microscopy

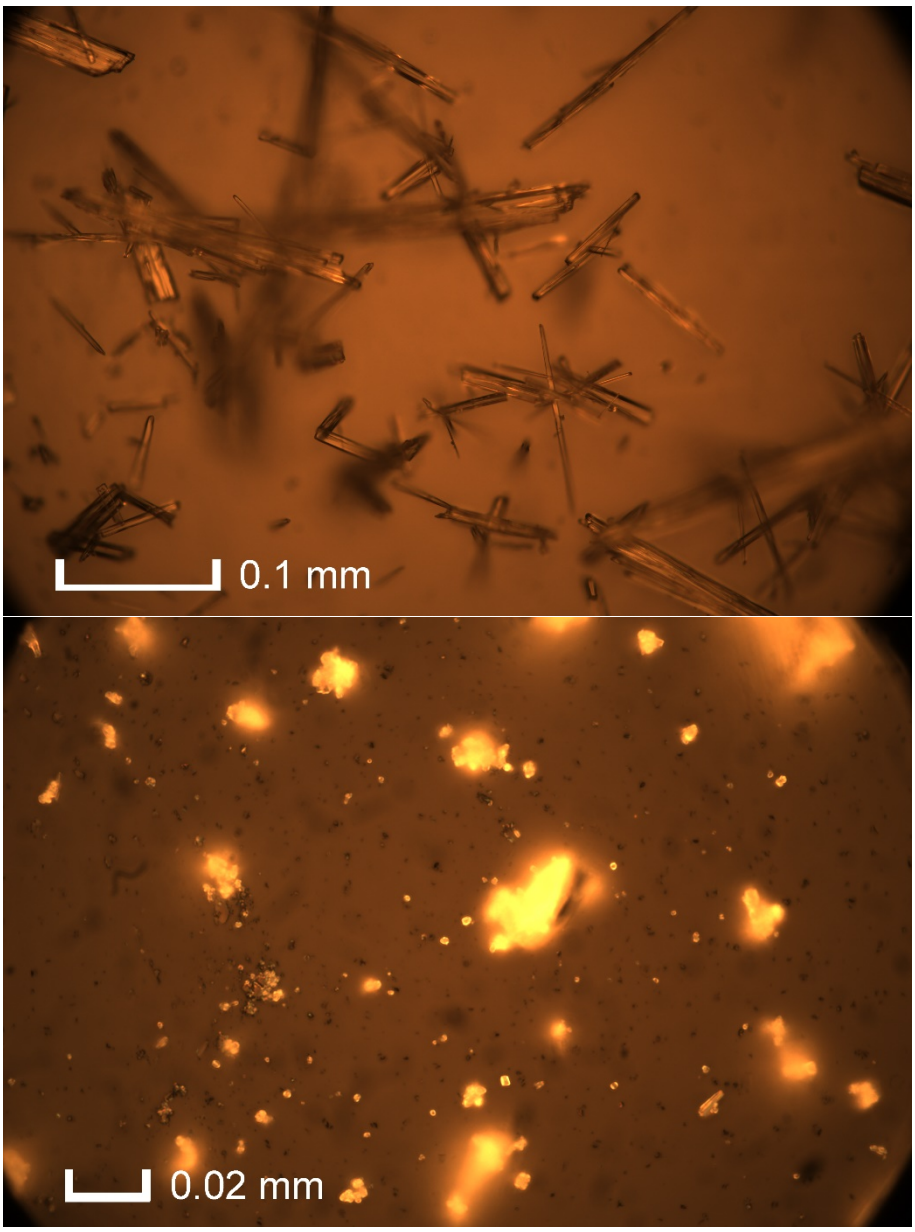

Figure S11: Light field microscope images of **1-Tb^{D}** (above) and **1-Tb^{D}-a** (below).

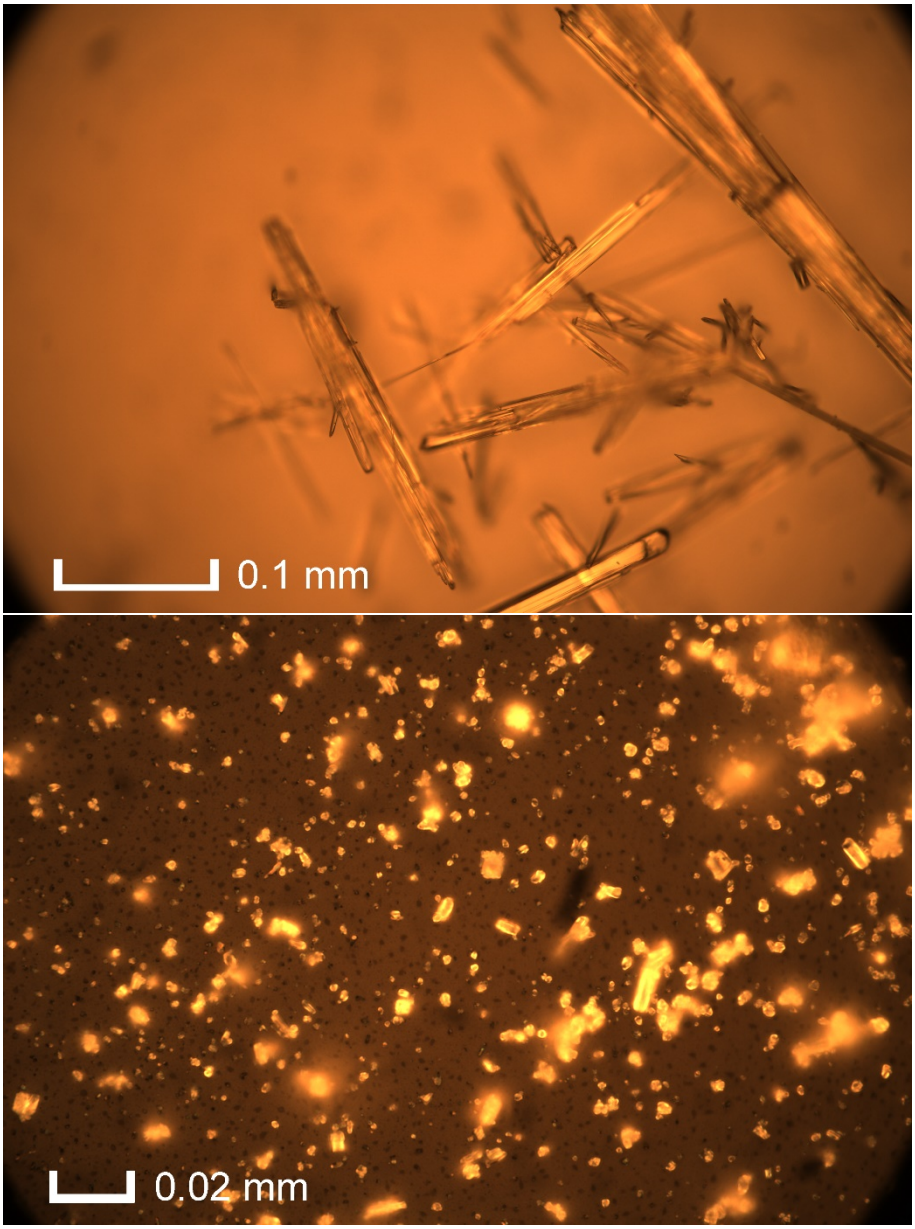

Figure S12: Light field microscope images of **1-Dy^{D}** (above) and **1-Dy^{D}-a** (below).

Inelastic neutron scattering spectra of 1-La^{D}

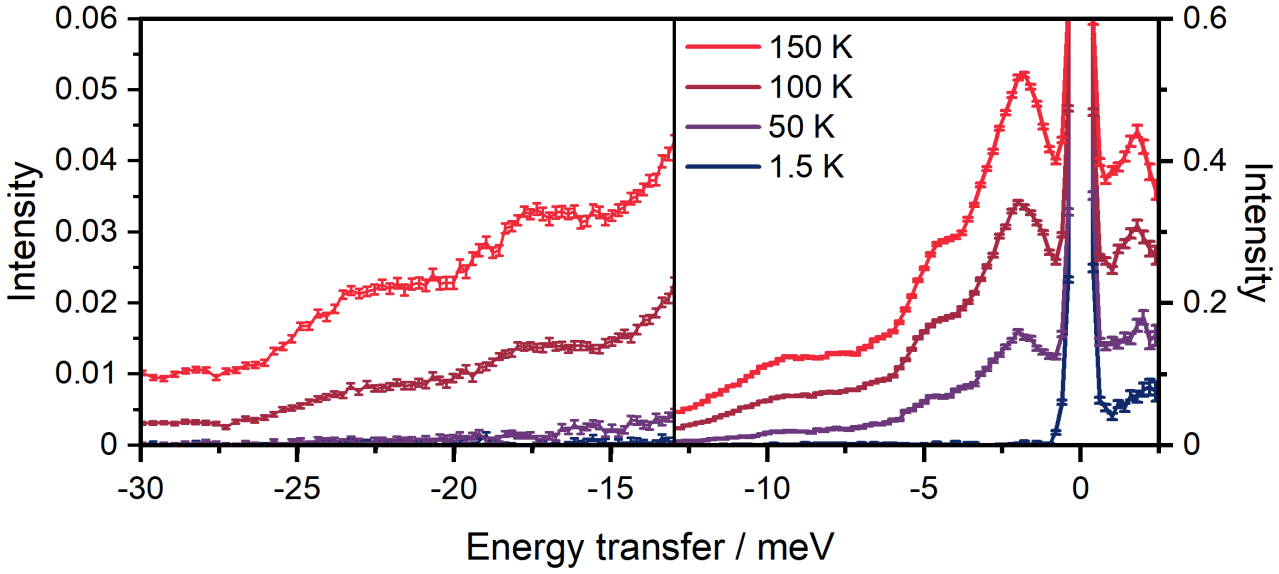

Figure S13: Variable temperature INS spectra of **1-La^{D}**, integrated over all *Q*.

Phonon Generalized Density of States of 1-La^{D}

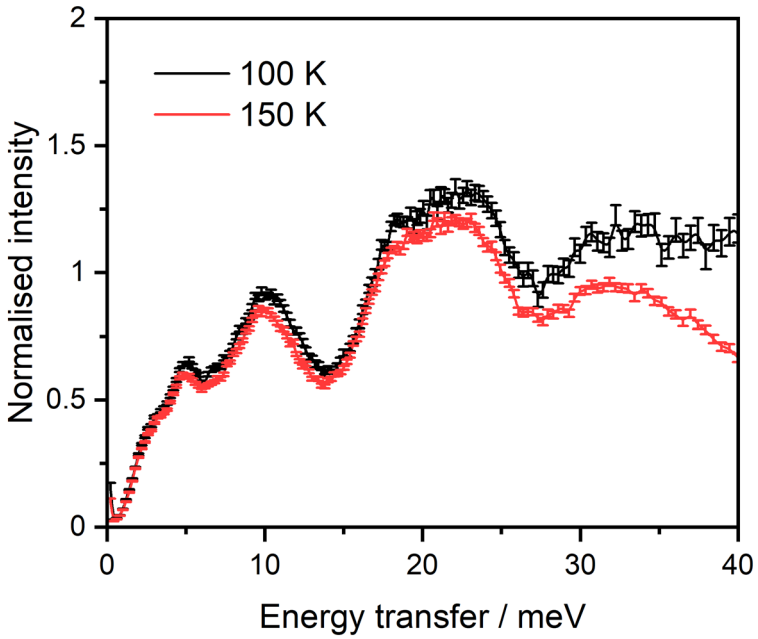

Figure S14: Phonon GDOS calculated for **1-La^{D}** at T = 100 K (black) and 150 K (red).

Dynamic magnetic susceptibility of Tb(III) analogues

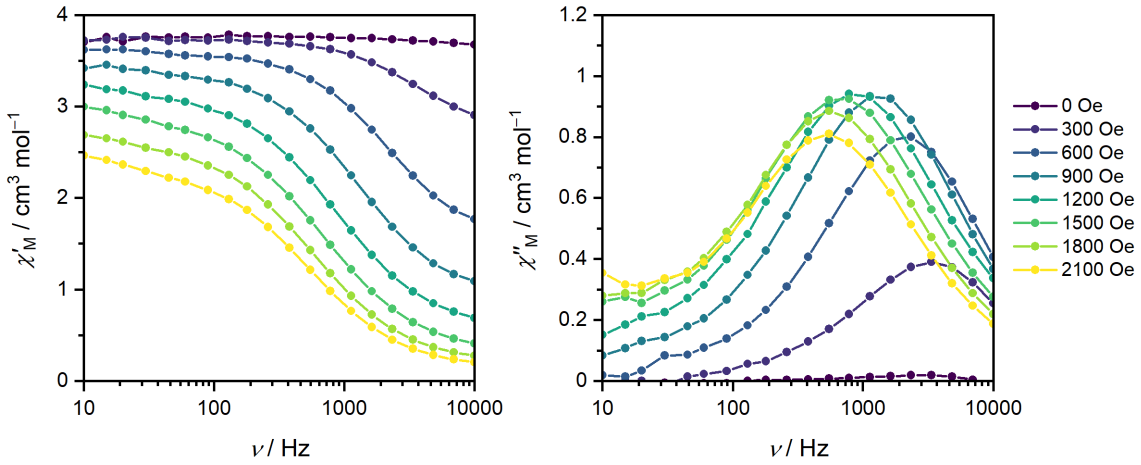

Figure S15: Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Tb^{D}** measured at T = 2.5 K

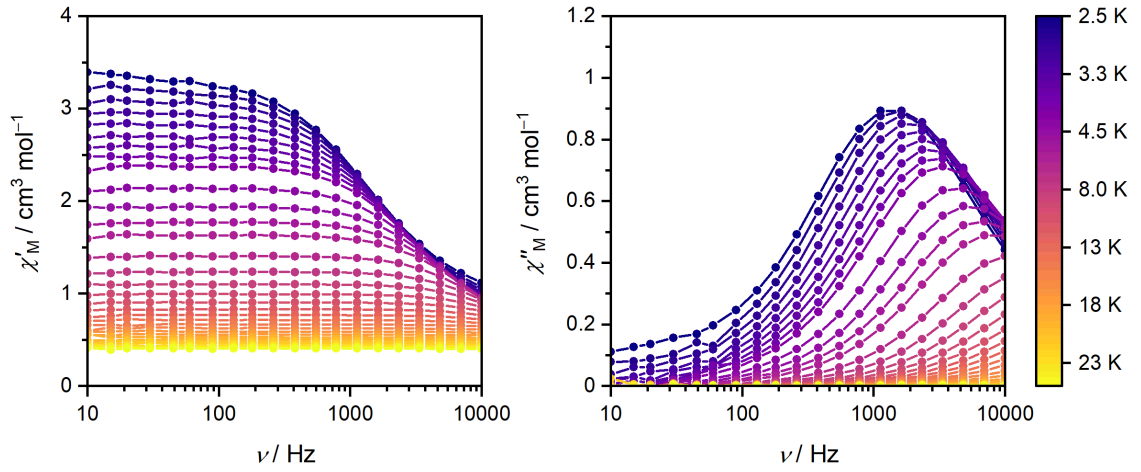

Figure S16: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Tb^{D}** measured in an applied field of B_{dc} = 1,000 Oe.

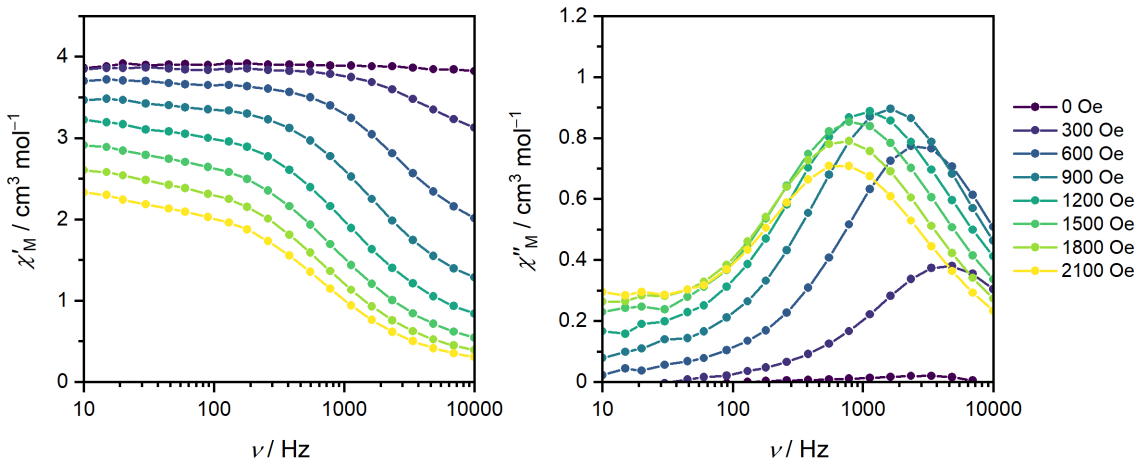

Figure S17: Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Tb^{D}-a** measured at T = 2.5 K

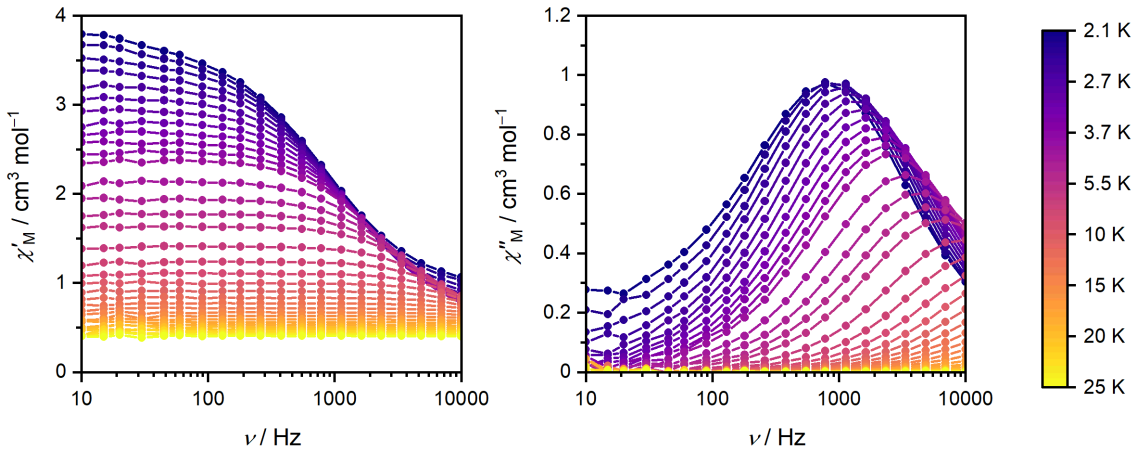

Figure S18: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Tb^{D}-a** measured in an applied field of B_{dc} = 1,000 Oe.

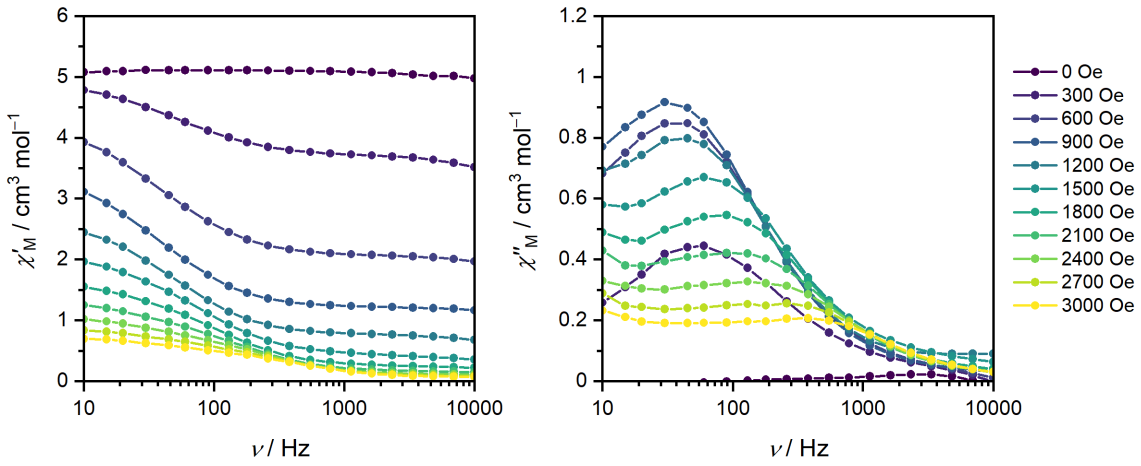

Figure S19: Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **2-Tb** measured at $T = 2.0$ K

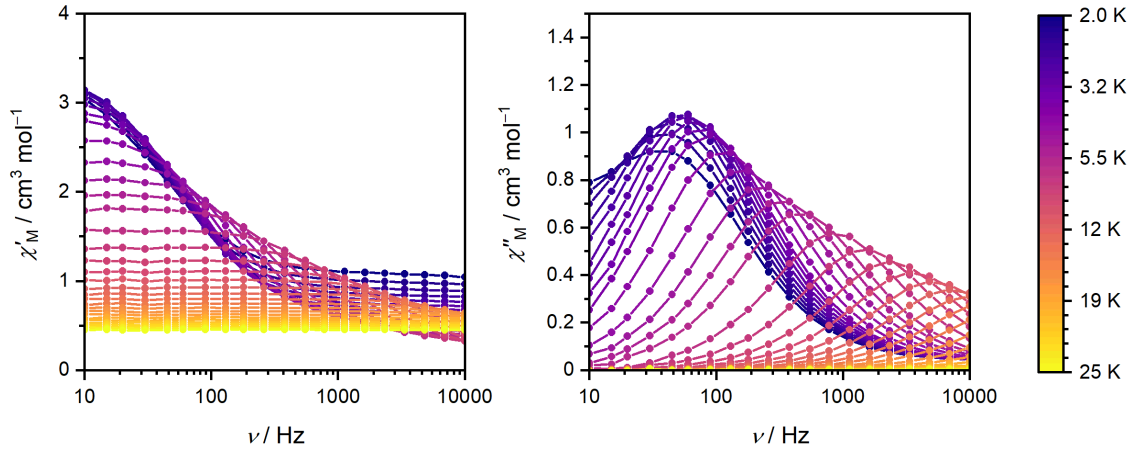

Figure S20: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **2-Tb** measured in an applied field of B_{dc} = 1,000 Oe.

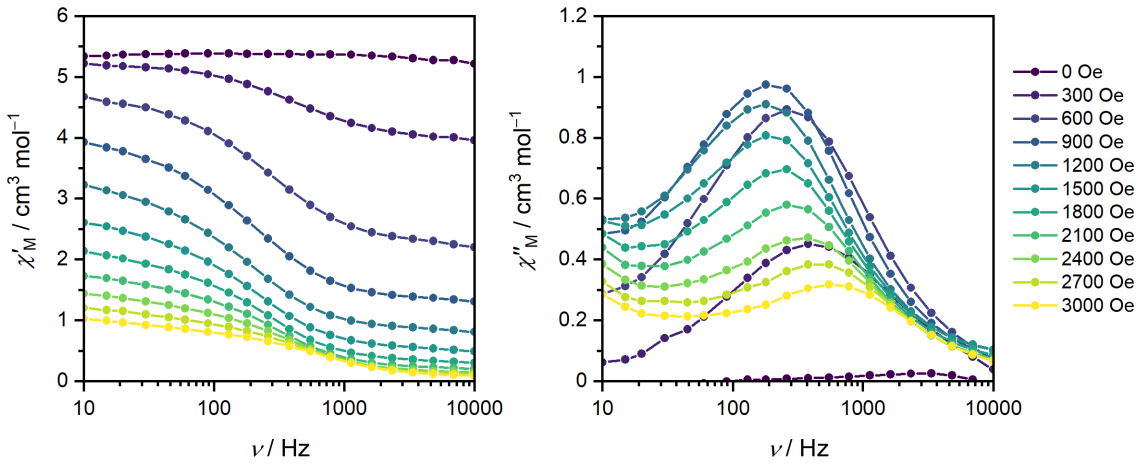

Figure S21: Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **3-Tb** measured at $T = 2.0$ K

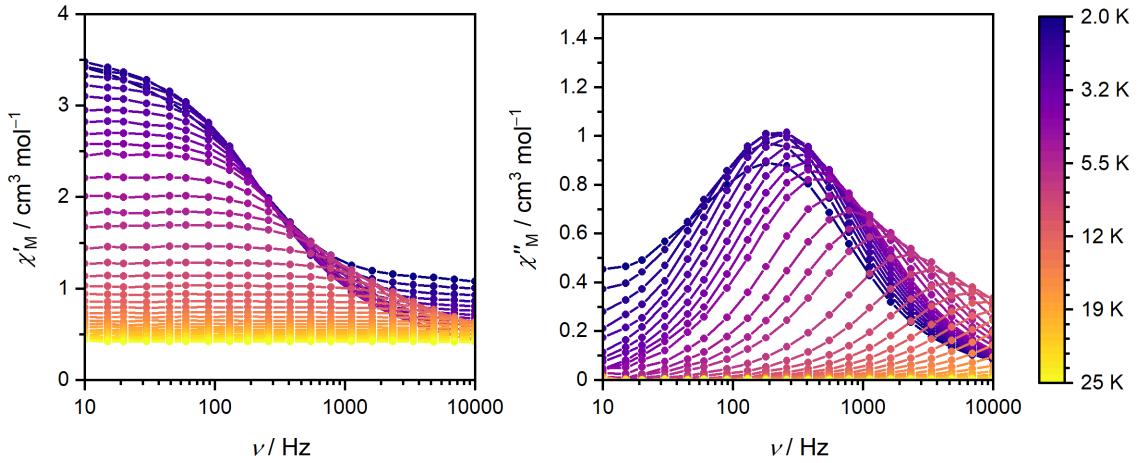

Figure S22: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **3-Tb** measured in an applied field of B_{dc} = 1,000 Oe.

Dynamic magnetic susceptibility of Dy(III) analogues

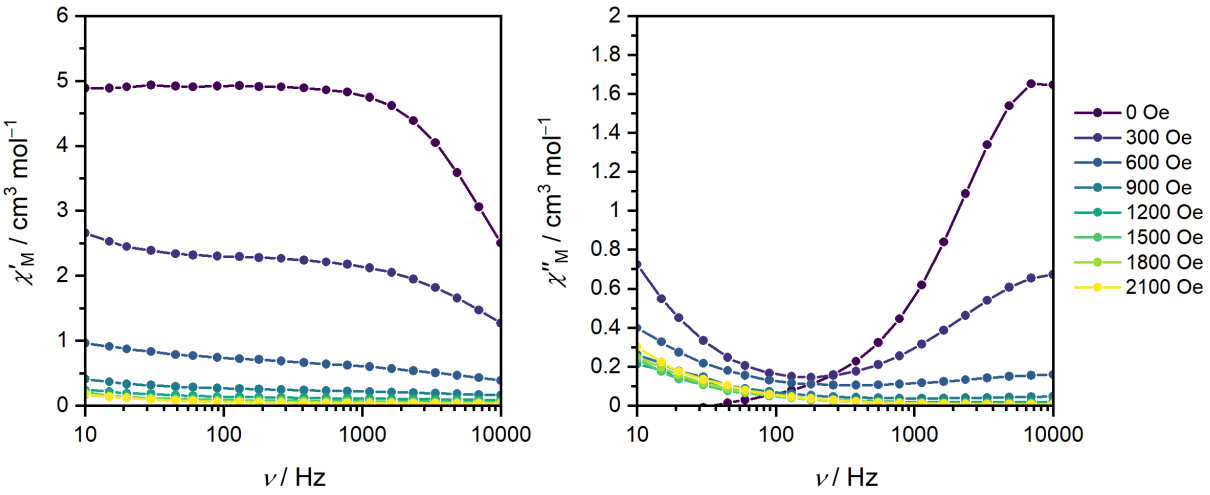

Figure S23: Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Dy^{D}** measured at T = 2.5 K

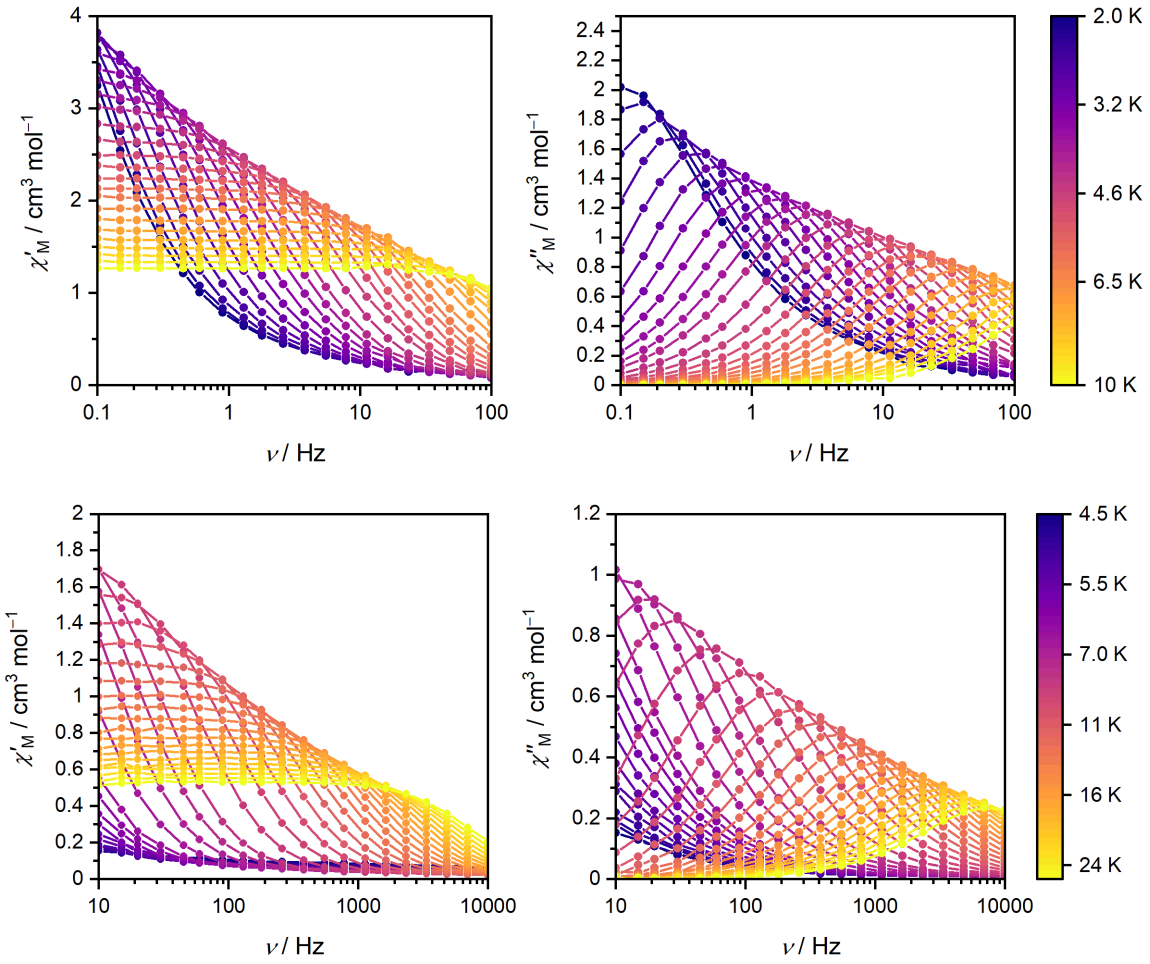

Figure S24: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Dy^{D}** measured in an applied field of B_{dc} = 1,500 Oe.

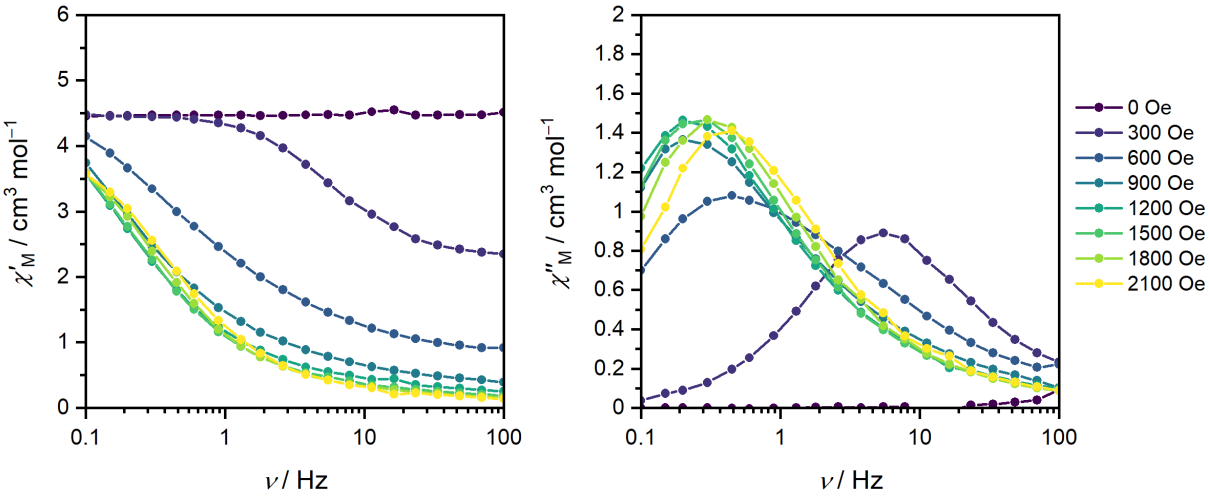

Figure S25 Magnetic field dependence of in-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Dy^{D}-a** measured at T = 2.5 K

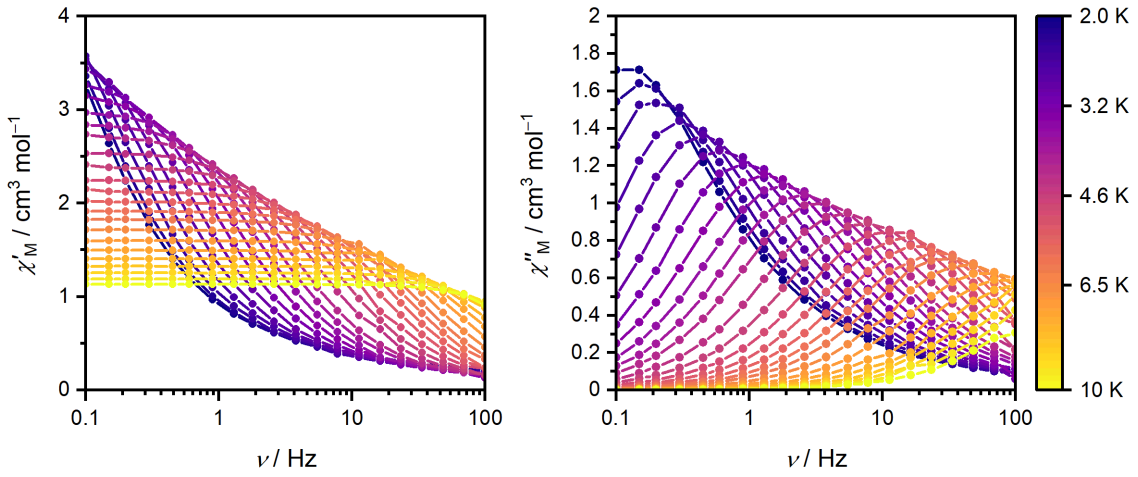

Figure S26: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **1-Dy^{D}-a** measured in an applied field of B_{dc} = 1,500 Oe.

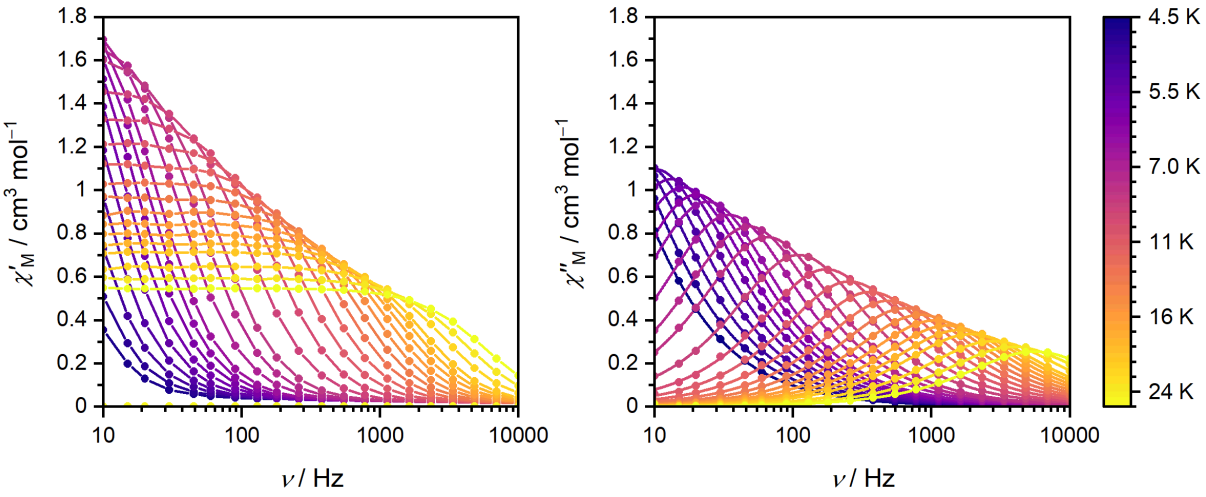

Figure S27: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **2-Dy** measured in an applied field of B_{dc} = 1,500 Oe.

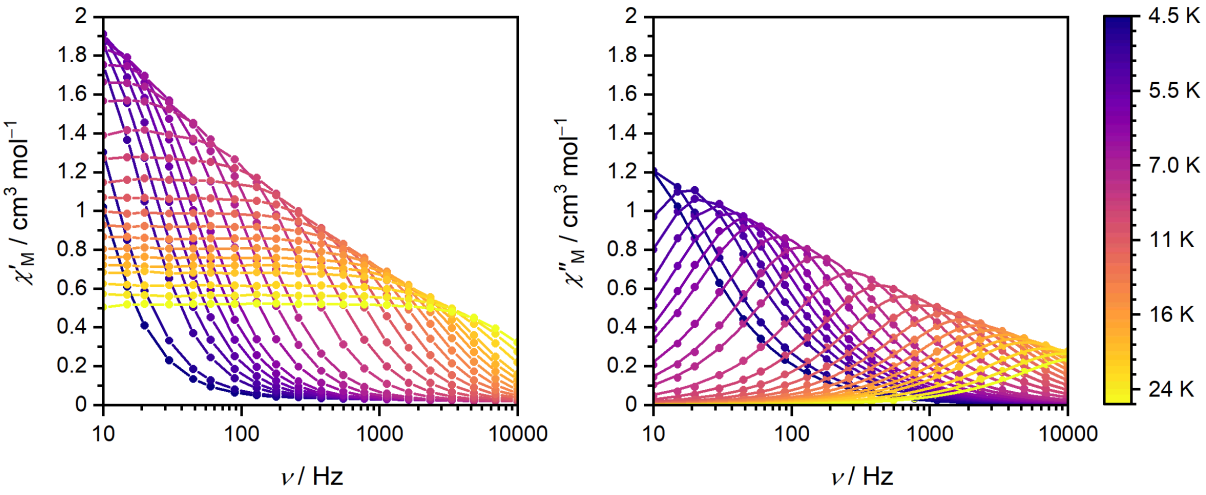

Figure S28: In-phase and out-of-phase components of the ac molar magnetic susceptibility of **3-Dy** measured in an applied field of B_{dc} = 1,500 Oe.