A new family of [$Cu^{II}Ln^{III}M^{V}$] heterotrimetallic complexes (Ln = La, Gd, Tb; M = Mo, W): Model systems to probe exchange interactions and Single-Molecule Magnet properties

Electronic Supplementary Information

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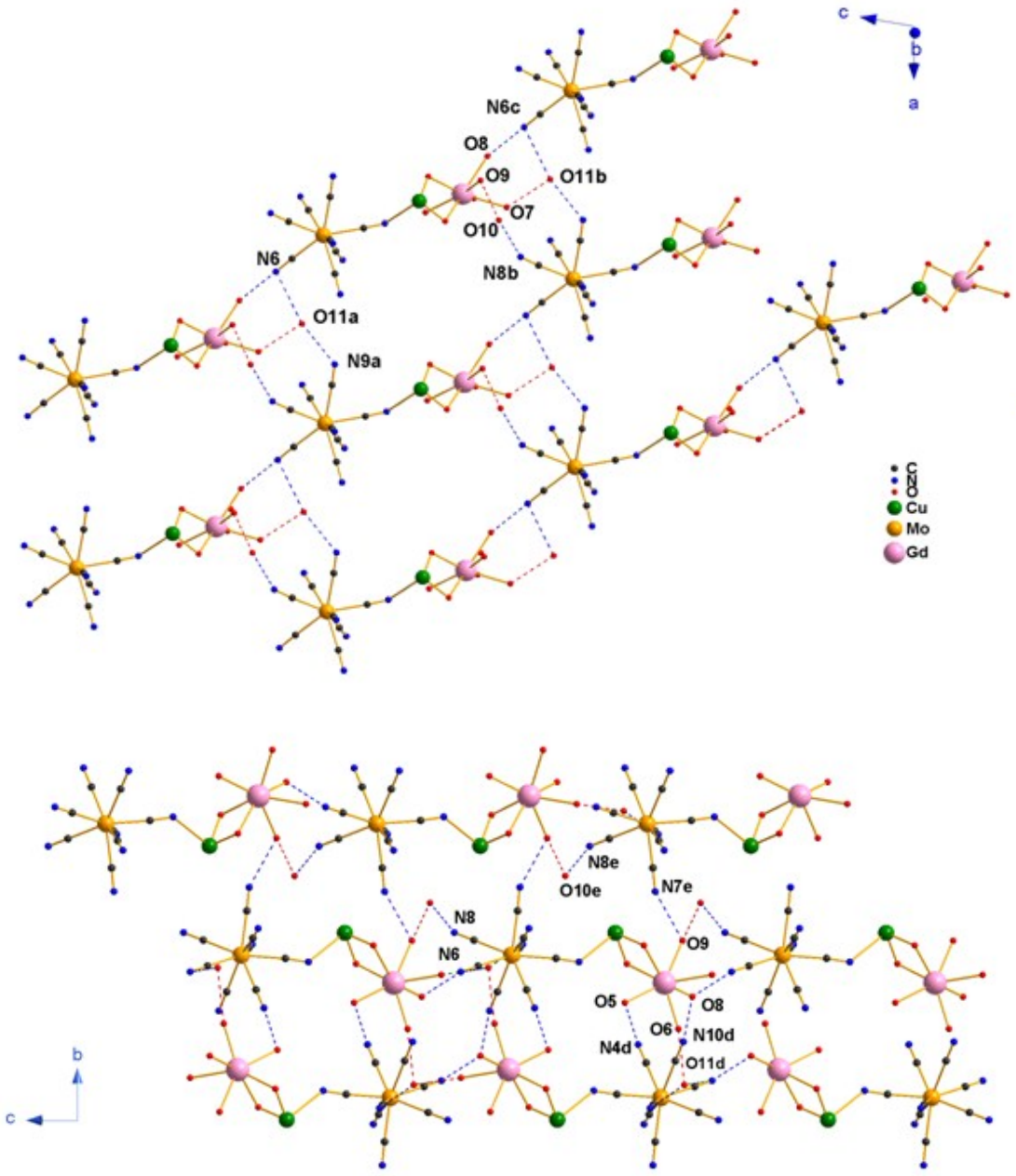

Figure S1. Structural details of the packing diagram in **3** viewed in: (a) *ac* and (b) *bc* planes, showing the hydrogen bond pattern of the O···O (red-dotted lines) and N···O (blue-dotted lines) types (symmetry codes *a* = 1+*x*, *y*, *z*; *b* = *x*, *y*, -1+*z*; *c* = -1+*x*, *y*, -1+*z*; *d* = 2-*x*, -*y*, 2-*z*; *e* = ½+*x*, ½-*y*, -1/2+*z*). The carbon and nitrogen atoms belonging to the Schiff-base ligand and hydrogen atoms were omitted for the sake of clarity.

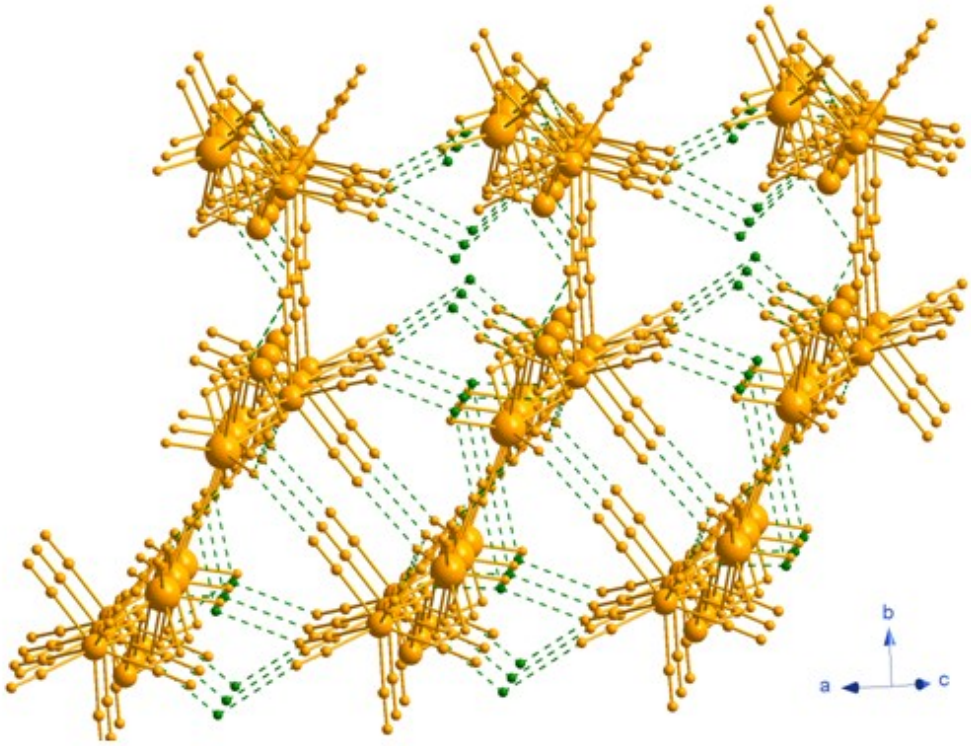

Figure S2. Fragment of the packing diagram in **3** showing the supramolecular three-dimensional network, resulting from the inter-connection of the trinuclear units (orange color) and the crystallization of water molecules (green color) by means of hydrogen-bonds (green dotted lines). The carbon and nitrogen atoms belonging to the Schiff-base ligand and hydrogen atoms were omitted for the sake of clarity.

Table S1. Selected hydrogen-bonds distances (Å) for compounds **2**-**4**.

	2	**3**	**4**
O(5)···N(4)^{d}	2.8028(7)	2.8179(3)	2.8141(6)
O(8)···N(6)^{c}	2.7962(6)	2.8515(3)	2.8318(5)
O(8)···N(10)^{d}	2.8329(7)	2.8238(3)	2.8586(5)
O(9)···N(7)^{e}	2.8534(7)	2.8798(3)	2.8843(6)
O(10)^{d}···N(8)	2.8932(8)	2.8955(4)	2.8889(7)
O(11)^{a}···N(6)	-	3.0655(4)	3.0494(6)
O(11)^{a}···N(9)^{a}	2.7964(7)	2.8301(4)	2.8326(6)
O(6)···O(11)^{d}	2.7699(7)	2.8012(3)	2.8016(6)
O(7)···O(11)^{b}	2.7619(5)	2.7520(3)	2.7575(4)

* symmetry codes *a* = 1+*x*, *y*, *z*; *b* = *x*, *y*, -1+*z*; *c* = -1+*x*, *y*, -1+z; *d* = 2-*x*, -*y*, 2-*z*; *e* = ½+*x*, ½-*y*, -1/2+*z*)

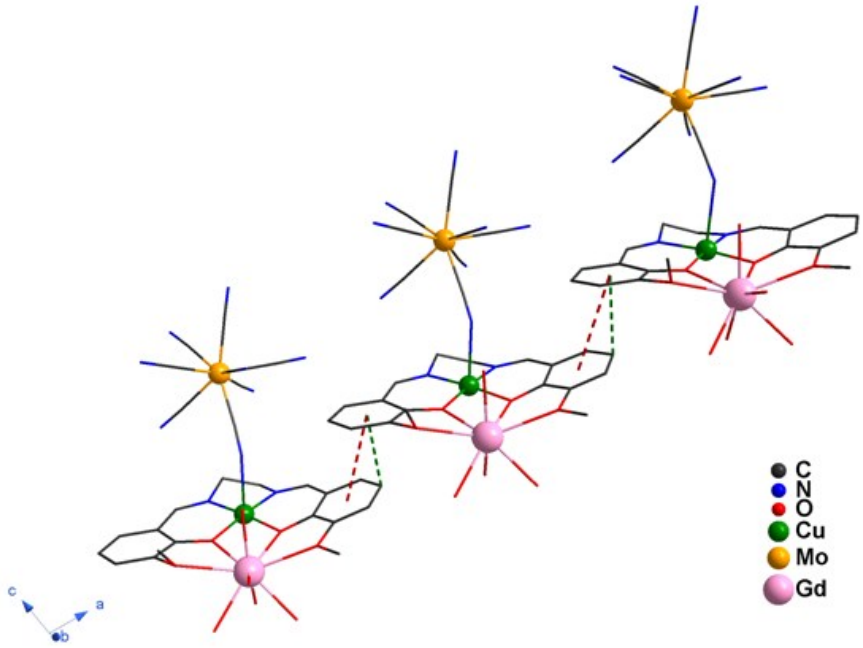

Figure S3. Structural details of the packing diagram in **3** showing the π-π stacking interaction established along *a* axis between the aromatic rings of the Schiff-base ligands.

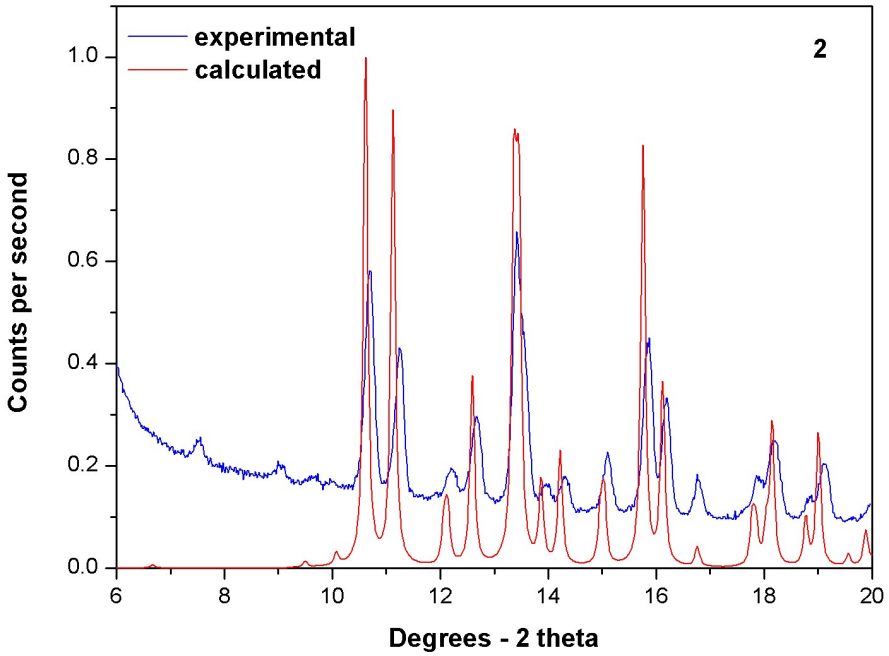

Figure S4. Experimental and calculated powder X-ray diffractograms at room temperature for compound **2**.

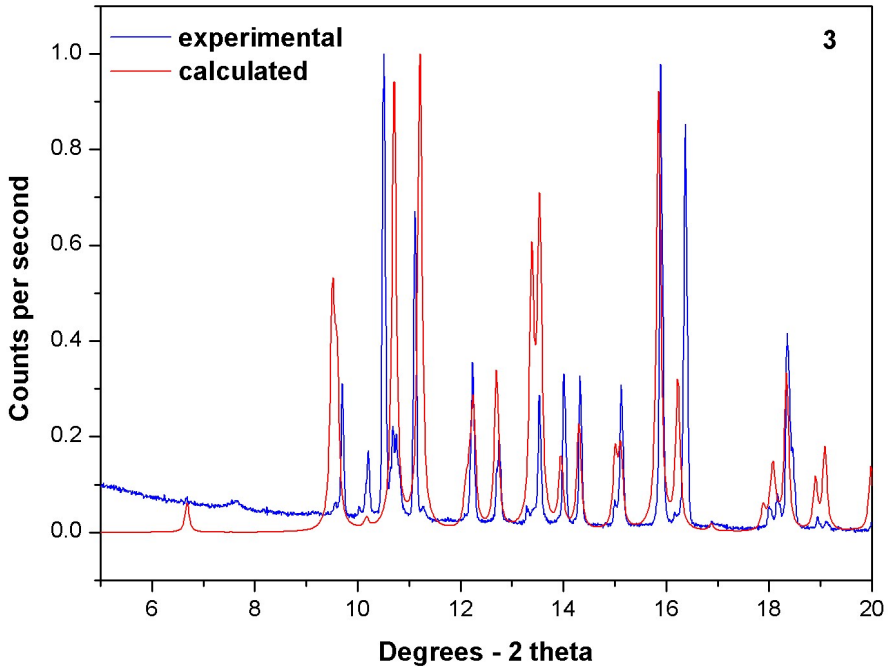

Figure S5. Experimental and calculated powder X-ray diffractograms at room temperature for compound **3**.

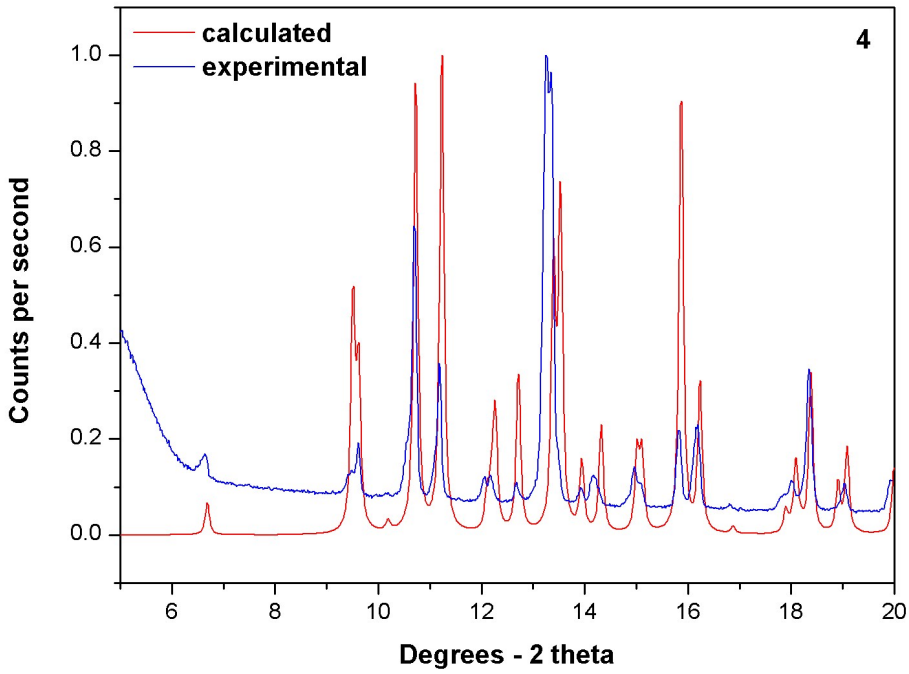

Figure S6. Experimental and calculated powder X-ray diffractogram at room temperature for compound **4**.

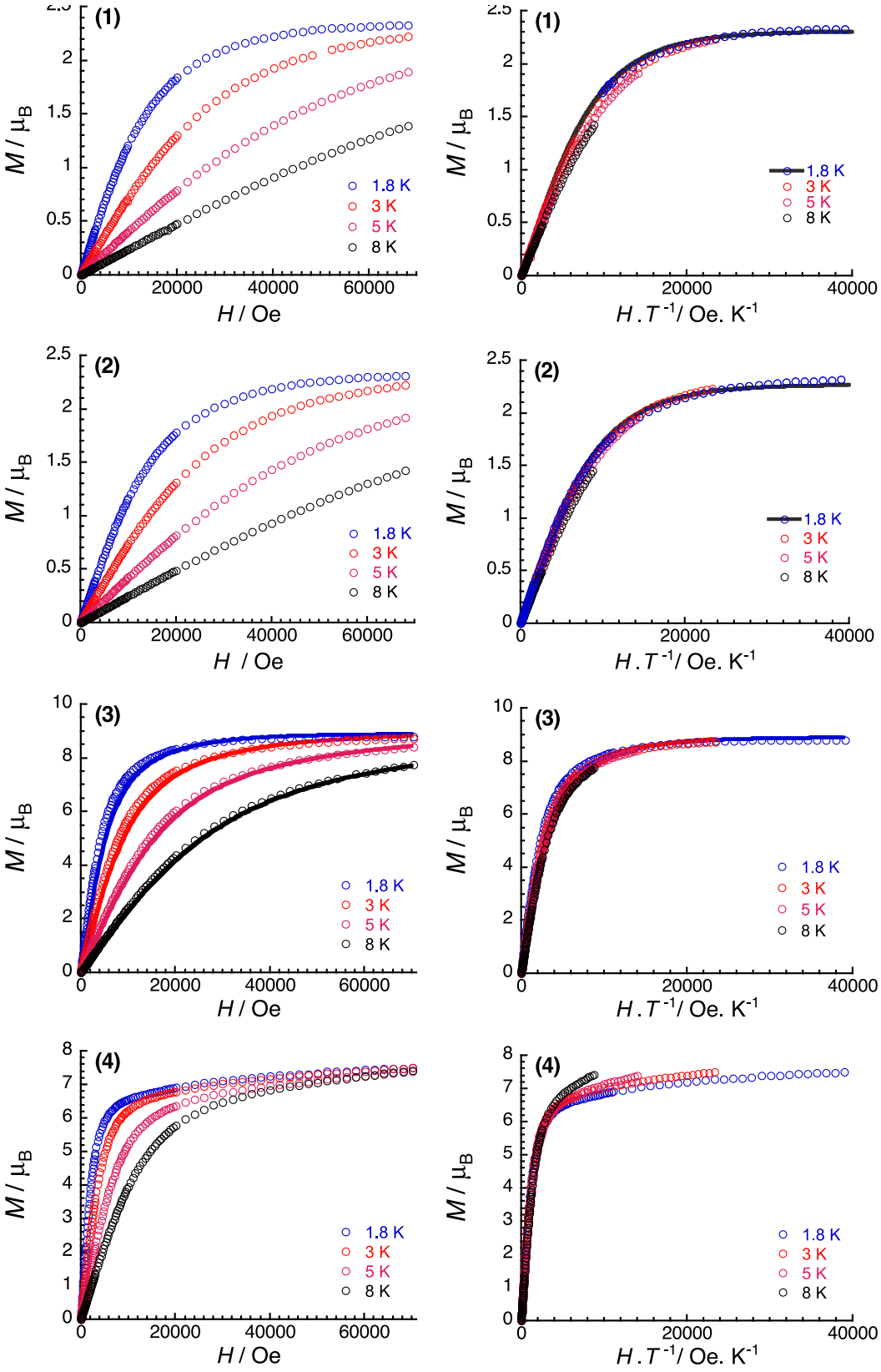

Figure S7. Field, *H*, dependences of the magnetization, *M*, below 8 K plotted as *M* vs *H* (left) and *M* vs *H/T* (right) between 0 and 7 T for compounds **1**, **2**, **3** and **4**. Solid lines are the best fits or simulations discussed in the main text.

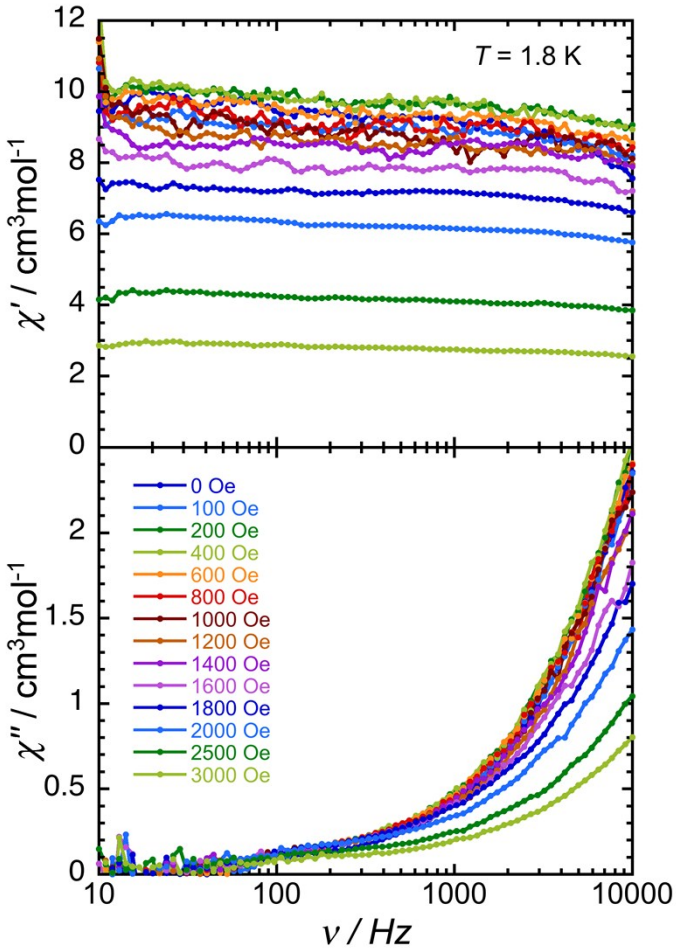

Figure S8. Frequency dependence of the real (χ', top) and imaginary (χ'', bottom) parts of the ac susceptibility, between 10 and 10000 Hz for dc field up to 0.3 T for **4** at 1.8 K. Solid lines are visual guides.